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APPLICATIONS OF INFORMATICS IN ENVIRONMENT ENGINEERING AND MEDICINE

Editors:
Jan Studzinski
Ludosław Drelichowski
Olgierd Hryniewicz

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Systems Research Institute of Polish Academy of Science
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CHAPTER 1

Water and Air Quality Management

MISSING DATA IN WATER QUALITY TIME SERIES

Albrecht GNAUCK, Bernhard LUTHER
Brandenburg University of Technology at Cottbus, Germany
<umweltinformatik@tu-cottbus.de; luther@tu-cottbus.de>

Missing data in water quality time series lead to some general problems in many fields of environmental research and simulation. They cause not only difficulties in process identification and parameter estimation but also misinterpretations of spatial and temporal variations of water quality indicators. Mostly, time series represent samples of data at discrete time events based on various sampling intervals. For modelling and simulation of water quality processes time series must be mapped on a regular time grid. This procedure is known as re-sampling of time series and consists on data interpolation or, in the case of disturbed signals, on data approximation. Some well-known linear and nonlinear interpolation methods exist while data approximation can be done by static and dynamic procedures. Regression type functions or in the case of cycling time series Fourier approximations are mainly used. By these procedures equidistant data will be obtained. In opposite of that, digital filtering procedures deliver consistent equidistant data estimates based on major signal frequencies. In the paper different algorithms of data interpolation and approximation are applied on irregularly sampled water quality time of rivers with different hydraulic conditions. Additionally, low pass filters are checked to find out the best filter function for each water quality indicator.

Keywords: Water quality, time series, interpolation, approximation, digital filtering.

1. Introduction

Water quality time series of freshwater ecosystems characterise not only complex ecological processes but also levels of water pollution due to anthropogenic activities as well as industrial and agricultural land use in a river basin. The goals of administrative freshwater monitoring programs consist of information mining of the actual ecosystem state including the historic development of ecological processes (Gnauck, 1982). The intensity of water pollution and the impact on ecosystem functioning as well as on biodiversity of freshwater organisms can be estimated on the base of water quality time series. They form a decision platform for complex and complicated water quality management alternatives. Time series of water quality express the results of interacting and networking ecological processes. Only regularly sampled data represent the full ecosystem information. For modelling and simulation of environmental processes it is necessary that all data sets are based on a regularly time grid. But in practice, water quality time series often contain missing and/or irregularly sampled data. Data gaps entail not only information lacks, but lead also to misinterpretations of statistical measures and results of water quality simulation models (Little and Rubin 1983).

From this background the question arises how to fill in data gaps in time series. Gentili et al. (2004) reported on some methods of linear interpolation and imputation techniques. Meloun et al. (1994) have used simple interpolation and approximation methods to fill gaps in chemical data series. Gnauck et al. (1976) and Gnauck and Winkler (1983) estimated missing data in water quality time series by static recursive regression estimation procedures. Hirsch et al. (1982) used trend techniques to estimate monthly water quality data from incomplete data sets. Dynamic estimation procedures to solve modelling problems caused by missing data are applied by Young and Beck (1974), Pagano (1978), Vecchia (1985), Vecchia and Ballerini (1991), Franses (1994, 1999), McLeod (1994), Drepper et al. (1994), Hondzo and Stefan (1996), Bhangu and Whitfield (1997), Franses and Draisma (1997), Lehmann and Weber (1998), Franses (1999), Young (1999). Various stationary and instationary trend functions, simple data filter and approximation methods for water quality time series are discussed by Hipel and McLeod (1994). Haan (2002) applied trend functions on hydrologic time series.

The efficiency of all these procedures is quite different. For modelling and simulation of water quality processes it is necessary that all data sets are based on a regularly time grid. On the other hand, filling the data gaps in water quality time series by information theory based methods (Lange 1999), by wavelet analysis (Gnauck and Tesche 1998) or by transfer function using *z*-transformation (Young 1999, Romanowicz and Petersen 2003) is at the beginning and commonly not used. The question how to handle missing data in water quality, or more general, in environmental time series is unsolved up to now (Nittner 2003, Latini and Passerini 2004). In the following chapters some proposals are given how to fill in data gaps in water quality time series, and to get not only equidistant but consistent data.

