

Automatic Analysis for Time-Series with Large Gaps

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model:

$$\mathbf{m} = \mathbf{s} + \mathbf{r} \quad \mathbf{m} = (m_j), \quad \mathbf{s} = (s_j), \quad \mathbf{r} = (r_j), \quad j = 1, \dots, M$$

$$\begin{aligned} s_j &= A_0 + \sum_{i=1}^N A_i \cos(2\pi f_i t_j + \phi_i) \\ &= a_0 + \sum_{i=1}^N a_i \cos(2\pi f_i t_j) + \sum_{i=1}^N b_i \sin(2\pi f_i t_j) \end{aligned}$$

m_j measured value at time t_j

s_j computed value at time t_j

r_j error in measurement

aim:

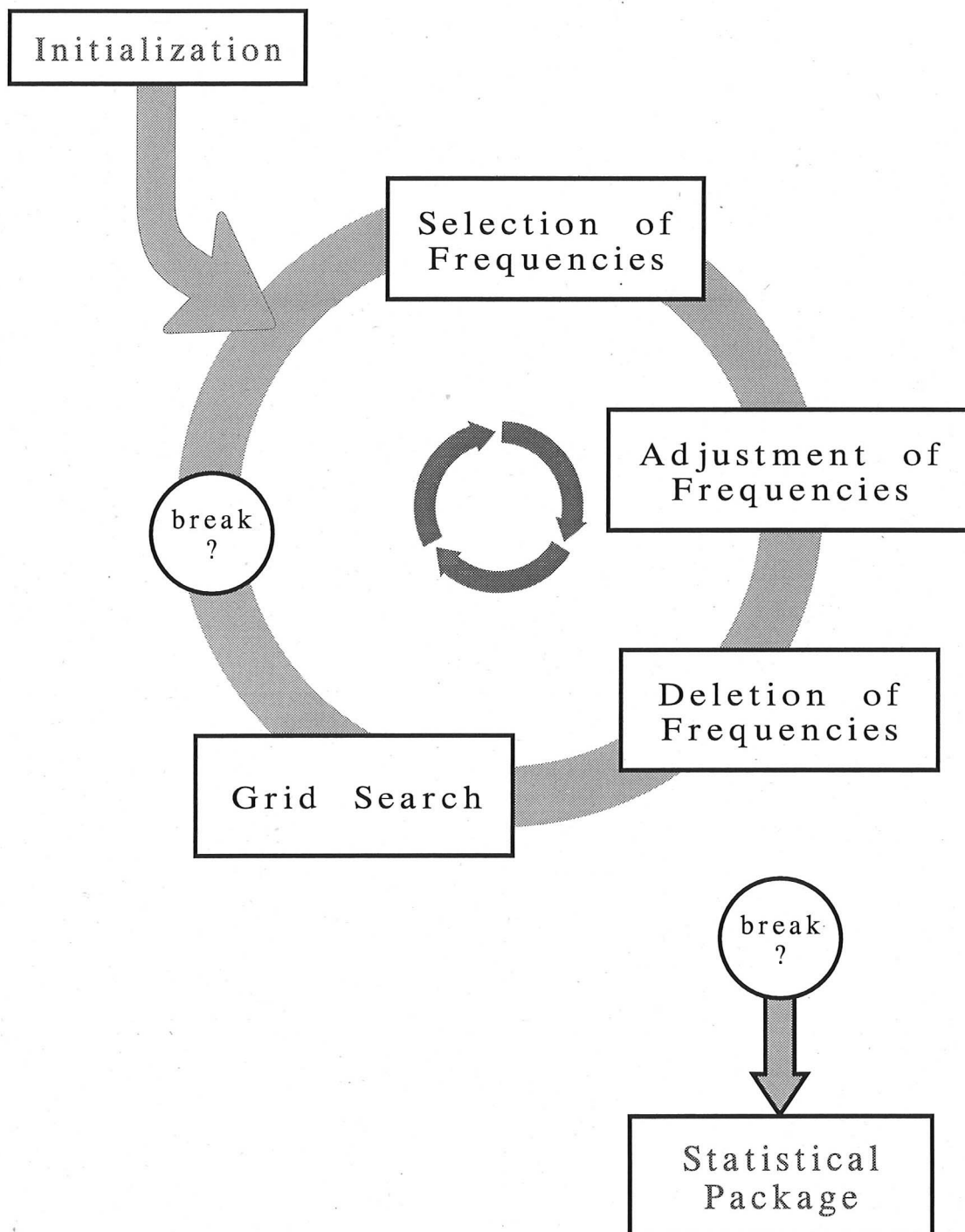
choose N (number of frequencies)

frequencies f_i ,

amplitudes A_i , and phases ϕ_i (resp. a_i and b_i)

which minimize

$$\|\mathbf{r}\| = \|\mathbf{m} - \mathbf{s}\| = \min !$$



Selection of Frequencies

Our main criterion for selection of frequencies gives the power function. We use:

$$(1) \quad p(f) = \sqrt{\frac{\left(\sum_{j=1}^M \cos(2\pi f t_j) m_j\right)^2}{\sum_{j=1}^M \cos^2(2\pi f t_j)} + \frac{\left(\sum_{j=1}^M \sin(2\pi f t_j) m_j\right)^2}{\sum_{j=1}^M \sin^2(2\pi f t_j)}}$$

and if possible we change to:

$$(2) \quad p(f) = \sqrt{\frac{2}{M}} \sqrt{\left(\sum_{j=1}^M \cos(2\pi f t_j) m_j\right)^2 + \left(\sum_{j=1}^M \sin(2\pi f t_j) m_j\right)^2}$$

- $p(f)$ is a very rapidly oscillating function. Therefore, high resolution for a clear image is necessary.
- In order to overcome local oscillations we smooth $p(f)$ by taking the maximum over small intervals. We build a second table to remember the location of the maxima in these small intervals.
- Up to n_{ins} maxima of the smoothed power-function are added to the frequency vector. This enlarged frequency vector is used as starting value for the minimization routine.
- If there are more than n_{max} frequencies only the strongest n_{max} signals of the composed frequency vector are taken.

