Quantum Wave ToolBox documentation

BETA version

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Contents

Abstract

Press a button with bold title AMPLITUDE
. . . drink a coffee . . .
and get the result

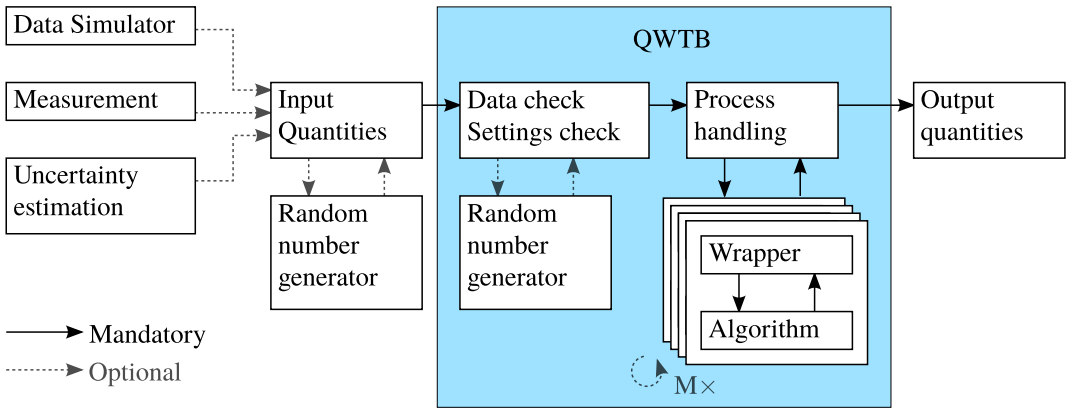
Quantum Wave Tool Box (QWTB) is a toolbox for evaluation of measured data. QWTB consist of data processing algorithms from very different sources and unificating application interface. The toolbox gives the possibility to use different data processing algorithms with one set of data and removes the need to reformat data for every particular algorithm. Toolbox is extensible. The toolbox can variate input data and calculate uncertainties by means of Monte Carlo Method (MCM) [1].

Chapter 1

Basic description of the toolbox

1.1 Toolbox overall scheme

The basic scheme of the toolbox is following:



User have to prepare the data, either based on a real measurement or simulated, into a specified format. If needed, user can generate randomized data for selected quantities (e.g. with special probability density functions) and prepare for Monte Carlo uncertainty calculation. Next user calls toolbox to apply a selected algorithm on the data and review results. Toolbox will:

1. Check user data.
2. Check or generate calculation settings.
3. If required, quantities are randomized according uncertainties to prepare for MCM uncertainty calculation.

4. Data are handled to a wrapper. If needed, wrapper is run multiple times according MCM.

5. Output data are the result of the toolbox.

Another algorithm can be used immediately on the same data. User interface of the toolbox is represented by the function qwtb defined in the file `qwtb.m`.

1.2 Toolbox use

The toolbox is used in several modes according to a number and character of input arguments.

1.2.1 Get list of implemented algorithms

```
alginfo = qwtb()
```

With no input arguments, toolbox returns informations on all available algorithms. Result array alginfo contains structures for every algorithm found in the same directory as `qwtb.m`. Format of structures is defined in 2.2.

1.2.2 Application of an algorithm on the data

```
dataout = qwtb('algid', datain)
```

The algorithm is selected by first input argument algid. It is a string with designator of the algorithm, according structrue 2.2.

The second input argument is the user data. Data have to be formatted in a structure with fields named as quantities required by the algorithm (see 2.3).

The output variable is the structure with fields named as quantities.

In this case, standard calculation settings are used. If the user specifies calculation settings in structure according 2.4, it can be used as third input argument calcset:

```
dataout = qwtb('algid', datain, calcset)
```

For some calculation settings some fields of datain or calcset are generated automatically. To review automatically generated fields, user can get these structure in second and third output argument:

```
[dataout, datain, calcset] = qwtb('algid', datain)
[dataout, datain, calcset] = qwtb('algid', datain,
   calcset)
```

1.2.3 Running an example of algorithm use

Algorithm can have implemented an example of the use. This can be run by following syntax:

```
qwtb('algid', 'example')
```

The algorithm is selected by first input argument algid. It is a string with designator of the algorithm, according structrue 2.2. The second argument is a string. Toolbox will run a script alg_example.m located in a algorithm directory.

After finish user can review input and output data or resulted figures if any.