2. Missing data in water quality time series

Mostly, water quality time series consist of data which are based regular sampling intervals as daily, weekly, and two weekly or monthly intervals. But medium-term and long-term water quality time series often contain missing and/or irregularly sampled data. Figure 1 shows an example of an irregular sampled data set. The reasons for incomplete water quality time series are manifold: Failures in measurement devices, inaccurate laboratory analytics, errors in data management, interruption of transmission lines, data storage errors, changes in sampling program design and others. Little and Rubin (1987) classified missing data as missing completely at random, as missing at random and as non-ignorable.

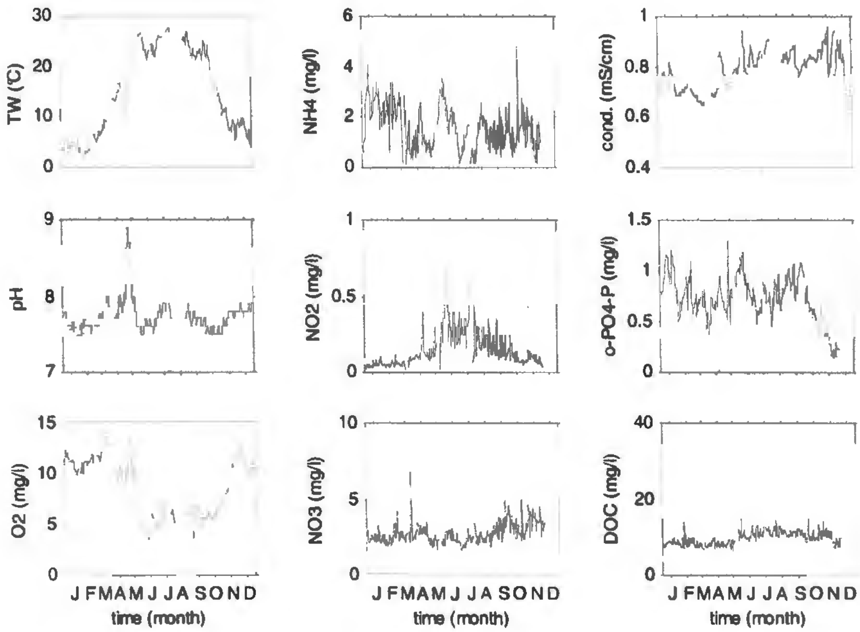

Figure 1. Irregular sampled water quality time series

All missing data have to be replaced. Known procedures are replacing by smoothing, by interpolation, by application of trend functions or by data from reference curves according to standards and conventional rules. But the efficiency of all these procedures is quite different. Applying interpolation procedures on irregular sampled raw data sets time series with equidistant sampling intervals will be obtained. The application of approximation methods on such time series results in functional relationships. Another procedure is the so-called re-sampling method (Adorf 1995) which requires data interpolation and, in the case of noisy information, data approximation to place sampled data on a regularly time scale. The goal of this method is to reconstruct time series with small sampling intervals. The following tasks are equivalent to re-sampling:

1. Filling the gaps of irregularly recorded data by interpolation.
2. Reconstruction of data of regularly recorded time series by means of analytical functions or signal estimations.
3. Filling the gaps of irregularly recorded data by means of measuring values of reference curves.

The re-sampling procedure can be extended by application of digital filtering methods (figure 2). On the base of equidistant data consistent time series based on major process frequencies will be obtained.