Deletion Criteria

- If there is a pair of frequencies, which are close together, a special routine is called. This routine inserts new frequencies and checks whether there exists a better fit or not. If the old pair was a resonance phenomenon, it will be deleted in a later stage.
- Frequencies which are very close together are substituted by its mean value.
- Frequencies with small amplitudes are deleted.
- Take only the strongest $n_{max} - 2$ signals. This enables the code to try new frequencies, if the frequency vector is already full.
- After $iter1 \approx 5$ iterations a special deletion routine is called. This simulates a restart with better initial data.

Adjustment of Frequencies – Nonlinear Minimization

Given a start frequency vector $\mathbf{f} = (f_1, \dots, f_N)$ we solve the following overdetermined system of nonlinear equations:

$$\mathbf{g}(\mathbf{f}) = \left(a_0(\mathbf{f}) + \sum_{i=1}^N a_i(\mathbf{f}) \cos(2\pi f_i t_j) + \sum_{i=1}^N b_i(\mathbf{f}) \sin(2\pi f_i t_j) \right)_j \approx \mathbf{m} \quad (1)$$

For the amplitudes $a_0(\mathbf{f})$, $a_i(\mathbf{f})$, $b_i(\mathbf{f})$ we take the best fit at the current frequency vector (see below). Because $M > N$, the code tries to minimize

$$\|\mathbf{g}(\mathbf{f}) - \mathbf{m}\|_2 = \min!, \quad (2)$$

by varying \mathbf{f} , in the least squares sense. For this we use the damped Gauss-Newton code **nlscon** (see Deuffhard, coding Novak and Weimann). For testing purposes we used the lecture program **newton** (Hairer), which works quite well.

Determination of Amplitudes – Linear Minimization

The minimization routine needs a function which computes the amplitudes \mathbf{a} :

$$\mathbf{A} \cdot \mathbf{a} \approx \mathbf{m}$$

$$\mathbf{A} = \begin{pmatrix} 1 & \cos(2\pi f_1 t_1) & \cdots & \cos(2\pi f_N t_1) & \sin(2\pi f_1 t_1) & \cdots & \sin(2\pi f_N t_1) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 1 & \cos(2\pi f_1 t_M) & \cdots & \cos(2\pi f_N t_M) & \sin(2\pi f_1 t_M) & \cdots & \sin(2\pi f_N t_M) \end{pmatrix} \quad (3)$$

$$\mathbf{a} = (a_0, a_1, \dots, a_N, b_1, \dots, b_N)^t \quad \mathbf{m} = (m_1, \dots, m_M)^t$$

There exist two ways of solving the given system of equations:

- least squares solution (lsq)
- total least squares solution (tlsq)

If the given equation has full rank, then there exists a unique \mathbf{a} which minimizes $\|\mathbf{A}\mathbf{a} - \mathbf{b}\|_2$. This solution is called the least squares solution.

Least squares solution assumes an exact matrix \mathbf{A} and tries to get the best fit for the data \mathbf{m} , which are assumed to contain errors. However, in our situation time data are given with a precision of 10^{-5} d. We search for frequencies of the order of magnitude of 15 d^{-1} . This leads to relative errors in \mathbf{A} of size 10^{-3} . On the other side luminosity data have errors which are bounded by one to two thousands of a magnitude. Both sides of the equation show errors of the same order of magnitude. Therefore we use the method of total least squares (see Golub and Van Loan, Van Huffel and Vandewalle).

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$$\mathbf{a} = (a_0 \ a_1 \ \cdots \ a_N \ b_1 \ \cdots \ b_N)^t \quad \mathbf{m} = (m_1 \ \cdots \ m_M)^t$$

Least Squares Solution (lsq)

This algorithm assumes an exact matrix \mathbf{A} and tries to get the best fit for the data \mathbf{m} . We compute

$$\min \left\{ \|\mathbf{r}\| \mid \mathbf{r} = \mathbf{m} - \mathbf{m}', \exists \mathbf{a} : \mathbf{A}\mathbf{a} = \mathbf{m}' \right\}$$

The implementation is based on the QR-decomposition of \mathbf{A} and uses Lapack [6]

Total Least Squares Solution (tlsq)

Both, matrix \mathbf{A} and right side \mathbf{m} are assumed to be incorrect. In our case, one measurement requires about a minute. Within this time, our oscillation goes on some few degrees. Therefore \mathbf{A} should be treated as inexact. In this case we compute

$$\min \left\{ \|(\mathbf{r}|\mathbf{E})\|_F \mid \mathbf{r} = \mathbf{m} - \mathbf{m}', \mathbf{E} = \mathbf{A} - \mathbf{A}', \exists \mathbf{a} : \mathbf{A}'\mathbf{a} = \mathbf{m}' \right\}$$

For theoretical investigations see Van Loan [7], coding is due to Mössner.

Here $\|(\mathbf{r}|\mathbf{E})\|_F$ denotes the Frobenius Norm of the composed matrix $(\mathbf{r}|\mathbf{E})$

$$\|(\mathbf{r}|\mathbf{E})\|_F = \sqrt{\sum_{j=1}^M r_j^2 + \sum_{j=1}^M \sum_{i=1}^N e_{ji}^2}$$

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For the amplitudes $a_0(\mathbf{f})$, $a_i(\mathbf{f})$, $b_i(\mathbf{f})$ we take the best fit at the current frequency vector (see below). Because $M > N$, the code tries to minimize