1.2.4 Running a test of algorithm

Algorithm can have implemented a self test. This can be run by following syntax:

```
qwtb('algid', 'test')
```

The algorithm is selected by first input argument algid. It is a string with designator of the algorithm, according structrue 2.2. The second argument is a string. Toolbox will run a script alg_test.m located in a algorithm directory.

Test should prepare data, run algorithm and check results. If implementation of algorithm behaves incorrectly, an error will occur.

1.2.5 Adding or removing algorithm path

Algorithms are stored in different directories, which are not in MATLAB/GNU Octave load path. To add directory with selected path to MATLAB/GNU Octave load path, following syntax is used:

```
qwtb('algid', 'addpath')
```

To remove path, use:

```
qwtb('algid', 'rempath')
```

Adding or removing path should be required only in special cases, such as debugging etc.

1.2.6 Displaying license of an algorithm

To display a license of an algorithm, following syntax is used:

```
license = qwtb('algid', 'license')
```

For details on licensing, see chapter 3.

Chapter 2

Detailed description of the toolbox

2.1 Algorithm directory structure implementation

Every algorithm is placed in a directory of following name:

`alg_X`

These directories have to be located in the directory containing the toolbox main script `qwtb.m`.

Every algorithm directory contains following files:

`X1`, `X2`, ... — Mandatory. One or more files with the algorithm itself.

`alg_info.m` — Mandatory. Description of the algorithm. See 2.1.1.

`alg_wrapper.m` — Mandatory. Wrapper of the algorithm. See 2.1.2.

`alg_test.m` — Recomended. Testing function. See 2.1.3.

`alg_example.m` — Recomended. Example script. See 2.1.4.

2.1.1 File `alg_info.m`

File contains a function with definition:

```
function alginfo = alg_info()
```

The output `alginfo` is a structure with informations about the algorithm. Structure is defined in 2.2.

File is mandatory. If file is missing in algorithm directory, QWTB will not recognize this algorithm as part of the toolbox.

2.1.2 File `alg_wrapper.m`

File contains a function with definition:

```
function dataout = alg_wrapper(datain, calcset)
```

The input datain is a structure with input data (see), calcset is a structure with definition of calculation settings (see 2.4).) and dataout is a structure containing output data (see).

The wrapper does following:

1. Formats input data structure datain into variables wuitable for algorithm.
2. Runs the algorithm.
3. Format results of the algorithm into data structure dataout.

File is mandatory. If file is missing in algorithm directory, QWTB will not recognize this algorithm as part of the toolbox.

2.1.3 File `alg_test.m`

File contains a function with following definition:

```
function alg_test(calcset)
```

Test should generate sample data, run algorithm and check results by a function assert. QWTB will provide a standard calculation settings structure calcset (see 2.4).

This file is not mandatory, however is recommended.

2.1.4 File `alg_example.m`

Example contains a script showing a basic use of the algorithm. The format of the file should conform to the publishing markup defined in Matlab documentation. See matlab help on keyword *Publishing markup*). The QWTB runs this script in base context, thus all variables defined in the example script will be accessible to the user.

To create a documentation of the QWTB, function publish is applied to the example script and resulting file is attached to the documentation file.

2.2 Algorithm informations structure

Structure defines properties and possibilities of the algorithm. All fields are mandatory but . fullpath .

.id — Designator of the algorithm.

.name — Name of the algorithm.

.desc — Basic description.

.citation — Reference.

.remarks — Any remark.

.license — License of the algorithm.

.requires — Required quantities.

.reqdesc — Short description of required quantities.

.returns — Output quantities.

.retdesc — Short description of output quantities.

.providesGUF — Algorithm/wrapper calculates GUF uncertainty.

.providesMCM — Algorithm/wrapper calculates MCM uncertainty.

.fullpath — Full path to the algorithm. Automatically generated by the toolbox.

2.2.1 .id

String. Designator of the algorithm. It is unique identifier, no two algorithms can have same id.

2.2.2 .longname

String. Full name of the algorithm.

2.2.3 .desc

String. Basic description of the algorithm.

2.2.4 .citation

String. A reference to the paper, book or other literature with full description of the algorithm.

2.2.5 .remarks

String. Remarks or others related to the algorithm.

2.2.6 .license

String. License of the algorithm. This is not license of the toolbox but of the algorithm!

2.2.7 .requires

Cell array of strings. Names of quantities required by the algorithm.

2.2.8 .reqdesc

Cell array of strings. Short description of quantities required by the algorithm.

2.2.9 .returns

Cell array of strings. Names of quantities returned by the algorithm.

2.2.10 .retdesc

Cell array of strings. Short description of quantities returned by the algorithm.