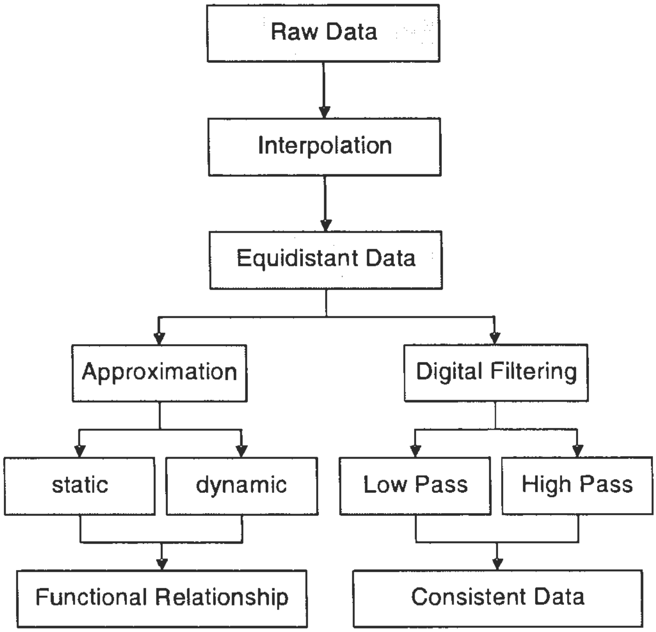

Figure 2. Re-sampling and digital filtering of data

3. Interpolation

To obtain water quality time series with equidistant daily sampling intervals from irregularly sampled raw data Gnauck and Luther (2004) compared four interpolation methods (table 1) for rivers with different hydraulic conditions. The methods are distinguished by the degree of continuity of derivatives of the interpolation function $\tilde{x}(t)$ on an interval $[t_k, t_{k+1}]$. Nearest neighbour method gives out discontinuous interpolated data while the other ones produce continuous interpolated time series. 3rd order polynomial and cubic splines interpolation functions are distinguished by parameters only. Because of random, but not normal distributed raw data and nonlinear effects within the water quality processes observed no R^2 like statistics was used. The suitability of interpolation method was valuated by standard error $SE = s/\sqrt{n}$ between interpolated and original time series (table 2). For all investigated time series mostly linear interpolation method was found out the best one to get daily data. This can be explained by the time step of interpolation of one day in comparison with most ecological process rate constants. Nearest neighbour method can easily be applied to irregular sampled time series, but continuous interpolated data should be preferred.

Table 1. Interpolation algorithms used

Method	Algorithm	Remark
Nearest neighbour	$\tilde{x}(t) = \begin{cases} x_k & t < (t_k + t_{k+1})/2 \\ x_{k+1} & t \geq (t_k + t_{k+1})/2 \end{cases}$	$\tilde{X} \notin C^{(0)}[t_0, t_n]$ $\tilde{X}$ discontinuous
Linear	$\tilde{x}(t) = \dfrac{x_{k+1} - x_k}{t_{k+1} - t_k}(t - t_k) + x_k$	$\tilde{X} \in C^{(0)}[t_0, t_n]$ $\tilde{X}$ continuous
Cubic Hermite polynomial	$\tilde{x}(t)\Big\vert_{[t_k, t_{k+1}]} = a_k t^3 + b_k t^2 + c_k t^3 + d_k$	$\tilde{X} \in C^{(1)}[t_0, t_n]$ $\tilde{X}$ continuous differentiable
Cubic splines	$\tilde{x}(t)\Big\vert_{[t_k, t_{k+1}]} = e_k t^3 + f_k t^2 + g_k t^3 + h_k$	$\tilde{X} \in C^{(2)}[t_0, t_n]$ $\tilde{X}, \tilde{X}$ continuous differentiable

Table 2. Comparison of standard errors of interpolation algorithms used

Year	Method	NH4-N	NO2-N	NO3-N	o-PO4-P	DOC
1994	neighbour	0,12	0,020	0,27	0,020	1,47
1994	linear	**0,09**	**0,017**	**0,23**	**0,019**	**1,14**
1994	spline	0,11	0,019	**0,23**	**0,019**	**1,41**
1994	cubic	0,11	0,019	**0,23**	**0,019**	**1,41**
1995	neighbour	0,09	0,016	0,22	0,027	0,73
1995	linear	**0,08**	**0,015**	**0,20**	**0,025**	**0,69**
1995	spline	0,10	0,016	0,22	0,026	0,71
1995	cubic	0,10	0,016	0,22	0,026	0,71

Polynomial and cubic splines interpolation are also helpful, but they result for some intervals in the opposite time structure compared with raw data. Mainly linear interpolation functions show acceptable results. Table 3 contains results for daily interpolations from two-weekly irregularly sampled data for rivers with different hydraulic flow regimes. It comes out from table 3 that linear interpolation method can be used to get regularly sampled data independent from river hydraulics.

