CONTENTS

Contents

| 2 | | Nota | ation | | i |
|----|---|-------|----------|-------------------------------------|-----------|
| 3 | 1 | | | escription 75 GDD | 1 |
| 5 | 2 | Inte | rpolatio | on Methods | 2 |
| 6 | | 2.1 | Setting | g | 2 |
| 7 | | 2.2 | Param | netric Regression | 2 |
| 8 | | | 2.2.1 | Double Logistic | 4 |
| 9 | | | 2.2.2 | Fourier Approximation | 4 |
| 10 | | 2.3 | Non-P | Parametric Regression | 5 |
| 11 | | | 2.3.1 | Kernel Regression | 5 |
| 12 | | | 2.3.2 | Kriging | 6 |
| 13 | | | 2.3.3 | Savitzky-Golay Filter (SG Filter) | 7 |
| 14 | | | 2.3.4 | Locally Weighted Regression (LOESS) | 8 |
| 15 | | | 2.3.5 | B-splines | 10 |
| 16 | | | 2.3.6 | Natural Smoothing Splines | 11 |
| 17 | | | 2.3.7 | Other Methods to study: | 11 |
| 18 | 3 | NDV | VI Corr | rection / Improve NDVI Data | 15 |
| 19 | | 3.1 | Consid | dering other SCL Classes | 15 |
| 20 | | Bibli | iograph | ny | 17 |
| 21 | A | Hi N | /Iom | | 18 |

Notation

```
c: a (vector of) constant(s)
\lambda \in \mathbb{R}: a scalar
n \in \mathcal{N}: sample size
i, j are indices in \{1, \ldots, n\}
x \in \mathbb{R}^n: covariable in 1-dim interpolation setting
w \in \mathbb{R}^n: a vector of weights for each location x
y \in \mathbb{R}^n: response in 1-dim interpolation setting
\hat{y} \in \mathbb{R}^n: estimate of y
r \in \mathbb{R}^n: residuals given by y - \hat{y}
Pixel: A pixel describes a specific location in a field. It has the size of 10 x 10 meters
and coincides with the resolution (and location) of the sentinel-2 pixels. Such pixels are
illustrated in figure ??.
P_t: this describes the observed data (weather and spectral bands) at pixel P and at time
P: a pixel. More formally we see it as a collection of all the observations at the specified
location within one season.
SCL: scene classification layer. This indicates what one can expect at a pixel at a sampled
time. For an overview c.f. table ??
P^{scl45}: similar to P but we only consider observations which belong to the classes 4 and
5. This is used done to get a subset of observations which are less contaminated by clouds
and shadows.
NDVI: normalized vegetation difference index
DAS: days after sowing
GDD: growing degree days – cumulative sum of (temperature – threshold)<sup>+</sup>
```

Chapter 1

48 Problem Description

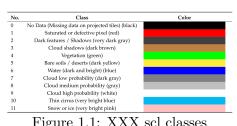


Figure 1.1: XXX scl classes

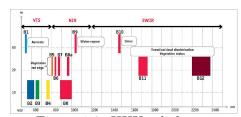


Figure 1.2: XXX scl classes

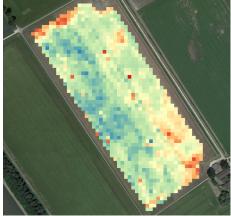


Figure 1.3: XXX yield raster

DAS vs GDD 1.1

XXX

Chapter 2

Interpolation Methods

- In this section we take a closer look at several interpolation methods, which will be used
- to interpolate and smooth the NDVI time series.
- First, we give a brief overview in table 2.1.
- 56 Second, we introduce and discuss each method.
- 57 Then, we try to extract the main ingredients of each method to forge our own one.
- Finally, using leave-one-out cross validation we tune the parameters (where necessary) and
- 59 get a first idea of the performance of each method.

o 2.1 Setting

We are given data in the form of (x_i, Y_i) for i = 1, ..., n). Assume that it can be represented by

$$Y_i = m(x_i) + \varepsilon_i,$$

where ε_i is some noise and $m : \mathbb{R} \to \mathbb{R}$ being some (parametric or non-parametric) function. If we assume that $\varepsilon_1, \ldots, \varepsilon_n$ i.i.d. with $\mathbb{E}\left[\varepsilon_i\right] = 0$ then

$$m(x) = \mathbb{E}[Y \mid x]$$

Different assumptions on m will lead to the following methods:

2.2 Parametric Regression

- Parametric Curve estimation tries to fit a parametric function (e.g. a Gaussian function
- with parameter μ and σ) to a dataset. In the following we introduce 2 such parametric
- 65 approaches.