2.2.11 .providesGUF

Boolean. If nonzero, the wrapper or the algorithm calculates uncertainty by means of GUM Uncertainty Framework.

2.2.12 .providesMCM

Boolean. If nonzero, the wrapper or the algorithm calculates uncertainty by means of Monte Carlo Method.

2.2.13 .fullpath

String. Full path to the algorithm. This field is automatically generated by QWTB.

2.3 Quantity structure

Every quantity is a structure with following fields:

.v — Value.

.u — Uncertainty.

.d — Degree of freedom.

.c — Correlation.

.r — Randomized uncertainty.

2.3.1 .v

Value of the quantity. Can be a scalar, *row* vector or matrix. More dimensions are not supported.

2.3.2 .u

Standard uncertainty of the quantity. Dimensions are the same as of the value field.

2.3.3 .d

Degrees of freedom the uncertainty according GUM Uncertainty Framework. Dimensions are the same as of the value field.

This field is automatically generated by the toolbox if missing, required and calcset.dof.gen is set to nonzero. The value will be set to 50.

2.3.4 .c

Correlation matrix for quantity. 2DO XXX.

This field can be automatically generated by the toolbox if missing, required and calcset.cor.gen is set to nonzero. The value will be set to 0.

2.3.5 .r

Randomized uncertainties according Monte Carlo method. In the case of scalar quantity it is *column* vector of length equal to calcset.mcm.repeats. For a vector quantity it is a matrix with number of columns equal to length of value of the quantity and number of rows equal to calcset.mcm.repeats. For a matrix quantity it is a matrix with three dimensions, first two equal to the dimensions of value quantity, third dimension equal to calcset.mcm.repeats.

This field is required if Monte Carlo uncertainty calculation is required. In this case it can be automatically generated by the toolbox if missing and calcset.mcm.randomize is set to boolean. The pdf will be normal, sigma will be equal to the standard uncertainty of the quantity.

2.3.6 Quantity structure examples

Example of scalar quantity of mean value 1, standard uncertainty 0.1, degrees of freedom 9, correlation has no sense for scalar quantity, and radnomized matrix has number of elements equal to calcset.mcm.randomize.

$$\begin{aligned} \text{.v:} &\quad (1) \\ \text{.u:} &\quad (0.1) \\ \text{.d:} &\quad (9) \\ \text{.c:} &\quad (0) \\ \text{.r:} &\quad \begin{pmatrix} 1.02076 \\ 1.22555 \\ \vdots \\ 0.89727 \end{pmatrix} \end{aligned}$$

Example of vector quantity with i elements, M is equal to calcset.mcm.randomize (only symbolic representation):

$$\begin{aligned} \text{.v:} &\quad (v_1, v_2, \ldots, v_i) \\ \text{.u:} &\quad (u_1, u_2, \ldots, u_i) \\ \text{.d:} &\quad (d_1, d_2, \ldots, d_i) \\ \text{.c:} &\quad \begin{pmatrix} c_{11} & \ldots & c_{1i} \\ \vdots & \ddots & \vdots \\ c_{i1} & \ldots & c_{ii} \end{pmatrix} \\ \text{.r:} &\quad \begin{pmatrix} r_{11} & \ldots & r_{1i} \\ \vdots & \ddots & \vdots \\ r_{M1} & \ldots & r_{Mi} \end{pmatrix} \end{aligned}$$

Example of matrix quantity with i times j elements, M is equal to calcset.

mcm.randomize (only symbolic representation):

$$
\begin{array}{ll}
\text{.v:} & \begin{pmatrix} v_{11} & \dots & v_{1j} \\ \vdots & \ddots & \vdots \\ v_{i1} & \dots & v_{ij} \end{pmatrix} \\
\text{.u:} & \begin{pmatrix} v_{11} & \dots & u_{1j} \\ \vdots & \ddots & \vdots \\ u_{i1} & \dots & u_{ij} \end{pmatrix} \\
\text{.d:} & \begin{pmatrix} d_{11} & \dots & d_{1j} \\ \vdots & \ddots & \vdots \\ d_{i1} & \dots & d_{ij} \end{pmatrix} \\
\text{.c:} & (XXX???) \\
\text{.r:} & \begin{pmatrix} r_{111} & \dots & r_{1j1} \\ \vdots & \ddots & \vdots \\ r_{i11} & \dots & r_{ij1} \end{pmatrix} \\
 & \vdots \\
 & \begin{pmatrix} r_{11M} & \dots & r_{1jM} \\ \vdots & \ddots & \vdots \\ r_{i1M} & \dots & r_{ijM} \end{pmatrix}
\end{array}
$$

2.4 Calculation settings structure

Structure defines calculation methods.