Table 3. Interpolation methods applied on rivers

Variable	Spree	Havel	Upper Elbe	Lower Elbe	Oder
NH4-N	linear	linear	linear	linear	linear
NO2-N	linear	linear	linear	linear	linear
NO3-N	linear	linear	linear	linear	linear
o-PO4-P	linear, spline, polynomial	linear, spline, polynomial	*no data*	*no data*	*no data*
DOC	linear	linear	linear	linear	linear
UV	*no data*	linear, spline, polynomial	*no data*	*no data*	linear, spline
Turbidity	*no data*	linear	linear	linear	linear
Conductivity	spline, polynomial	spline, polynomial	linear, spline, polynomial	linear, spline, polynomial	linear, polynomial
DO	linear	linear	linear	linear	linear

4. Approximation

A second step in re-sampling of water quality time series is the estimation of missing data due to approximating functions. For parameter estimation mostly least squares method or maximum likelihood method are used. Valuations of linear approximations by multiple linear regression functions are expressed by performance index R^2 (Straškraba and Gnauck 1985). To approximate aperiodic water quality time series some procedures as multivariate regression models (Gnauck and Winkler 1983), polynomial models (Hirsch et al. 1982) or time-discrete transfer function models (Young 1999) are helpful. Haefner (1996) discussed data problems in the context of chaos of biological problems. Evaluations of the quality of fit are given by linear or nonlinear coefficients of determination. Table 4 contains results of an approximation study of the Havel River. The last column indicates the significance level of the approximation.

Table 4. Trend functions of water quality of the River Havel

Water quality indicator	Trend function	Order	R^2	P(95%)
Water flow	polynomial	2	0,8126	+
Temperature	polynomial	2	0,6177	+
Conductivity	polynomial	2	0,1971	-
Chloride	polynomial	2	0,0382	-
DO	polynomial	2	0,3858	+
BOD	polynomial	2	0,4264	+
CSV	polynomial	2	0,7611	+
NH4-N	exponential		0,5669	+
NO2-N	exponential		0,4879	+
NO3-N	exponential		0,4746	+
O-PO4-P	exponential		0,8683	+
TP	polynomial	2	0,0822	-
SiO2	polynomial	2	0,8888	+
Suspended matter	polynomial	2	0,0227	-
Chlorophyll-a	polynomial	2	0,6032	+
Inorg. part of biomass	polynomial	2	0,6742	+
Loss of organic matter	polynomial	2	0,1418	-

Trend functions or polynomials are well studied but their parameters are interpretable only in few cases. For a linear trend: $y(t) = a_0(t) + a_1(t)\ x(t)$ the parameter can be interpreted as follows: a_0 – mean start value, a_1 – mean rate of change. In case of a quadratic trend $y(t) = a_0(t) + a_1(t)\ x(t) + a_2(t)\ x^2(t)$ the following interpretation of parameters can be given: a_0 - mean start value, a_1 - mean rate of change, a_2 – mean process acceleration. For a higher order polynomial trend $y(t) = a_0(t) + a_1(t)\ x(t) + a_2(t)\ x^2(t) + ... + a_n(t)\ x^n(t)$ an interpretation of parameters is mostly impossible. The parameters of an exponential trend $x(t) = x(0)\ e^{\cdot kt} + E$ can be interpreted according to kinetics 1. order: x(0) – initial concentration value, k – rate of change, E – random quota.

Mathematical equations describe either the time dependency (function of time *t*) or the frequency dependency (function of frequency ω or cycles per time unit) (Pollock 1999). Because of water quality processes are often influenced by external cycling processes they will be approximated by Fourier polynomials which express characteristic cycles by harmonic frequencies. A water quality cycling (or periodic) process with period T_0 is described by a Fourier series of the form $x(t) = a_0/2 + \sum a_i \cdot \cos(i\omega_0 t) + \sum b_i \cdot \sin(i\omega_0 t)$ with $-\infty \le i \le +\infty$, $\omega_0 = 2\pi/T_0$ – frequency of the basic cycle, T_0 – period of cycle. Coefficients a_i and b_i are calculated as follows $a_i = 1/T_0 \int x(t) \cdot \cos(i\omega_0 t) dt$ and $b_i = 1/T_0 \int x(t) \cdot \sin(i\omega_0 t) dt$. The initial parameter a_0 is given by $a_0 = 1/2T_0 \int x(t) dt$. The Fourier polynomial is an approximation which represents the minimum mean squared deviation of the cycling process. The amplitudes of the approximating function are given by $A_i = \sqrt{a_i^2 + b_i^2}$, where phase shifts in the interval [0, 2π] are given by $\varphi_i = \arc\tan b_i/a_i$. The application of Fourier polynomials to water quality processes often leads to a shift of the approximated time series (figure 3).