$$\| \mathbf{g}(\mathbf{f}) - \mathbf{m} \| = \min !$$

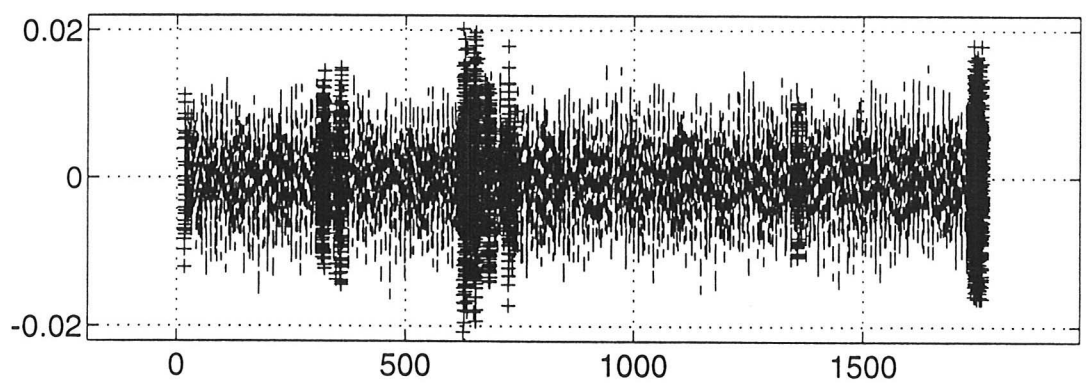
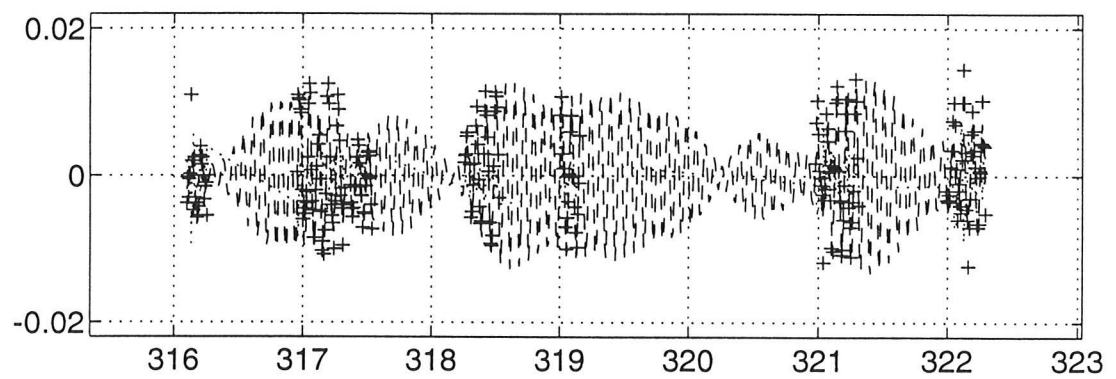
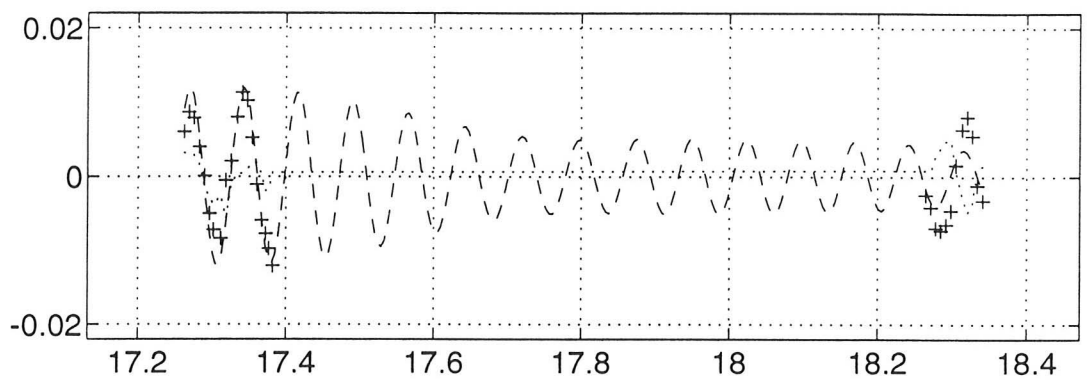
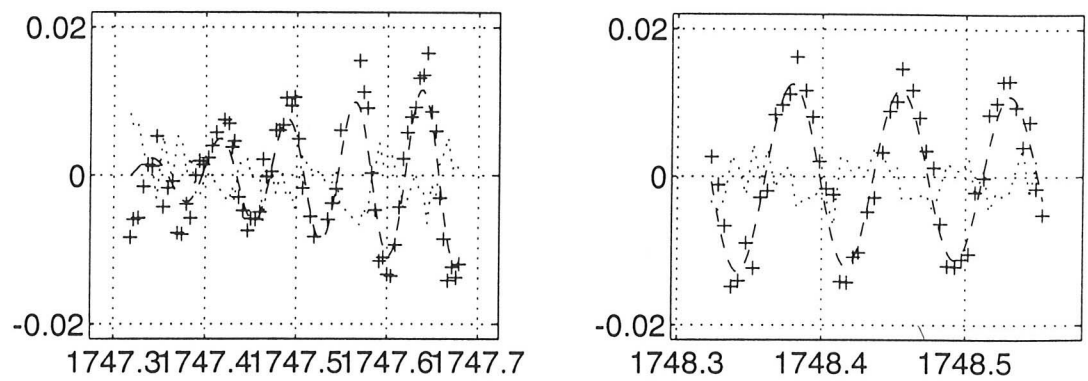
in the least squares sense.

Numerical Methods:

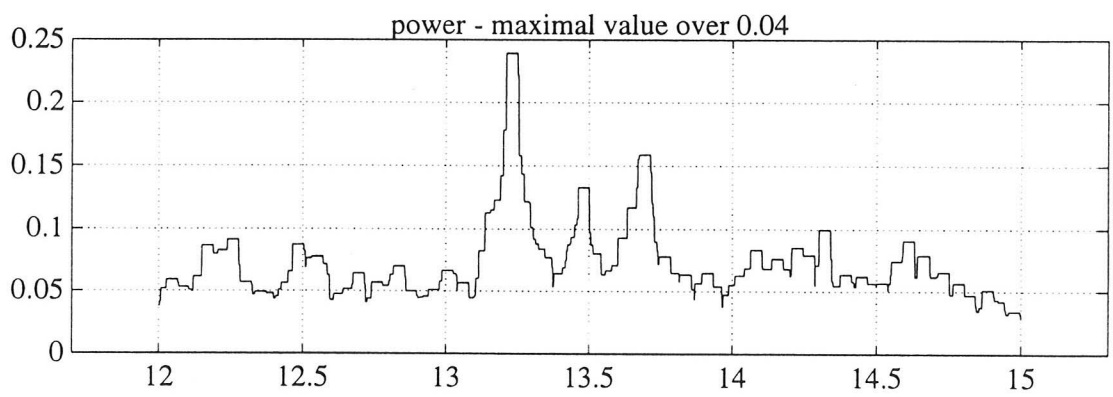
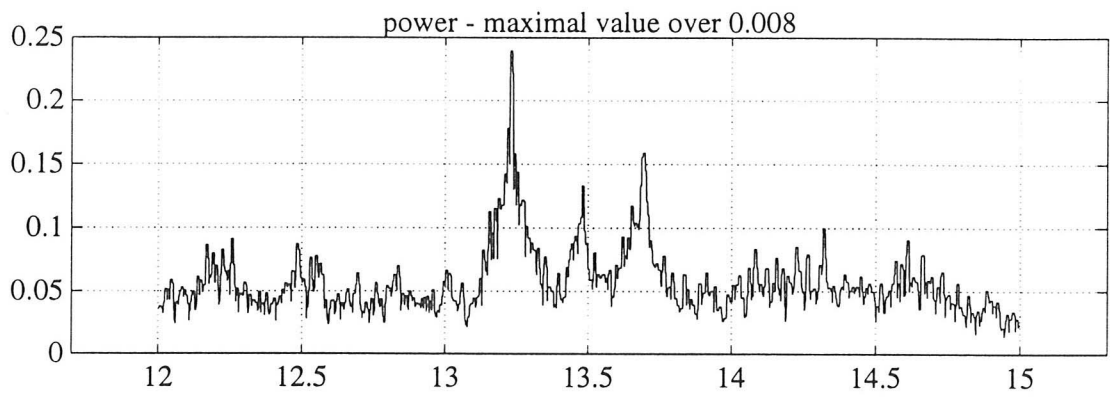
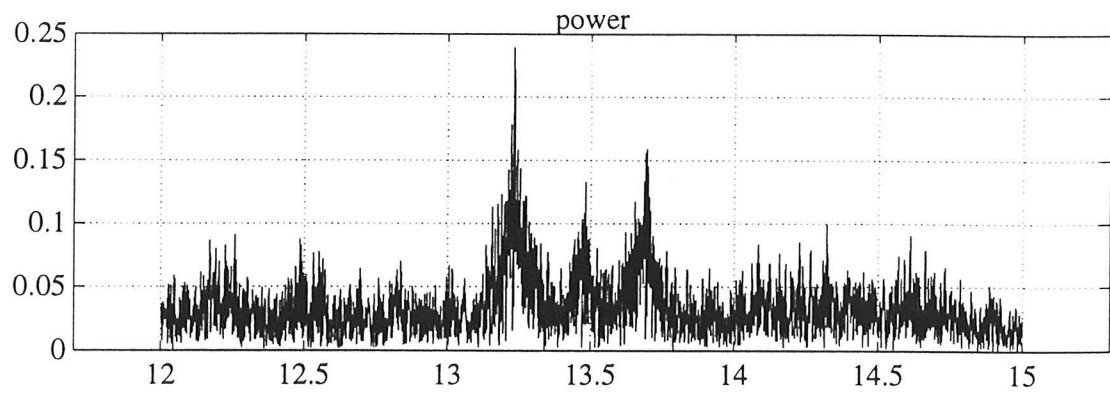
newton: method of Gauss-Newton with λ -strategy.
This method is due to Hairer [2] and Deuffhard [3].

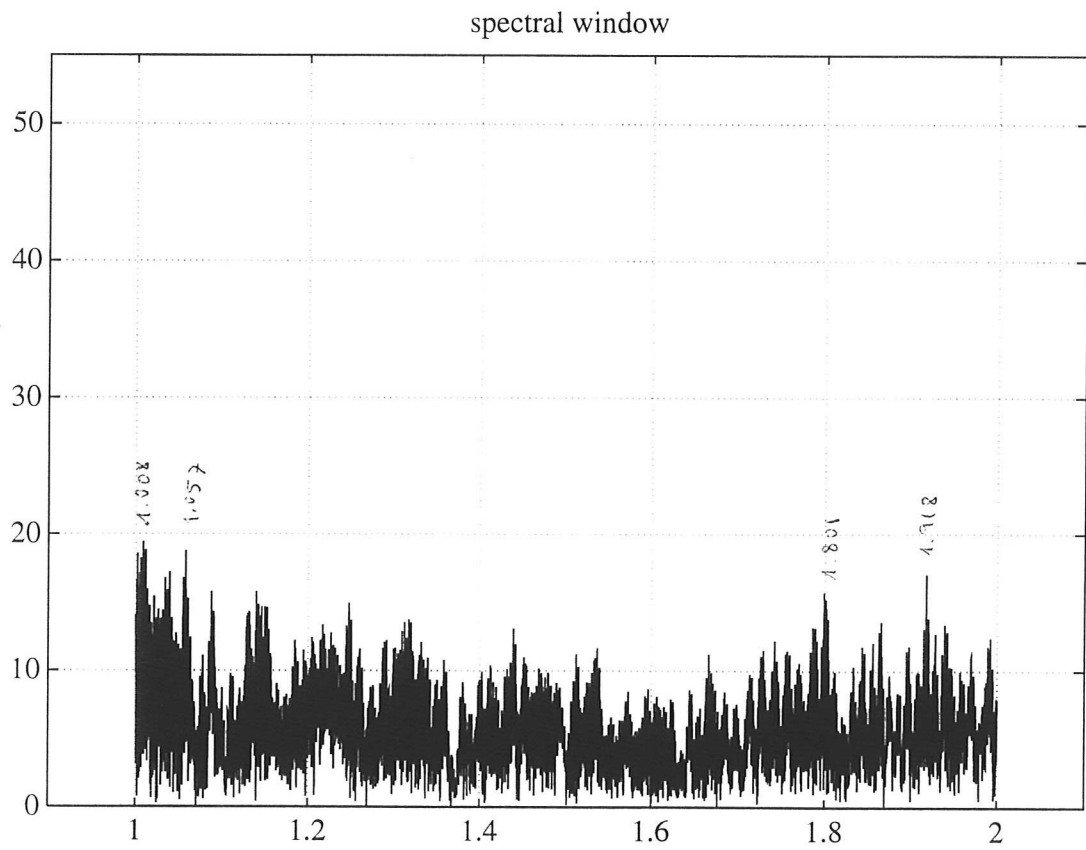
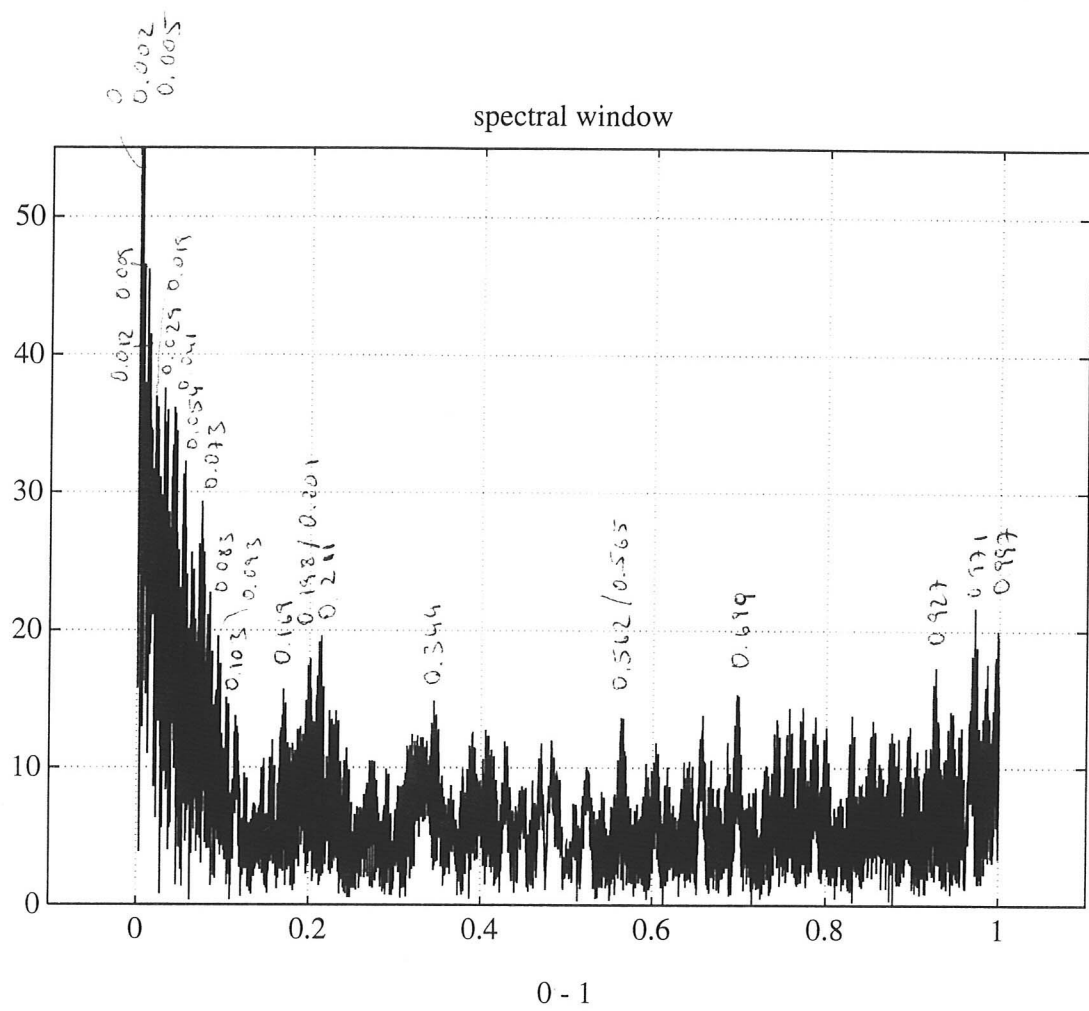
nlscon: damped Gauss-Newton method due to Deuffhard [4]
The code is due to Novak and Weimann [5]