Optimization Issues

- In the following we search for 5 or 6 parameters that minimize the residuals sum of squares.
- This is a non-convex optimization problem and thus the algorithm¹ either could not find
- the global minimum or failed to converge. This was fixed by providing for each parameter
- 70 reasonable initial values and generous bounds (which match our experience).

 $^{^{1}\}mathrm{We}$ used the python function <code>scipy.optimize.curve_fit</code>

| ; | assumtpions | pros | cons | weights | bounded |
|-------------------------------|---|--|---|---------|---------|
| Golay filter | high frequencies - are noise (low.pass filter) equidistant points local polynomials | | - cannot deal natively with missing data (need some interpolation) | no | mostly |
| SG + - | | - biological knowl- edge | bad "upper envelope" since weights are not used for the estimation itselfe | (no) | mostly |
| Loess – | local polynomial - with points closer - to the estimated point are more important | | computationally expensive | yes | mostly |
| Smoothing- Splines | | = | – unbounded | yes | no |
| | function can be approximated by a linear combination of B-splines basis functions | | unboundedno intuitive meaning for smoothing | | no |
| (Gaussian) Kernel Smooth- ing | | - simple - general assump- tions | bandwidh: failes if there are big data- gaps | yes | yes |
| Double- – Logistic | function first in- creases then de- creases ndvi has a minimal - value | plants (if snow masks ndvi) | parameterestimation can go seriously wrong strange behaviour for long data-gaps | · | mostly |
| Universal – Kriging | realization of a | - informative parameters - flexible | regression to the meanassumptions clearly not met | yes | mostly |

Table 2.1: A short summary of the studied interpolation methods

2.2.1 Double Logistic

The Double Logistic smoothing as described in Beck, Atzberger, Høgda, Johansen, and Skidmore (Beck et al.) heavily relies on shape assumptions of the fitted curve (i.e. the NDVI time series).

5 Assumptions:

- There is a minimum NDVI level Y_{\min} in the winter (e.g. due to evergreen plants), which might be masked by snow. This can be estimated beforehand, taking into several years into account.
 - The growth cycle can be divided into an increase and a decrease period where the time series follows a logistic function. The maximum increase (or decrease) is observed at t_0 (or t_1) with a slope of d_0 (or d_1).

The equation of the double-logistic fit is given by:

$$Y(t) = Y_{\min} + (Y_{\max} - Y_{\min}) \left(\frac{1}{1 + e^{-d_0(t - t_0)}} + \frac{1}{1 + e^{-d_1(t - t_1)}} - 1 \right)$$

- Where the five free parameters: Y_{max} , d_0 , d_1 , t_0 , t_1 are initially estimated by least squares. Such fit can be seen in figure 2.1.
- Similar as for the Savitzky-Golay Filter (c.f. section 2.3.3) we reestimate (only once) the parameters by giving less weight to the overestimated observations and more weight to the underestimated observations².

| Pros | | Cons | | | | |
|---|---|---|--|--|--|--|
| Incorperates subject specific knowledge in the case of evergreen plants covered | _ | Strong shape assumptions on the NDVI curve. | | | | |
| by snow. | _ | Parameter optimization might go | | | | |
| Optimized parameters have an intuitive meaning. | | wrong. This can be mitigated to some extend to provide bounds for the paramters | | | | |
| | _ | Strange behaviour in regrions with little observations. (cf. figure 2.1) | | | | |

2.2.2 Fourier Approximation

Similar as in section 2.2.1 we fit a parametric curve to the data by least squares. Here we take the second order fourier series:

$$NDVI(t) = \sum_{j=0}^{2} a_j \times \cos(j \times \Phi_t) + b_j \times \sin(j \times \Phi_t)$$

where $\Phi = 2\pi \times (t-1)/n$.