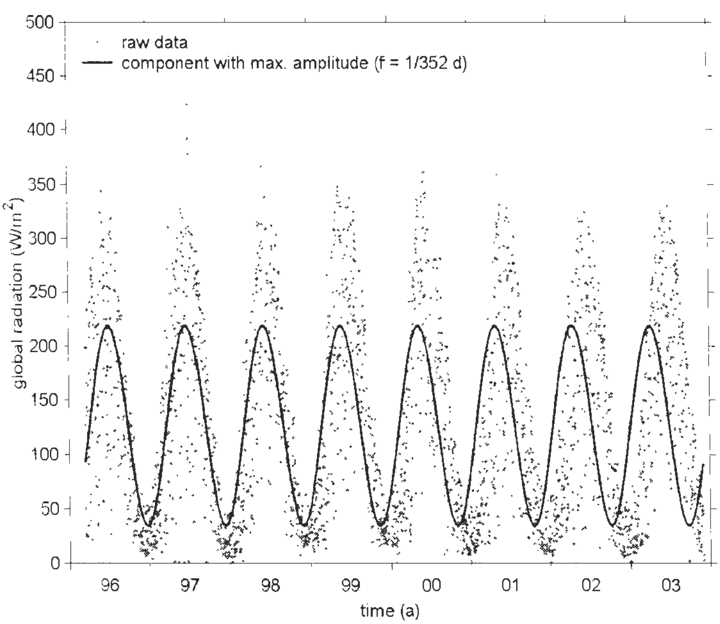

Figure 3. Cycling of an external driving force

Fourier approximations of cycling water quality processes of freshwater ecosystems are mostly expressed by the yearly dominant harmonic cycle. The frequency will be different in dependence from location (table 5).

Table 5. Fourier approximations of physical variables of freshwater ecosystems

Fourier approximation
Saidenbach reservoir
$TEMP(t) = 12.0 + 1.458 \cdot \cos((6\pi/180)t) - 4.462 \cdot \sin((6\pi/180)t$
Neunzehnhain reservoir
$TEMP(t) = 11.9 + 0.693 \cdot \cos((6\pi/180)t) + 4.415 \cdot \sin((6\pi/180)t$
Klicava reservoir
$TEMP(t) = 11.1 - 6.650 \cdot \cos((9\pi/180)t) - 7.820 \cdot \sin((9\pi/180)t$
Slapy reservoir
$TEMP(t) = 12.0 - 7.073 \cdot \cos((10\pi/180)t) - 6.684 \cdot \sin((10\pi/180)t$
River Havel
$TEMP(t) = 12.5 + 10.5 \cdot \sin((t+208) \cdot 2\pi/327)$
River Havel
$I(t) = 280 + 210 \cdot \sin((t+240) \cdot 2\pi/365)$

5. Digital Filtering

Time series of water quality are described by methods of linear systems theory. They are given by monitored data at discrete time events. Each real system causes distortions, attenuations and redundancies of the time structure of signals. These effects have to be measured and evaluated. Therefore, some characteristics of a reference system are needed which shows no distortions (Meyer 2003). Such a system is given by an ideal low pass filter. Filters are frequency dependent systems which let pass selected frequency ranges of signals (pass band), and lock other frequency ranges (lock band). Usually, a signal can be separated into two parts: The disturbance signal ($x_D(t)$) and in the useful part of signal ($x_U(t)$). A signal transfer of a linear transfer system of an input signal $x(t) = x_U(t) + x_D(t)$ results with an output signal $y(t) = y_U(t) + y_D(t)$ where $y_D(t) = 0$ is desired. In this case $y_N(t) = k\, x_N(t - \tau)$ is the distortion free transferred signal. In the case of $y_D(t) \rightarrow 0$ optimal filter as Wiener filter or Kalman filter will be get. Digital filters are subdivided into recursive (IIR-) filters and non-recursive (FIR-) filter. Other subdivisions are used by frequency range (low pass, band pass, high pass, band lock), by the kind of filter approximation, and by the order of approximating polynomial. To obtain consistent data signal transmission should be carried out by an ideal low pass filter with the gain characteristic $|H(\omega)|^2 = 1/(1+F(\omega^2))$. It works as a distortionless system (Kammeyer und Kroschel 2002, Meyer 2003, Werner 2003). The amplitude response $|H(\omega)|^2 = 1$, if $\omega \leq 1$ or $|H(\omega)|^2 = 0$, if $\omega > 1$.