The data of θ^2 -Tauri



The power spectrum of θ^2 -Tauri





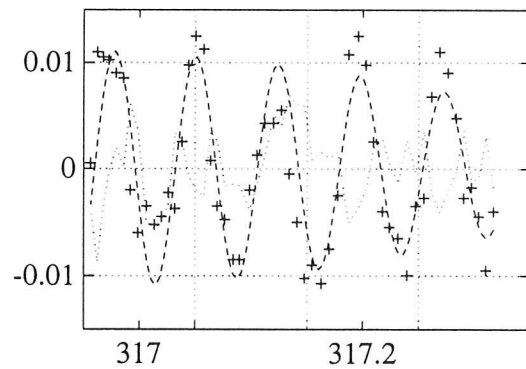
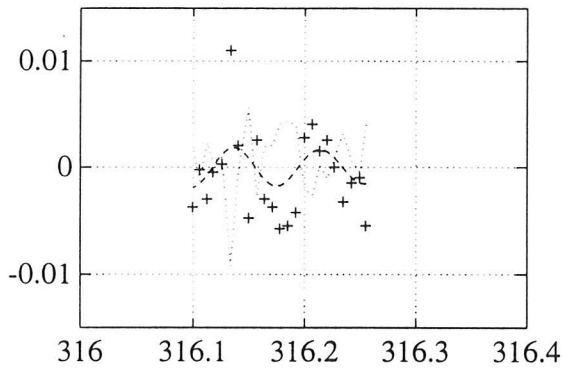
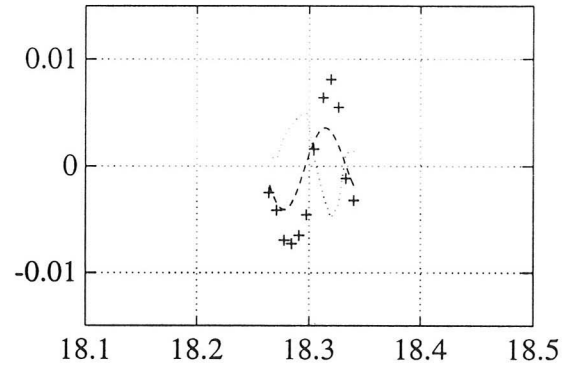
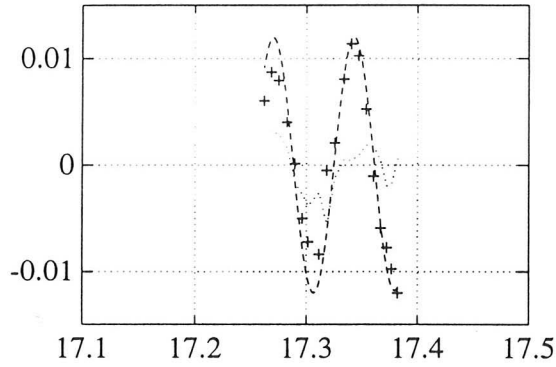
Example: Delta Scuti star θ^2 Tauri

- 2806 data sampled over 5 years.
- The data contain large gaps
 - about 20 hours between most days
 - about 300 days between every year.
- The first five frequencies are already published by Breger.

days	number of data
17-28	248
316-322	248
347-358	112
625-738	1145
1355-1359	80
1738-1759	1190

results of Breger	
frequency	amplitude
13.229653	0.0066
13.480733	0.0026
13.693597	0.0045
14.317637	0.0027
14.614537	0.0012