.strict — (0) If zero, other fields generated automatically.

.verbose — (1) Display various informations.

.unc — ('none') How uncertainty is calculated ('none', 'guf', 'mcm').

.cor.req — (0) Correlation matrix is required for all input quantities.

.cor.gen — (1) Zero correlation matrix is generated automatically if missing.

.dof.req — (1) Degrees of freedom are required for all input quantities.

.dof.gen — (1) Degree of freedom are generated automatically if missing with value 50.

.mcm.repeats — (100) Number of Monte Carlo iterations.

.mcm.verbose — (1) Display various informations concerning Monte Carlo method.

.mcm.method — ('singlecore') Parallelization method ('multicore', 'multistation').

.mcm.procno — (1) Number of processors to use.

.mcm.tmpdir — ('.') Directory for temporary data.

.mcm.randomize — (1) Randomized uncertainties are generated automatically if missing.

2.4.1 .strict

Boolean, default value 0. If set to zero, all other fields of the structure are generated automatically and set to a default value.

2.4.2 .verbose

Boolean, default value 1. If set to non-zero value, various messages are displayed during calculation, such as used uncertainty calculation method, automatic generation of matrices etc.

2.4.3 .unc

String, default value ''. Determines uncertainty calculation method. Only three values are possible:

'' — Uncertainty is not calculated.

'guf' — Uncertainty is calculated by GUM Uncertainty Framework [2].

'mcm' — Uncertainty is calculated by Monte Carlo Method [1].

See chapter XXX for uncertainty calculation details.

2.4.4 .cor

Structure sets handling of correlation matrices of quantities. Structure has two fields:

.req — Boolean, default value 0. If non-zero, correlation matrices are required for all quantities.

.gen — Boolean, default value 1. If non-zero, correlation matrices will be generated automatically if missing in quantity.

Automatically generated correlation matrices has all elements of zero value.

2.4.5 .dof

Structure sets handling of degrees of freedom of quantities. Structure has two fields:

.req — Boolean, default value 0. If non-zero, degrees of freedom are required for all quantities.

.gen — Boolean, default value 1. If non-zero, degree of freedom will be generated automatically if missing in quantity.

Automatically generated degree of freedom has value 50.

2.4.6 .mcm

Structure sets handling of Monte Carlo calculation of uncertainties. Structure has following fields:

.repeats — Positive non-zero integer, default value 100. Number of iterations of Monte Carlo method.

.verbose — Boolean, default value 1. If set to non-zero value, various messages are displayed during calculation of Monte Carlo method such as used parallelization method, number of calculated iterations etc.

.method — String, default value 'singlecore'. Parallelization method used for Monte Carlo method calculation. Only three values are possible:

'singlecore' — No parallelization, all is calculated on one CPU core.

'multicore' — Calculation is divided into cores of one computer.

'multistation' — Calculation is distributed on several computers.

Not all methods are possible to use on all computers. 'singlecore' is always possible to use. 'multicore' use parfor in Matlab or parcellfun in GNU Octave. 'multistation' use

.procno — Zero or positive integer, default value 0. Number of CPU cores exploitable by the parallelization method 'multicore'. If set to zero, all available CPU cores will be used. If desktop computer is used, it is good practice to set to number of CPU cores minus one, so the computer can be used by other task also. Works only in GNU Octave.

.tmpdir — String, default value '.' (current directory). Temporary directory for storing temporary data needed for some parallelization methods.

.randomize — Boolean, default value 1. If non-zero, randomized uncertainties will be generated automatically if missing, but only if uncertainty calculation method is set to 'mcm' (Monte Carlo) to prevent large memory usage.

2.5 How uncertainty calculation works

2.6 How to add a new algorithm

To add a new algorithm, several steps have to be done.