Filter procedures can be distinguished by differences in the pass band and by the ripple effects (Meyer 2003). An often applied family of linear discrete filters with infinite pulse response is given by Butterworth filters. Noise and outliers are strongly reduced by high limiting frequencies. For low cut-off frequencies the filtered time series does not follow the original time series and converges to zero. This is known from exponential filters. Some important low pass filters are listed in table 6. They are distinguished by band pass and ripple effects.

Table 6. Digital filters

Method	Equation	Comment
Butterworth (power low pass)	$\|H(\omega)\|^2 = 1/(1 + \omega^{2n})$	Amplitude response should be flat as possible in the pass band
Chebychev 1	$\|H(\omega)\|^2 = 1/(1 + \varepsilon^2 c_n^2(\omega))$	ε - ripple factor or eccentricity, $\varepsilon = 0.1526$, $c_n(\omega)$ is the Chebychev polynomial of order n. In the pass band a ripple is accepted. Transition from pass band to stop band is steeper than for Butterworth filter
Chebychev 2 (inverse Chebyshev filter)	$\|H(\omega)\|^2 = 1/(1 + \varepsilon^{*2} c_n^{2n}(\omega))$	$\varepsilon^* = 2\varepsilon/(1-\varepsilon)$, in the stop band a ripple is accepted
Cauer (elliptic filter)	$\|H(\omega)\|^2 = 1/(1 + \varepsilon^2 F_n^*(\omega^2))$	$F_n^*(\omega^2)$ - characteristic function. Ripples arise in the pass band and in the stop band. One gets the steepest transition between both frequency bands

Filter functions of water quality indicators were tested for different rivers. Higher order filters cause strong ripple effects in pass band as well as in stop band. Because of ripples cause unexplainable disturbances for signal reproduction filters of order 1 to 3 should be used only. In figures 4 and 5 two examples are given. Comparing standard errors it can be seen that filters of lower order lay out smaller standard errors. They show smoother frequency behaviour as filters of higher order.

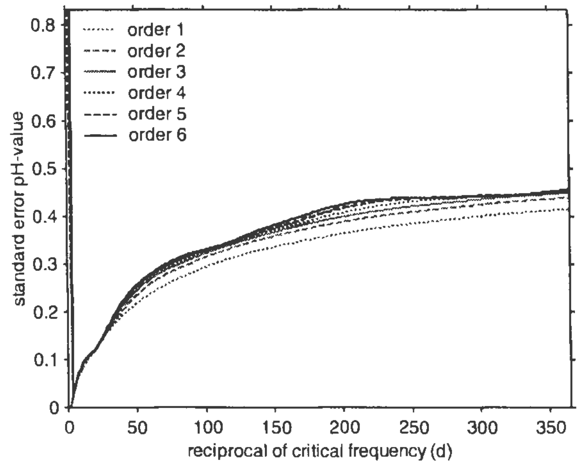

Figure 4. Standard errors of a Butterworth filter for pH

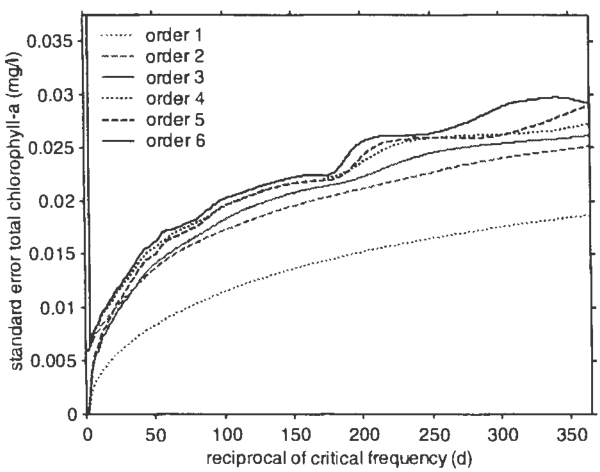

Figure 5. Standard errors of Chebychev 1 filter for phytoplankton biomass

Mostly, Butterworth filters, Chebychev 1 filters and Cauer filters are found out as useful for water quality indicators. Chebychev 2 filters were found acceptable in a few cases only. For this filter type standard errors of lower order filters are higher than those for higher orders.