²For the details on the weights we refer to Beck, Atzberger, Høgda, Johansen, and Skidmore (Beck et al.)

| Pros | Cons | | | |
|---|--|--|--|--|
| — Assumtion of periodicity can be helpful | 9 | | | |
| if we are modelling multiyear grow cycles | (cf. figure 2.1) | | | |
| — Flexible curve shape | — Hard to interpret estimated parameters | | | |

— Parameter estimation can go wrong. Introducing bounds can help.

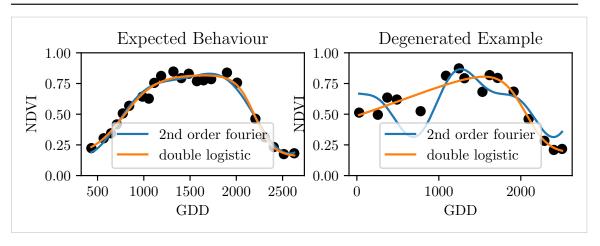


Figure 2.1: Here we observe the nice fitting possibilities of the two parametric methods but notice also some misbehavior

2.3 Non-Parametric Regression

In non-parametric curve estimation we no longer demand our curve to be fully determined by several parameters, but we allow it to also dependent on the data. That said we might still use some tuning-parameters sometimes.

2.3.1 Kernel Regression

4 As described previously, we would like to estimate

$$\mathbb{E}[Y \mid X = x] = \int_{\mathbb{R}} y f_{Y|X}(y \mid x) dy = \frac{\int_{\mathbb{R}} y f_{X,Y}(x,y) dy}{f_{X}(x)}, \tag{2.3.1.1}$$

where $f_{Y|X}, f_{X,Y}, f_X$ denote the conditional, joint and marginal densities. This can be done with a kernel K:

$$\hat{f}_X(x) = \frac{\sum_{i=1}^n K\left(\frac{x-x_i}{h}\right)}{nh}, \hat{f}_{X,Y}(x,y) = \frac{\sum_{i=1}^n K\left(\frac{x-x_i}{h}\right) K\left(\frac{y-Y_i}{h}\right)}{nh^2}$$

By plugging the above into equation 2.3.1.1 we arrive at the *Nadaraya-Watson* kernel estimator:

$$\hat{m}(x) = \frac{\sum_{i=1}^{n} K((x - x_i)/h) Y_i}{\sum_{i=1}^{n} K((x - x_i)/h)}$$

Examples: Normal, Box For local bandwidth selection see Brockmann et al. (1993)
 XXX

| Pros | Cons |
|------|------|
| Pros | Con |

- flexible due to different possible kernels
- can be assigned degrees of freedom (trace of the hat-matrix)
- estimation of the noise variance $\hat{\sigma}_{\varepsilon}^2$ (XXX c.f. CompStat 3.2.2)
- if the $x \mapsto K(x)$ is not continuous, \hat{m} isn't either
- choice of bandwidth, especially if x_i are not equidistant.

2.3.2 Kriging

Kriging was developed in geostatistics to deal with autocorrelation of the response variable at nearby points. By applying the notion that two spectral indices which are (timewise) close should also take similar values we justify the application of Kriging. In the end we would like to fit a smooth Gaussian process to the data. For this subsection we will follow Diggle and Ribeiro (dig).

Definitions and Assumptions

A Gaussian Process $\{S(t): t \in \mathbb{R}\}$ is a stochastic process if $(S(t_1), \dots, S(t_k))$ has a multivariate Gaussian distribution for every collection of times t_1, \dots, t_k . S can be fully characterized by the mean $\mu(t) := E[S(t)]$ and its covariance function $\gamma(t, t') = \text{Cov}(S(t), S(t'))$

Assumption: We will assume the Gaussian process to be stationary. That is for $\mu(t)$ to be constant in t and $\gamma(t,t')$ to depend only on h=t-t'. Thus, we will write in the following only $\gamma(h)$.³

We also define the variogram of a Gaussian process as

$$V(h) := V(t, t+h) := \frac{1}{2} \operatorname{Var}(S(t) - S(t+h)) = (\gamma(0))^2 (1 - \operatorname{corr}(S(t), S(t+h)))$$