1. Select an algorithm ID. Usually it is an acronym or abbreviation of the new algorithm name.
2. Create a directory named `alg_SOMEID`, where `SOMEID` is a selected ID. For a directory structure, see 2.1.
3. Put all files required by the algorithm (i.e. scripts, libraries) into the directory `alg_SOMEID/`.
4. Create a file `alg_SOMEID/alg_info.m`. An example of such file follows.

```
        function info = alg_info() %<<<1
        % Part of QWTB. Info script for algorithm
SOMEALG.
        %
        % See also qwtb

        info.id = 'SOMEID';
        info.name = 'SOMEALG';
        info.desc = 'SOMEID is an super mega hyper
algorithm for calculation of the ultimate answer
 to everything.';
        info.citation = 'Some nifty paper in some
super journal.';
        info.remarks = 'Very simple implementation'
;
        info.license = 'MIT License';
        info.requires = {'a', 'b'};
        info.reqdesc = {'some input', 'some more
important input'};
        info.returns = {'x', 'y', 'z'};
        info.retdesc = {'some output', 'some more
important output', 'other output};
        info.providesGUF = 1;
        info.providesMCM = 0;
```

5. Create a wrapper for the algorithm in a file `alg_SOMEID/alg_wrapper.m`, see 2.1.2. An example of simple wrapper file follows.

```
      function dataout = alg_wrapper(datain,
calcset)
      % Part of QWTB. Wrapper script for
algorithm SOMEALG.
      %
      % See also qwtb

      % Format input data
------------------------------- %<<<1
      % SOMEALG definition is:
      % function [x, y, z] = SOMEALG(a, b);
      a = datain.a.v;
      b = datain.b.v;

      % Call algorithm
-------------------------------- %<<<1
      [x, y, z] = SOMEALG(a, b);

      % Format output data:
------------------------------- %<<<1
      dataout.x.v = x;
      dataout.y.v = y;
      dataout.z.v = z;

      end % function
```

6. Put a license of the algorithm into the file `alg_SOMEID/LICENSE.txt`.

7. Create a testing script `alg_SOMEID/alg_test.m`. This is optional, however recomended. An example follows.

```
      function alg_test(calcset) %<<<1
      % Part of QWTB. Test script for algorithm
SOMEALG
```

```
%
% See also qwtb

% Generate sample data
------------------------------- %<<<1
DI = [];
U = 1; V = 2;
DI.a.v = [U:V];
DI.b.v = U/V;

% Call algorithm
DO = qwtb('SOMEID', DI);

% Check results ------------------------------------
 %<<<1
assert((DO.x.v > U.*(1-1e6)) & (DO.x.v < U.
*(1+1e6)));
assert((DO.y.v > V.*(1-1e6)) & (DO.y.v < V.
*(1+1e6)));
assert((DO.z.v > sqrt(U).*(1-1e6)) & (DO.z.
v < sqrt(U).*(1+1e6)));

end % function
```

8. Create an example script `alg_SOMEID/alg_example.m`. This is optional, however recomended. An example follows.

```
%% SOMEALGNAME
% Example for algorithm SOMEID.
%
% SOMEID is an super mega hyper algorithm
for calculation of the ultimate answer to
% everything.
%

%% Generate sample data
% Two quantities are prepared: |a| and |b|,
 representing something and something even more
% important.
```

```
        DI = [];
        U = 1; V = 2;
        DI.a.v = [U:V];
        DI.b.v = U/V;

        %% Call algorithm
        % Use QWTB to apply algorithm |SOMEID| to
    data |DI|.
        CS.verbose = 1;
        DO = qwtb('SOMEID', DI, CS);

        %% Display results
        % Results is the very answer.
        x = DO.x.v
        y = DO.y.v
        z = DO.z.v
        %%
        % Errors of estimation in parts per milion:
        xerrppm = (DO.x.v - U)/U .* 1e6
        yerrppm = (DO.y.v - V)/V .* 1e6
        zerrppm = (DO.z.v - sqrt(U)/sqrt(U) .* 1e6
```

9. Check and test everything. Send your contribution to qwtb authors. Ask them to generate a new documentation. Celebrate.

Chapter 3

Licensing

Every algorithm has its own license. License of every algorithm is placed in the directory of the algorithm in a file named `LICENSE.txt`. Type of the license is included in the algorithm information structure, see chapter 2.2. The license of an algorithm can be displayed by following syntax:

```
license = qwtb('algid', 'license')
```

The license of the toolbox itself is MIT License, please see file `LICENSE.txt` in the directory containing script `qwtb.m`.

Chapter 4

Bilbiography

[1] JCGM, *Evaluation of measurement data - Supplement 1 to the "Guide to the expression of uncertainty in measurement" - Propagation of distributions using a Monte Carlo method*, JCGM, Ed. Bureau International des Poids et Measures, 2008.

[2] ——, *Evaluation of measurement data - Guide to the expression of uncertainty in measurement*, JCGM, Ed. Bureau International des Poids et Measures, 1995, ISBN: 92-67-10188-9.