Following we show the first four days of data:



+ data points
dashed computed signal
dotted error in measurement

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Results:

The given confidence intervals have an error probability of $\beta = 0.001$

	frequency [d ⁻¹]	amplitude [mag]	phase [deg]
	0.000000	-0.00003 (± 0.00016)	
7	12.172308 (± 0.000088)	0.00075 (± 0.00025)	35 (± 39)
1	13.229653 (± 0.000010)	0.00654 (± 0.00026)	149 (± 5)
4	13.480717 (± 0.000027)	0.00246 (± 0.00025)	-106 (± 12)
6	13.647071 (± 0.000084)	0.00085 (± 0.00025)	-146 (± 37)
2	13.693601 (± 0.000017)	0.00428 (± 0.00024)	76 (± 7)
9	13.827642 (± 0.000104)	0.00063 (± 0.00024)	-153 (± 47)
3	14.317639 (± 0.000033)	0.00258 (± 0.00032)	47 (± 12)
8	14.323414 (± 0.000140)	0.00063 (± 0.00033)	175 (± 54)
5	14.613782 (± 0.000060)	0.00111 (± 0.00025)	2 (± 27)
10	26.189602 (± 0.000126)	0.00050 (± 0.00023)	-19 (± 56)

A Test Example

For testing purposes we created data sets for the following signal

$$(1) \quad s_j = 1 + 4 \cos(2\pi 6.5 t_j) + 6 \cos(2\pi 8.6 t_j + 1) + 5 \cos(2\pi 9.3 t_j - 2) + 3 \cos(2\pi 18.0 t_j - 3) + r_j$$

We selected the time distribution:

$$(2) \quad t_j = \frac{0.2 i}{n_{step} - 1} + d + 300 y \quad \text{with} \quad j = i + 1 + n_{step} \cdot (d + n_{day} \cdot y)$$

$$i = 0, \dots, n_{step} - 1, \quad d = 0, \dots, n_{day} - 1, \quad \text{and} \quad y = 0, \dots, n_{year} - 1.$$

The given test example uses $n_{step} = 20$, $n_{day} = 30$, and $n_{year} = 2$. Errors were simulated by a uniform random generator. Given two uniform random numbers U_1 and U_2 , one gets by the transformation: $G = \sigma \sqrt{-2 \ln U_1} \cos(2\pi U_2) + \mu$ a Gaussian random number with mean μ and variance σ (Devroye). The test example contains Gaussian errors with mean $\mu = 0$ and variance $\sigma = 0.2$. Errors in time data were simulated by adding to t_j , a uniformly distributed random number of range $\pm 10^{-4}$

This example shows strong aliasing structures. The power has maxima at 5.5, 7.5, 8.3, 9.6, 10.3, and 10.6. As starting vector for the frequencies we took the foolish input $\mathbf{f} = (3.0)$. Our algorithm stops after 5 iterations, because the residuals approach the statistical limit. The result for the error probability $\beta = 0.001$ is

	frequency [d ⁻¹]	amplitude [mag]	phase [rad]
	0.0000000	1.005 (±0.018)	
3	6.4999999 (±0.0000066)	4.006 (±0.026)	-0.001 (±0.009)
1	8.5999981 (±0.0000044)	6.016 (±0.025)	1.004 (±0.006)
2	9.3000030 (±0.0000054)	4.995 (±0.025)	-2.002 (±0.007)
4	17.9999847 (±0.0000090)	2.995 (±0.024)	2.986 (±0.013)

Statistical Package

After successful exit or at *itmax* iterations, iteration stops and the statistical package is called:

- Tests on the randomness of the residual vector are performed.
- Compute confidence intervals for the computed parameters.
- Test whether all frequencies are necessary or not (planned).

Our parameter vector is $\mathbf{p} = (A_0, A_1, \dots, A_N, f_1, \dots, f_N, \phi_1, \dots, \phi_N)$. With the Student's t distribution with ν degrees of freedom

$$A(t|\nu) = \frac{\Gamma\left(\frac{\nu+1}{2}\right)}{\sqrt{\nu\pi} \Gamma\left(\frac{\nu}{2}\right)} \int_{-\infty}^t \left(1 + \frac{\tau^2}{\nu}\right)^{-(\nu+1)/2} d\tau$$

and its β -fractil $t_{\beta,\nu}$, defined by:

$$A(t_{\beta,\nu}|\nu) = \beta,$$

we have the following probability [8]:

$$P\left(|p_{i,w} - p_i| < \delta_i\right) = 1 - \beta$$

$$\delta_i = S \sqrt{c_{ii}} t_{1-\beta/2, M-3N-1}$$

$$S = \frac{\|\mathbf{r}\|}{\sqrt{M-3N-1}} \quad c_{ii} = \left((\mathbf{J}^t \mathbf{J})^{-1}\right)_{ii}$$

- $p_{i,w}$ true value of computed parameter p_i
 β significance level of confidence interval.
 \mathbf{J} Jacobian of minimization function $\mathbf{g}(\mathbf{f})$.

This gives the confidence interval

$$[p_i - \delta_i, p_i + \delta_i]$$

with error probability β .

Statistical Package

The statistical package has following aims:

- Decide whether weak signals are real or not
 - Compare point to point sigma to model sigma. Fisher test.
 - Test randomness of residual vector.
 - Compute confidence limits.
- Decide which one of closely aliased signals is the real one.
 - Compare point to point sigma to model sigma.
 - Test randomness of residual vector.

For this we perform following tests:

- Do basic statistics:
 - mean, standard deviation, ...
- Test randomness of the residual vector:
 - Do runs test.
 - Compute confidence intervals for the mean and the variance of the residual distribution.
 - Perform Kolmogorov-Smirnov type tests.
 - * Two Kolmogorov-Smirnov tests.
 - * Cramer-von Misés Test.
 - * Anderson-Darling test.
- Compute accuracy of the result.
 - Compute confidence intervals.
 - possible further tests are:
 - * Tests on the reliability of the results.
 - * Fisher test for the safety of weak signals.

Runs Test

The runs test tests the randomness of the sign changes in the residual vector.