And decide to use a gaussian Variogram defined by

$$V(h) = p \cdot \left(1 - e^{-\frac{h^2}{\left(\frac{4}{7}r\right)^2}}\right) + n,$$

where h is the distance, n is the nugget, r is the range and p is the partial sill visuilized in figure 2.2.⁴

| Pros | Cons | | | |
|--|--|--|--|--|
| — It is a well-studied method | — Regression to the mean | | | |
| — Parameters have an intuitive meaning | — Assumption of constant mean and con- | | | |
| — Flexible covariance structure | stant variance is clearly violated. Thus | | | |
| | the NVI is not a stationary process. | | | |
| | — Skewness of errors is not taken into ac- | | | |
| | count. | | | |

³Note that the process is also *isotropic* (i.e. $\gamma(h) = \gamma(\|h\|)$ since we are in a one-dimensional setting and the covariance is symmetric.

⁴Strictrly speaking we use a scaled version of the variogram. Thus only the ratio of p/n matters.

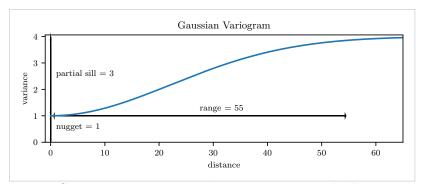


Figure 2.2: Gaussian Variogram with nugget=1, partial sill=3, range=55

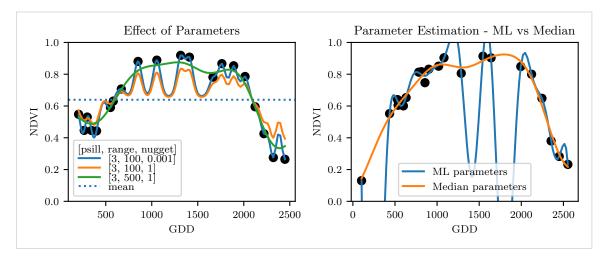


Figure 2.3: On the left we see how the interpolation change if we increase the nugget and the range parameter. On the right we compare two kriging interpolations where one takes parameters by numerically maximizing the (which results in a very small nugget) and the other takes the median of many such numerical optimizations.

2.3.3 Savitzky-Golay Filter (SG Filter)

The Savitzky-Golay Filter, introduced in Savitzky and Golay (Savitzky and Golay) is a technique in signal processing and can be used to filter out high frequencies (low-pass filter) as argued in Schafer (Schafer). Furthermore, it also can be used for smoothing by filtering high frequency noise while keeping the low frequency signal. First we choose a window size m. Then, for each point $j \in \{m, m+1, \ldots, n-m\}$ we fit a polynomial of degree k by:

$$\hat{y}_j = \min_{p \in P_k} \sum_{i=-m}^m (p(x_{j+i}) - y_{i+j})^2,$$

were P_k denotes the Polynomials of degree k over \mathbb{R} .

For equidistant points this can efficiently be calculated by

$$\hat{y}_j = \sum_{i=-m}^m c_i y_{j+i},$$

where the c_i are only dependent on the m and k and are tabulated in the original paper.

Adaptation to the NDVI

In a rather famous paper Chen, Jönsson, Tamura, Gu, Matsushita, and Eklundh (Chen et al.) a "robust" method based on the Savitzky-Golay has been used. The method is based on the assumption that due to atmospheric effects the observed NDVI tends to be underestimated and that it cannot increase too quickly⁵.

Algorithm:

- i.) Remove points which are labeled as cloudy
- ii.) Remove points which would indicate an increase greater than 0.4 within 20 days
- iii.) Linearly interpolate to obtain an equidistant time series X^0
- 4 iv.) Apply the Savitzky-Golay Filter to obtain a new time series X^1
- v.) Update X^1 by applying again a Savitzky-Golay Filter. Repeat this until $w^T|X^1-X^0|$ stops decreasing, where w is a weight vector with $w_i = \min\left(1, 1 \frac{X_i^1 X_i^0}{\max_i \|X_i^1 X_i^0\|}\right)$. This reduces the penalty introduced by outliers⁶ and by repeating this step we approach the "upper NDVI envelope".