Appendix A

Quick reference

Toolbox use:

```
                    alginfo = qwtb()
                    dataout = qwtb('algid', datain)
[dataout, datain, calcset] = qwtb('algid', datain)
                    dataout = qwtb('algid', datain, calcset)
[dataout, datain, calcset] = qwtb('algid', datain, calcset)
                                 qwtb('algid', 'example')
                                 qwtb('algid', 'test')
                                 qwtb('algid', 'addpath')
                                 qwtb('algid', 'rempath')
                    license = qwtb('algid', 'license')
```

Algorithm informations structure:

.id — Designator of the algorithm.
.name — Name of the algorithm.
.desc — Basic description.
.citation — Reference.
.remarks — Any remark.
.license — License of the algorithm.
.requires — Required quantities.
.reqdesc — Description of required quantities.
.returns — Output quantities.
.retdesc — Description of output quantities.
.providesGUF — Algorithm/wrapper calculates GUF uncertainty.
.providesMCM — Algorithm/wrapper calculates MCM uncertainty.
.fullpath — Full path to the algorithm. Automatically generated by the toolbox.

Quantity structure:

.v — Value.
.u — Uncertainty.
.d — Degree of freedom.
.c — Correlation.
.r — Randomized uncertainty.

Calculation settings structure:

.strict — (0) If zero, other fields generated automatically.
.verbose — (1) Display various informations.
.unc — ('none') How uncertainty is calculated ('none', 'guf', 'mcm').
.cor.req — (0) Correlation matrix is required for all input quantities.
.cor.gen — (1) Zero correlation matrix is generated automatically if missing.
.dof.req — (1) Degrees of freedom are required for all input quantities.
.dof.gen — (1) Degree of freedom are generated automatically if missing with value 50.
.mcm.repeats — (100) Number of Monte Carlo iterations.
.mcm.verbose — (1) Display various informations concerning Monte Carlo method.
.mcm.method — ('singlecore') Parallelization method ('multicore', 'multistation').
.mcm.procno — (1) Number of processors to use.
.mcm.tmpdir — ('.') Directory for temporary data.
.mcm.randomize — (1) Randomized uncertainties are generated automatically if missing.

Appendix B

Simple example of QWTB use

Simple example of the QWTB use

Sample data are simulated. QWTB is used to apply two different algorithms on the same data. Uncertainty of the results is calculated by means of Monte Carlo Method.

Contents

- Generate sample data
- Analyzing data
- Uncertainties

Generate sample data

Two quantities are prepared: t and y, representing 0.5 second of sinus waveform of nominal frequency 1 kHz, nominal amplitude 1 V and nominal phase 1 rad, sampled at sampling frequency fsnom 10 kHz.

```
DI = [];
Anom = 1; fnom = 1e3; phnom = 1; fsnom = 1e4;
DI.t.v = [0:1/fsnom:0.5];
DI.y.v = Anom*sin(2*pi*fnom*DI.t.v + phnom);
```

Add noise of standard deviation 1 mV:

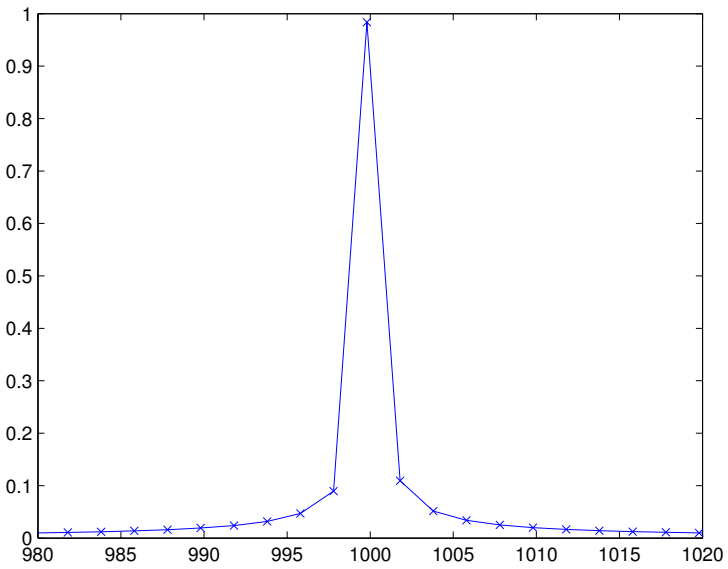
```
DI.y.v = DI.y.v + normrnd(0, 1e-3, size(DI.y.v));
```

Analyzing data

To get a frequency spectrum, algorithm SP−FFT can be used. This algorithm requires sampling frequency, so third quantity fs is added.

```
DI.fs.v = fsnom;
DO = qwtb('SP-FFT', DI);
plot(DO.f.v, DO.A.v, '-xb'); xlim([980 1020])
```

```
QWTB: no uncertainty calculation
```