- p number of positive residuals.
- n number of negative residuals.
- k number of runs (= number of sign changes + 1)

If X is the random variable which gives the number of runs, then the probability $P(X = k)$ is given by (Brownlee):

$$(1) \quad P(X = k) = \begin{cases} \frac{2 \binom{n-1}{l-1} \binom{p-1}{l-1}}{\binom{n+p}{n}}, & \text{if } k = 2l, \\ \frac{\binom{n-1}{l} \binom{p-1}{l-1} + \binom{n-1}{l-1} \binom{p-1}{l}}{\binom{n+p}{n}}, & \text{if } k = 2l + 1. \end{cases}$$

$$(2) \quad \begin{aligned} E(X) &= 1 + \frac{s}{t}, & V(X) &= \frac{s(s-t)}{t^2(t-1)} \\ s &= 2pn & t &= p+n \end{aligned}$$

Tests: Let x be the realization of X

- Check whether x is in the interval $[E(X) - V(X), E(X) + V(X)]$.
- Compute $P(|X - E(X)| > |x - E(X)|)$

Efficient computing:

$$(3) \quad \binom{a}{b} = \exp(\ln \Gamma(a+1) - \ln \Gamma(b+1) - \ln \Gamma(a-b+1))$$

$$(4) \quad \ln \Gamma(x) = \left(x - \frac{1}{2}\right) \ln \left(x + \gamma - \frac{1}{2}\right) - \left(x + \gamma - \frac{1}{2}\right) \\ + \ln(2\pi) + \ln \left(c_0 + \sum_{i=1}^N \frac{c_i}{x+i-1}\right) + \epsilon$$

This representation is due to Lanczos, coefficients for $\epsilon = 10^{-14}$ are due to Mössner.

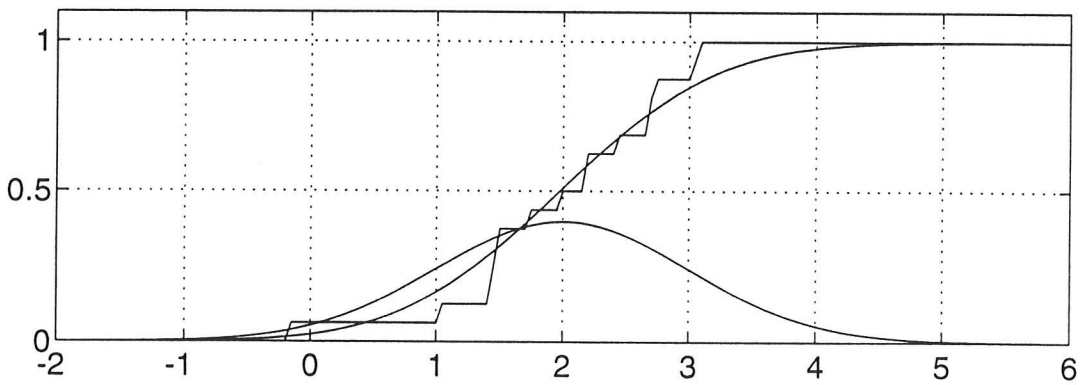
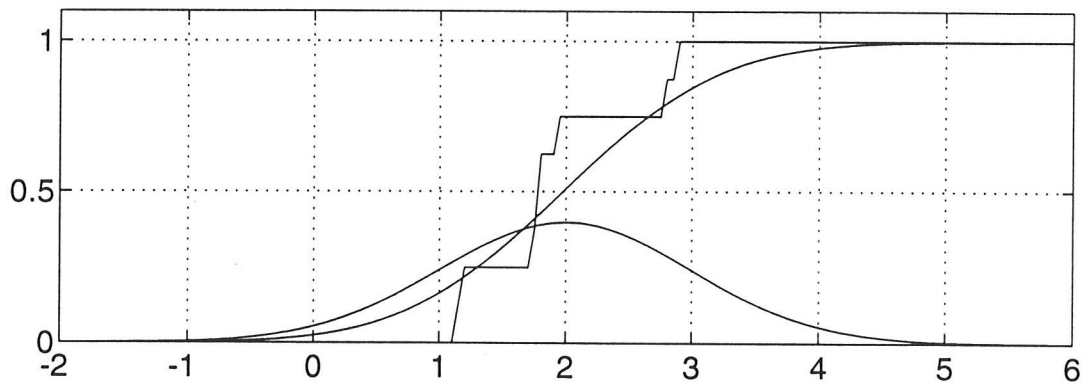
The Anderson-Darling Test

$$\begin{aligned}
 (1) \quad A_n &= n \int_{-\infty}^{\infty} \frac{(F_n(x) - F(x))^2}{F(x)(1 - F(x))} dF(x) \\
 &= -n - \frac{1}{n} \sum_{i=1}^n (2i - 1) \ln Y_i + (2(n - i) + 1) \ln(1 - Y_i)
 \end{aligned}$$

with

$$(2) \quad F_n(x) = \frac{1}{n} \sum_{i=1}^n \chi(x - X_i), \quad \text{with} \quad \chi(t) = \begin{cases} 1, & \text{for } t \geq 0, \\ 0, & \text{else.} \end{cases}$$

X_i sample of observations
 $F(x)$ the hypothesized distribution
 Y_i $Y_i := F(X_i)$



Limiting distribution

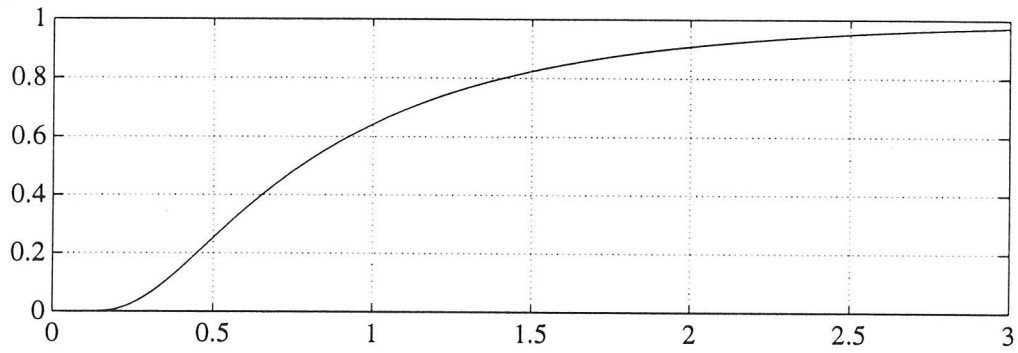
$A(x) = \lim_{n \rightarrow \infty} P(A_n < x)$ (Anderson and Darling):