After filter selection limiting frequencies are determined by means of power spectra. Figures 6 - 7 show results of signal reconstructions of long-term water quality data of River Spree at Berlin by digital filters.

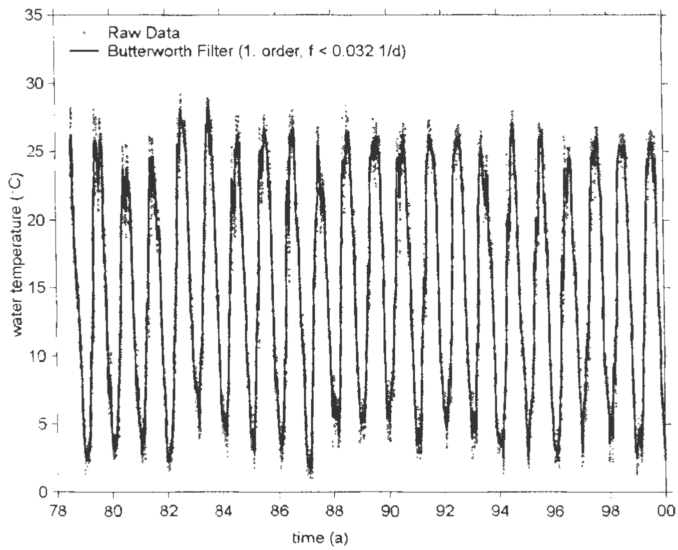

Figure 6. Filtered signal of water temperature for Spree River

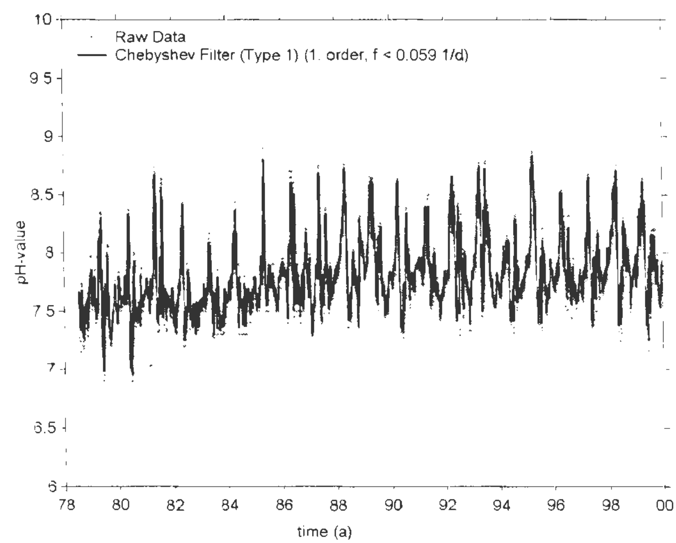

Figure 7. Filtered signal of pH for Spree River

In figures 8 and 9 show applications of elliptic filters to reconstruct irregularly sampled water quality and quantity data.

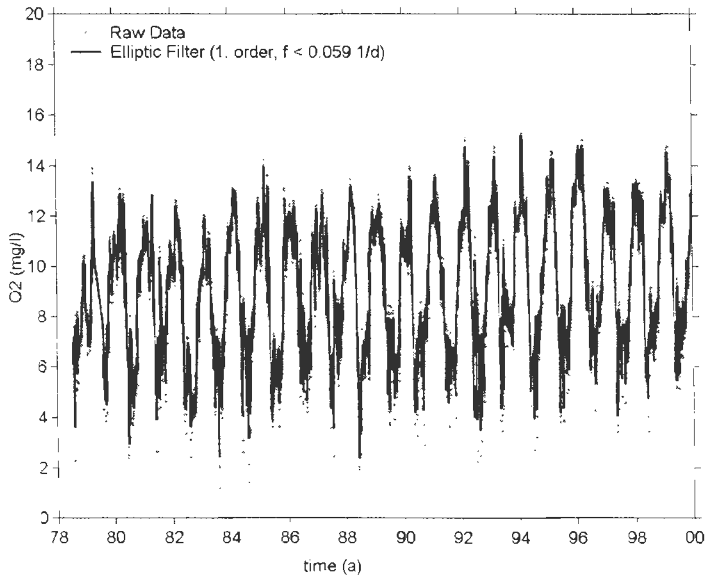

Figure 8. Reconstruction of DO time series by an elliptic filter function of 1st order