Pros Cons

- Popular technique in signal processing
- Efficient calculation for equidistant points
- Upper envelope matches intuition for the NDVI. Therefore, it is robust against outliers with small values.
- No natural way of how to estimate points which are not in the data.
- Not generalizable to other spectral indices.
- Linear interpolation to account for missing data might be not appropriate.
- No smooth interpolation between two measurements.

Extension: Spatial-Temporal-Savitzky-Golay Filter

One notable adaptation of the Savitzky-Golay is the presented by Cao, Chen, Shen, Chen, Zhou, Wang, and Yang (Cao et al.). The key difference is the additional assumption of the cloud cover being discontinuous and that we can improve by looking at adjacent pixels⁷. Because we are working with rather high resolution satellite data, and we need the variance in the predictors we will waive this extension.

2.3.4 Locally Weighted Regression (LOESS)

Introduced by: Cleveland (Cleveland) implemented here Cappellari, McDermid, Alatalo, Blitz, Bois, Bournaud, Bureau, Crocker, Davies, Davis, de Zeeuw, Duc, Emsellem, Khochfar, Krajnović, Kuntschner, Morganti, Naab, Oosterloo, Sarzi, Scott, Serra, Weijmans, and Young (Cappellari et al.)

⁵The latter is argued by the biological impossibility of such fast vegetation changes

⁶Here we call a point i an outlier if $X_i^0 < X_i^1$.

⁷Here, we say that a pixel is adjacent if it is the same pixel but from a different year (keeping the same day of the year) or (if not enough of such temporal-adjacent pixel are found) it is spatially adjacent

The Locally Weighted Regression (LOESS) can be understood as a generalization of the Savitzky-Golay Filter (c.f. sec. 2.3.3).

Given a proportion $\alpha \in (0,1]$, we estimate each y_i separately by fitting a polynomial of order d by weighted least squares. The weights are (usually) defined by

$$w_i(x_j) = \begin{cases} \left(1 - \left(\frac{x_j}{h_i}\right)^3\right)^3, & \text{for } |x_j| < h_i \\ 0, & \text{for } |x_j| \geqslant h_i \end{cases}$$

where h_i is the minimal distance such that $\lceil \alpha n \rceil$ observations are in the ball $B_{h_i}(x_i)$. So for each y_i we only consider a proportion α of the observations.

4 How does the Robust LOESS differ from the SG Filter?

The LOESS smoother takes a fraction of points instead of a fixed number and therefore automatically adapts to the size of the data we wish to interpolate. However, we run into the danger of considering to little observations since the estimation breaks down if $\lceil \alpha n \rceil < d+1$. Furthermore, LOESS gives less weight to points further away. This yields a "smoother" estimate, since when we slide the window (e.g. for estimating the next value) an influential point at the border does not suddenly get zero weight from being weighted equally before. Finally, the LOESS also can be used for non-equidistant data and allows for arbitrary interpolation.

Robustify

Cleveland (Cleveland) also proposes an iterative method how to reduce the impact of outliers.⁹

First we define a function which will determine the weight given to each observation such that observations with large scaled residuals will have less weight. That is the bisquare function B:

$$B(x) := \begin{cases} (1 - x^2)^2, & \text{if } |x| < 1\\ 0, & \text{else} \end{cases}$$

Now, we do something similar to what is done in iteratively reweighted least squares. Simply, reiterate with updating the weights of each observation with

$$w_i^{\text{new}} := w_i^{\text{old}} B\left(\frac{|r_i|}{6 \max(r_1, \dots, r_n)}\right)$$
 (2.3.4.1)

where $r_i = y_i - \hat{y}_i$ denotes the residuals. Stop the reiteration after several steps or till the change of the values is smaller than some tolerance.

Examples of such iterative fits are illustrated in fig. 2.4.

XXX Our Adjustment: Since we usually observe outliers with negative residuals we decide to divide the negative residuals by two before updating the weights. Furthermore, we want

⁸If too many weights are set to zero, we might end up considering not enough observations and thus get a singular design-matrix (for the least squares estimation). Therefore, we substitute h_i with $1.01h_i$, so that the observation on the boundary of $B_{h_i}(x_i)$ does not get completely ignored.