One can see it is not a coherent measurement. Therefore to get 'unknown' amplitude and frequency of the signal algorithm PSFE can be used:

```
DO = qwtb('PSFE', DI);
f = DO.f.v
A = DO.A.v
```

```
QWTB: no uncertainty calculation

f =
```

```
    1.0000e+03


A =

    1.0000
```

Uncertainties

Uncertainties are added to the t (time stamps) and y (sampled data) structures.

```
DI.t.u = zeros(size(DI.t.v)) + 1e-5;
DI.y.u = zeros(size(DI.y.v)) + 1e-4;
```

Calculations settings is created with Monte Carlo uncertainty calculation method, 1000 repeats and singlecore calculation.

```
CS.unc = 'mcm';
CS.mcm.repeats = 1000;
CS.mcm.method = 'singlecore';
```

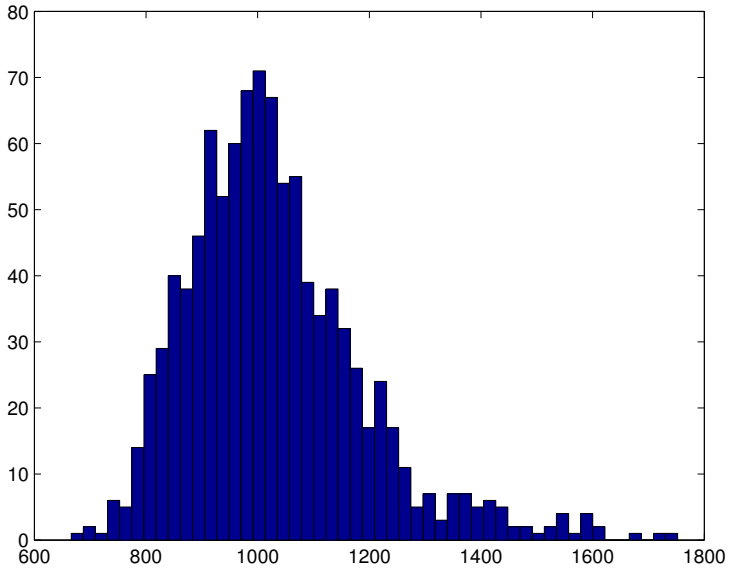
Run PSFE algorithm on input data DI and with calculattion settings CS.

```
DO = qwtb('PSFE',DI,CS);
```

```
QWTB: default correlation matrix generated for
    quantity 't'
QWTB: quantity t was randomized by QWTB
QWTB: default correlation matrix generated for
    quantity 'y'
QWTB: quantity y was randomized by QWTB
QWTB: general mcm uncertainty calculation
```

Result is displayed as a histogram of calculated frequency.

```
figure; hist(DO.f.r,50);
```



One can see the histogram is not Gaussian function. To get correct uncertainties, a shortest covariant interval has to be used.

Appendix C

Long example of QWTB use

Example of the QWTB use

Data are simulated, QWTB is used with different algorithms.

Contents

Generate ideal data

Sample data are generated, representing 1 second of sine waveform of nominal frequency fnom 1000 Hz, nominal amplitude Anom 1 V and nominal phase phnom 1 rad. Data are sampled at sampling frequency fsnom 10 kHz, perfectly synchronized, no noise.

```
Anom = 1; fnom = 1000; phnom = 1; fsnom = 10e4;
timestamps = [0:1/fsnom:0.1-1/fsnom];
ideal_wave = Anom*sin(2*pi*fnom*timestamps + phnom);
```

To use QWTB, data are put into two quantities: t and y. Both quantities are put into data in structure DI.

```
DI = [];
DI.t.v = timestamps;
DI.y.v = ideal_wave;
```

Apply three algorithms

QWTB will be used to apply three algorithms to determine frequency and amplitude: SP−FFT, PSFE and FPSWF. Results are in data out structure DOxxx. Algorithm FPSWF requires an estimate, select it to 0.1% different from nominal frequency. SP−FFT requires sampling frequency.

```
DI.f.v = fnom.*1.001;
DI.fs.v = fsnom;
DOspfft = qwtb('SP-FFT', DI);
DOpsfe = qwtb('PSFE', DI);
DOfpswf = qwtb('FPSWF', DI);
```

```
QWTB: no uncertainty calculation
QWTB: no uncertainty calculation
QWTB: no uncertainty calculation
Fitting started

Local minimum found.

Optimization completed because the size of the
    gradient is less than
the default value of the function tolerance.



Fitting finished
```