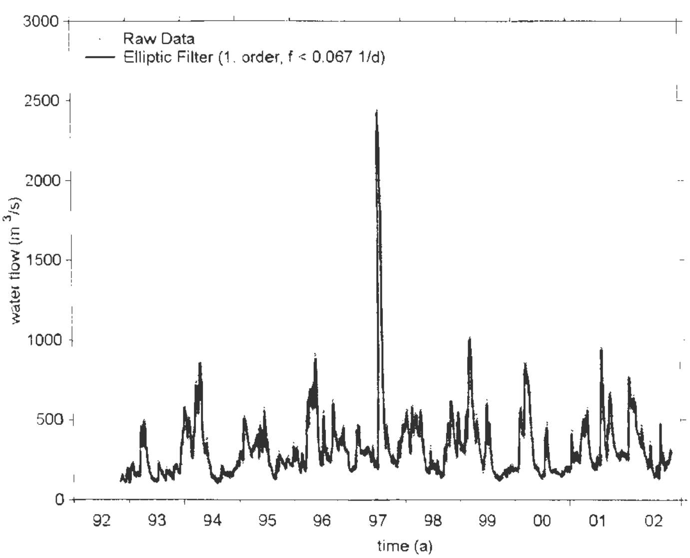

Figure 9. Elliptic filter of water flow for the Oder River at Frankfurt

Results from a filter study for rivers are summarised in table 7. It can be seen that elliptic filters are obtained for nutrients. All filter functions are determined on a 95% probability level. Some filter functions are valid for the 1% significance level. They are marked by brackets.

Table 7. Applications of digital filters on water quality indicators

Indicator	**1. order filter**	**2. order filter**	**3. order filter**
DOC	Cauer	(Cauer)	(Cauer)
conductivity	Butterworth, Cauer Chebychev1	Butterworth	Butterworth, Cauer, Chebychev1
NH4-N	Cauer	(Cauer)	(Cauer)
NO2-N	Cauer	(Cauer)	(Cauer)
NO3-N	Cauer	(Cauer)	(Cauer)
DO	Butterworth, Cauer Chebychev1	Butterworth	Butterworth, Cauer, Chebychev1
o-PO4-P	Cauer	(Cauer)	(Cauer)
pH	Butterworth, Cauer Chebychev1	Butterworth, Chebychev2	Butterworth, Cauer, Chebychev1, Chebychev2
water flow	Butterworth, Chebychev1, Cauer	Butterworth, Chebychev1	Butterworth, Cauer, Chebychev1,
water temperature	Butterworth, Chebychev1, Cauer	Butterworth, Chebychev1, Chebychev2, Cauer	Butterworth, Cauer Chebychev1, Chebychev2,

6. Conclusions

The question how to handle missing data in water quality time series depends not only from the problem to be solved but more from the data set available. Applying interpolation procedures time series with equidistant sampling intervals will be obtained. Linear interpolation method is suitable for most of time series of water quality indicators but cannot express the dynamics of ecological processes. The application of approximation methods series results in functional relationships which are valid for stationary environmental conditions only. Data processing of equidistant water quality time series by digital filters produces consistent time series which are suitable for modelling and simulation. These frequency dependent algorithms are able to follow the inherent dynamics of ecological signals which comes out by different networking processes. By means of such algorithms ecological signals can be reconstructed according to their dynamics. For rivers with different hydraulics digital filtering methods were not only successful but a prerequisite for modelling.

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Jan Studzinski, Ludosław Drelichowski, Olgierd Hryniewicz
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APPLICATIONS OF INFORMATICS IN ENVIRONMENT ENGINEERING AND MEDICINE

The purpose of the present publication is to popularize applications of informatics in environment and health engineering and protection. Runned papers are thematically chosen from the works presented during the conference *Multiaccessible Computer Systems* (*Komputerowe Systemy Wielodostępne*) that has been organized by the Systems Research Institute and University of Technology and Agriculture of Bydgoszcz for several years in Ciechocinek. Problems described in the papers concern quality management of the surface waters and the atmosphere, application of the mathematical modelling in environmental engineering, and development of computer systems in health and environmental protection. In several papers results of the research projects financed by the Polish Ministry of Science and Information Society Technologies are presented.

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