⁹Note that due to using the median for the normalization we gain a breakdown point of 50% for outliers in y.

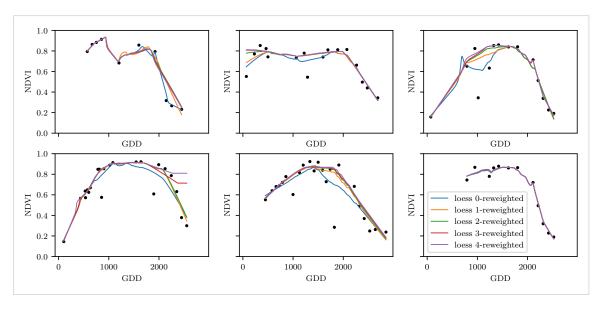


Figure 2.4: The loess smoother fitted to different (scl45-)NDVI time series. Iterations of a robustifing refit (as indicated in section 2.3.4) are also displayed

to prevent low-weighted observations to corrupt our estimation of scale (the median) and thus we use the weighted median. This can be defined as

$$\operatorname{med}_{\operatorname{weighted}}(r, w) := \arg\min_{\lambda \in \mathbb{R}} \sum_{i=1}^{n} |r_i w_i - \lambda|$$

for $r, w \in \mathbb{R}^n$

Pros
Cons

— Flexible generalization of SavitzkyGolay
— arbitrary interpolation possible
— Intuitive parameters
— Cons
— The nature of local regression might lead to suprising estimates (no smoothness guarantees for the second derivative)
— Multiple XXXXXXX

2.3.5 B-splines

from Lyche and Morken (Lyche and Morken)

$$S(x) = \sum_{j=0}^{n-1} c_j B_{j,k;t}(x)$$

$$B_{i,0}(x) = 1, \text{ if } t_i \le x < t_{i+1}, \text{ otherwise } 0$$

$$B_{i,k}(x) = \frac{x - t_i}{t_{i+k} - t_i} B_{i,k-1}(x) + \frac{t_{i+k+1} - x}{t_{i+k+1} - t_{i+1}} B_{i+1,k-1}(x)$$

Smoothing: We can relax the constrain that we have to perfectly interpolate. Thus we use the minimum number of knots¹⁰ such that: $\sum_{i=1}^{n} (w(y_i - \hat{y}_i))^2 \leq s$

 $[\]overline{\ }^{10}$ SciPy uses FITPACK and DFITPACK, the documentation suggests that smoothness is achieved by reducing the number knots used

| Pros | Cons | | | |
|--|---|--|--|--|
| can be assigned degrees of freedom extendable to "smooth" version performs also well if points are not equidistant | smoothing process does not translate well to a interpretation (unlike smoothing splines) choice of smoothing parameter s | | | |

2.3.6 Natural Smoothing Splines

Let \mathcal{F} be the Sobolev space (the space of functions of which the second derivative is integrable). Then the unique¹¹ minimizer

$$\hat{m} := \underset{f \in \mathcal{F}}{\operatorname{arg\,min}} \sum_{i=1}^{n} (Y_i - f(x_i))^2 + \lambda \int f''(x)^2 dx$$

is a natural¹² cubic spline (i.e. a piecewise cubic polynomial function). The objective function has an intuitive meaning, as to avoid lateral acceleration it is desirable to move the steering wheel as little as possible, when driving a car.

| Pros | Cons | | | |
|---|--------------------|--|--|--|
| can be assigned degrees of freedom (trace of the hat-matrix) efficient estimation (closed form solu- | — choose λ | | | |
| tion) — intuitive penalty (we don't want the function to be too "wobbly" — change | | | | |
| slopes) — performs also well if points are not equidistant | | | | |
| — fixes the Runge's phenomenon (fluctua- tion of high degree polynomial interpo- lation) | | | | |

2.3.7 Other Methods to study:

From inroduction of Chen, Jönsson, Tamura, Gu, Matsushita, and Eklundh (Chen et al.):
(1) threshold- based methods, such as the best index slope extraction algorithm (BISE)
(Viovy et al., 1992); (2) Fourier-based fitting methods (Cihlar, 1996; Roerink et al., 2000;
Sellers et al., 1994); and (3) asymmetric function fitting methods such as the asymmetric
Gaussian function fitting approach (Jonsson Eklundh, 2002) and the weighted least-squares
linear regression approach (Swets et al., 1999).