$$(3) \quad \begin{aligned} A(x) &= \frac{2}{\sqrt{x}} \exp\left(\frac{x}{8} - \frac{\pi^2}{8x}\right) \sum_{i=0}^{\infty} (-1)^i a_i I(x, b_i) \\ a_i &= \left(1 - \frac{1}{2i}\right) \exp\left(-\frac{(4i-1)\pi^2}{x}\right) a_{i-1}, \quad a_0 = 1 \\ b_i &= \frac{1}{8}(4i+1)^2 \pi^2 \end{aligned}$$

with

$$(4) \quad \begin{aligned} I(x, b) &= \int_0^{\infty} f(y; x, b) dy \quad x \geq 0, \quad b > 0. \\ f(y; x, b) &= \frac{2}{\sqrt{\pi}} \exp\left(-y^2 \left(1 + \frac{x^2}{8b} \cdot \frac{1}{1 + xy^2/b}\right)\right) \end{aligned}$$

FIGURE 1. The Anderson-Darling Function $A(x)$



Approximations to the Anderson-Darling test statistic

$$(5) \quad A_{m,n}(x) = \frac{1}{1 + \exp\left(\sum_{i=-m}^n c_i x^{i/2}\right)}, \quad c_{-m} > 0, \quad c_n < 0.$$

The unknown coefficients c_i , $i = -m, \dots, n$ were computed by least squares fitting the limiting distribution (Mössner, Netzer, and Pfeiderer).

TABLE 1. Coefficients for approximations of the Anderson-Darling function $A(x)$

model	m	n	c_{-i}	c_i
1	2	2	$c_{-1} = 0.0$ $c_{-2} = 0.90005634667$	$c_0 = 0.0$ $c_1 = 0.0$ $c_2 = -1.4486936792$
2	2	2	$c_{-1} = 0.0$ $c_{-2} = 1.0720379724$	$c_0 = -0.47672874207$ $c_1 = 0.0$ $c_2 = -1.1785883752$
3	3	2	$c_{-1} = 2.018$ $c_{-2} = -0.03287$ $c_{-3} = 0.2029$	$c_0 = -1.784$ $c_1 = 0.0$ $c_2 = -0.9936$
4	3	2	$c_{-1} = 2.7173177700$ $c_{-2} = -0.46999842833$ $c_{-3} = 0.29285553148$	$c_0 = -2.1714528342$ $c_1 = 0.0$ $c_2 = -0.95569185238$
5	6	6	$c_{-1} = -30.985724303897379$ $c_{-2} = 22.198442088714700$ $c_{-3} = -10.427567803868353$ $c_{-4} = 3.330806575355391$ $c_{-5} = -0.5942755083462223$ $c_{-6} = 0.04473918400266183$	$c_0 = 33.660074457587372$ $c_1 = -26.467806706020571$ $c_2 = 11.725227409412259$ $c_3 = -3.461437492448171$ $c_4 = 0.3647412183007341$ $c_5 = 0.03378178495561017$ $c_6 = -0.008249382832328045$
6	9	8	$c_{-1} = 504.96559880722138680323$ $c_{-2} = -361.15067999211410859866$ $c_{-3} = 205.95482419709786532568$ $c_{-4} = -91.74425625354047667882$ $c_{-5} = 31.09525679720687922258$ $c_{-6} = -7.64077211104759798805$ $c_{-7} = 1.26815570921344052725$ $c_{-8} = -0.126112815408544631380$ $c_{-9} = 0.00564542439518663198826$	$c_0 = -559.71696098878785161040$ $c_1 = 491.15232058574365070413$ $c_2 = -339.70147526769415082831$ $c_3 = 178.72304282215231741440$ $c_4 = -69.81115632571493771504$ $c_5 = 19.33154893753456654489$ $c_6 = -3.56347332952716023287$ $c_7 = 0.390428145406831375016$ $c_8 = -0.0191817094491927644459$

Models 1 and 2 give very fast approximations which use only 3 multiplications, one root, and one exponentiation. The achieved accuracy of 0.01 is high enough for practical purposes. Models 5 and 6 are approximations with enhanced precision, where the computation of equations (3,4) is quite expensive. These representations have an accuracy of approximately 7 digits. For a machine with a precision of $\epsilon \approx 10^{-15}$ model 5 gives the best approximation. The high precision approximation of model 6 needs – due to roundoff errors – a machine with a precision of better than $\epsilon < 10^{-20}$.

Confidence Intervals

For the computation of the confidence intervals we assume the model

$$(1) \quad s(t_j) = a_0 + \sum_{i=1}^N a_i \cos(2\pi f_i t_j + \phi_i), \quad j = 1, \dots, M$$

We use the parameter vector:

$$(2) \quad \mathbf{p} = (f_1, \dots, f_N, a_0, a_1, \dots, a_N, \phi_1, \dots, \phi_N).$$

With the Student's t distribution with ν degrees of freedom

$$(3) \quad A(t|\nu) = \frac{\Gamma\left(\frac{\nu+1}{2}\right)}{\sqrt{\nu\pi} \Gamma\left(\frac{\nu}{2}\right)} \int_{-\infty}^t \left(1 + \frac{\tau^2}{\nu}\right)^{-(\nu+1)/2} d\tau$$

and its β -fractil $t_{\beta,\nu}$, defined by:

$$(4) \quad A(t_{\beta,\nu}|\nu) = \beta,$$

we have the following probability:

$$(5) \quad \begin{aligned} P(|p_{i,w} - p_i| < \delta_i) &= 1 - \beta, \\ \delta_i &= S \sqrt{c_{ii}} t_{1-\beta/2, M-3N-1}, \\ S &= \frac{\|\mathbf{r}\|_2}{\sqrt{M-3N-1}} \quad c_{ii} = \left((\mathbf{J}^t \mathbf{J})^{-1}\right)_{ii} \end{aligned}$$

$p_{i,w}$ true value of computed parameter p_i

β significance level of confidence interval.

\mathbf{r} residuals of model. $\mathbf{r} = (r_j)$, $r_j = s(t_j) - data_j$.

\mathbf{J} Jacobian of model function $\mathbf{J} = (jac_{j,i})$, $jac_{i,j} = \partial s(t_j) / \partial p_i$.

This gives the confidence interval

$$(6) \quad [p_i - \delta_i, p_i + \delta_i]$$

with error probability β .

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