TEMP — Figures

¹¹Strictly speaking it is only unique for $\lambda > 0$

¹²It is called natural since it is affine outside the data range $(\forall x \notin [x_1, x_n] : \hat{m}''(x) = 0)$

| | SS | loess | dl | bspl | fourier | ss rob | loess rob | dl rob | bspl rob | fourier rob |
|----------|-------|-------|-------|-------|---------|--------|-----------|--------|----------|-------------|
| rmse | 0.066 | 0.062 | 0.061 | 0.077 | 0.062 | 0.073 | 0.068 | 0.064 | 0.082 | 0.137 |
| qtile 50 | 0.035 | 0.032 | 0.026 | 0.042 | 0.029 | 0.031 | 0.029 | 0.021 | 0.035 | 0.045 |
| qtile75 | 0.061 | 0.057 | 0.047 | 0.074 | 0.050 | 0.058 | 0.053 | 0.042 | 0.067 | 0.088 |
| qtile85 | 0.078 | 0.074 | 0.063 | 0.098 | 0.067 | 0.078 | 0.072 | 0.059 | 0.092 | 0.139 |
| qtile90 | 0.090 | 0.085 | 0.080 | 0.111 | 0.083 | 0.099 | 0.087 | 0.071 | 0.113 | 0.183 |
| qtile95 | 0.120 | 0.110 | 0.112 | 0.133 | 0.119 | 0.130 | 0.117 | 0.118 | 0.160 | 0.335 |

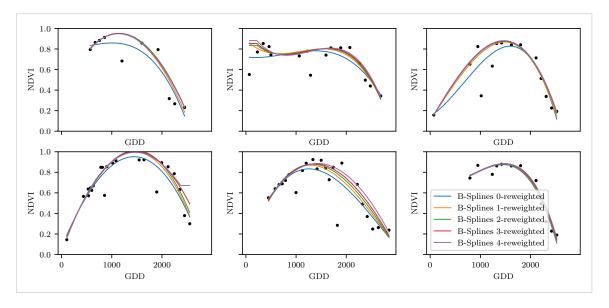


Figure 2.5: B-Splines fitted to different (scl45-)NDVI time series. Iterations of a robustifing refit (as indicated in section 2.3.4) are also displayed

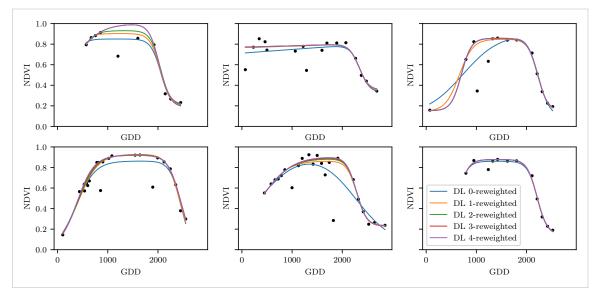


Figure 2.6: A Double Logistic curve fitted to different (scl45-)NDVI time series. Iterations of a robustifing refit (as indicated in section 2.3.4) are also displayed

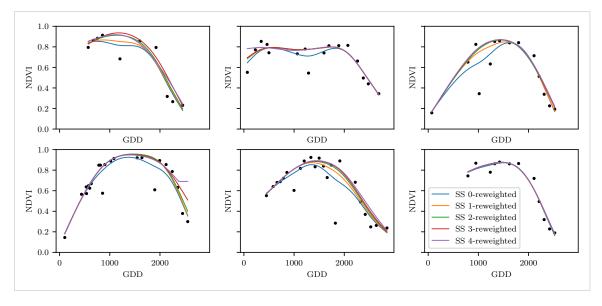


Figure 2.7: Smoothing Splines fitted to different (scl45-)NDVI time series. Iterations of a robustifing refit (as indicated in section 2.3.4) are also displayed

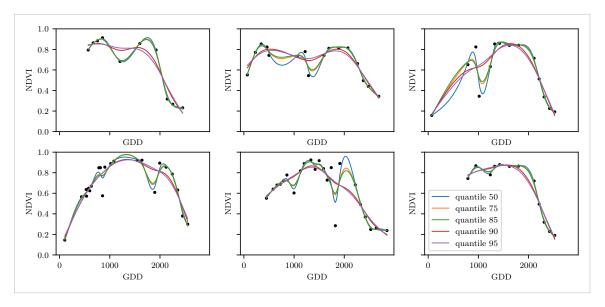


Figure 2.8: Smoothing splines fit with smoothing parameter optimized by minimizing the "..."-quantile of the absolute leave-one-out residuals. Note that the larger the considered quantile is, the smoother the resulting curve becomes.

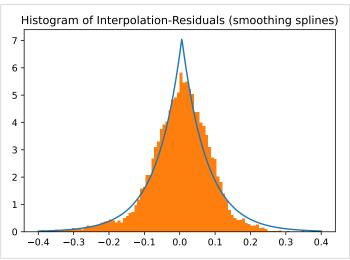


Figure 2.9: XXX caption XXX

Chapter 3

NDVI Correction / Improve NDVIData

Let's remind ourselves that the data from the Sentinel-2 is equipped with a scene classification layer (scl) and we therefore have some information of what is observed at each pixel for each sampled time (c.f. table ??). In this chapter we would like to improve the observed NDVI values by using more information than just the two bands used to calculate the NDVI (B4 and B8).

3.1 Considering other SCL Classes

In figure 3.1 we see for example that some blue points¹ follow the interpolated line closely and that they might be useful in improving an interpolation fit.

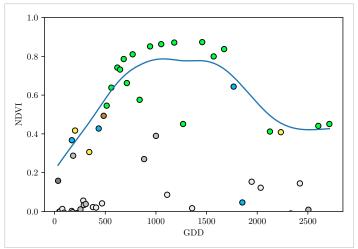


Figure 3.1: A smoothing splines fit considering green and yellow points (scl-classes 4 and 5)

To get an impression whether there is some useful information contained in the remaining scl-classes (all except 4 and 5) we would like to compare the observed NDVI with the

¹The blue points correspond to the scl-class 10: Thin cirrus clouds

true NDVI. But since we do not have any ground truth data we will make the following assumtion:

Definition 3.1.0.1. XXXAssumption (true NDVI) The true NDVI value at time t can be successfully estimated by out-of-bag interpolation using high quality observations. That is the interpolated value (using XXX) considering the points $P^{scl45} \setminus P_t$. In the following we will call this estimate the "true"-NDVI

i.) For each pixel and for each observation (every scl-class): estimate the NDVI value (via out-of-the-box interpolation²)

ii.)

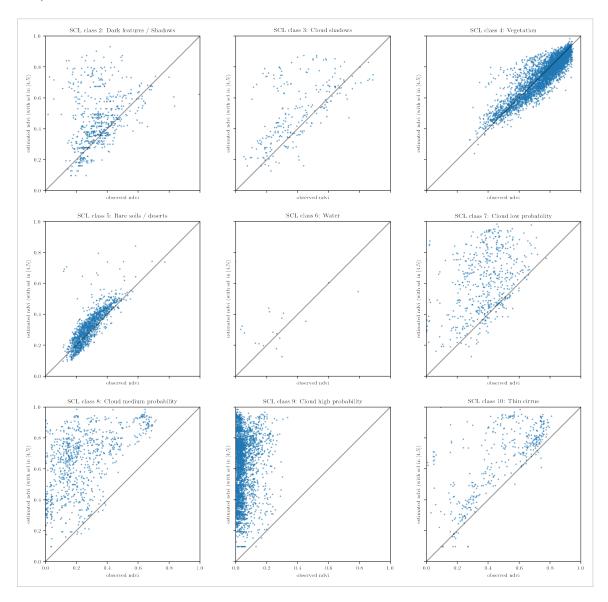


Figure 3.2: XXX caption XXX

²That is, we use all observations (with scl-class 4 or 5) but the current one.

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Appendix A

Hi Mom