Compare results for ideal signal

Calculate relative errors in ppm for all algorithm to know which one is best. SP−FFT returns whole spectrum, so only the largest amplitude peak is interesting. One can see for the ideal case all errors are very small.

```
disp('SP-FFT errors (ppm):')
[tmp, ind] = max(DOspfft.A.v);
ferr  = (DOspfft.f.v(ind) - fnom)/fnom .* 1e6
Aerr  = (DOspfft.A.v(ind) - Anom)/Anom .* 1e6
pherr = (DOspfft.ph.v(ind) - phnom)/phnom .* 1e6

disp('PSFE errors (ppm):')
ferr  = (DOpsfe.f.v - fnom)/fnom .* 1e6
Aerr  = (DOpsfe.A.v - Anom)/Anom .* 1e6
pherr = (DOpsfe.ph.v - phnom)/phnom .* 1e6

disp('FPSWF errors (ppm):')
ferr  = (DOfpswf.f.v - fnom)/fnom .* 1e6
Aerr  = (DOfpswf.A.v - Anom)/Anom .* 1e6
pherr = (DOfpswf.ph.v - phnom)/phnom .* 1e6
```

```
SP-FFT errors (ppm):

ferr =

     0


Aerr =

     0


pherr =

  -4.2920e+05

PSFE errors (ppm):
```

```
ferr =

   -2.2737e-10


Aerr =

    4.8850e-09


pherr =

    2.3093e-08

FPSWF errors (ppm):

ferr =

   -3.4106e-10


Aerr =

   -4.0479e-07


pherr =

    3.7526e-08
```

Noisy signal

To simulate real measurement, noise is added with normal distribution and standard deviation sigma of 100 microvolt. Algorithms are again applied.

```
sigma = 100e-6;
DI.y.v = ideal_wave + normrnd(0, 100e-6, size(
    ideal_wave));
DOspfft = qwtb('SP-FFT', DI);
```

```
DOpsfe = qwtb('PSFE', DI);
DOfpswf = qwtb('FPSWF', DI);
```

```
QWTB: no uncertainty calculation
QWTB: no uncertainty calculation
QWTB: no uncertainty calculation
Fitting started

Local minimum found.

Optimization completed because the size of the
   gradient is less than
the default value of the function tolerance.



Fitting finished
```

Compare results for noisy signal

Again relative errors are compared. One can see amplitude and phase errors increased to several ppm, however frequency is still determined quite good by all three algorithms. FFT is not affected by noise at all.

```
disp('SP-FFT errors (ppm):')
[tmp, ind] = max(DOspfft.A.v);
ferr  = (DOspfft.f.v(ind) - fnom)/fnom .* 1e6
Aerr  = (DOspfft.A.v(ind) - Anom)/Anom .* 1e6
pherr = (DOspfft.ph.v(ind) - phnom)/phnom .* 1e6

disp('PSFE errors:')
ferr  = (DOpsfe.f.v - fnom)/fnom .* 1e6
Aerr  = (DOpsfe.A.v - Anom)/Anom .* 1e6
pherr = (DOpsfe.ph.v - phnom)/phnom .* 1e6

disp('FPSWF errors:')
ferr  = (DOfpswf.f.v - fnom)/fnom .* 1e6
Aerr  = (DOfpswf.A.v - Anom)/Anom .* 1e6
```

```
pherr = (DOfpswf.ph.v - phnom)/phnom .* 1e6
```

```
SP-FFT errors (ppm):

ferr =

     0


Aerr =

    0.4267


pherr =

  -4.2920e+05

PSFE errors:

ferr =

    0.0084


Aerr =

    0.4251


pherr =

   -4.2581

FPSWF errors:

ferr =

    0.0103
```

```
Aerr =

    0.4249


pherr =

   -4.7325
```

Non-coherent signal

In real measurement coherent measurement does not exist. So in next test the frequency of the signal differs by 20 ppm:

```
fnc = fnom*(1 + 20e-6);
noncoh_wave = Anom*sin(2*pi*fnc*timestamps + phnom);
DI.y.v = noncoh_wave;
DOspfft = qwtb('SP-FFT', DI);
DOpsfe = qwtb('PSFE', DI);
DOfpswf = qwtb('FPSWF', DI);
```

```
QWTB: no uncertainty calculation
QWTB: no uncertainty calculation
QWTB: no uncertainty calculation
Fitting started

Local minimum found.

Optimization completed because the size of the
    gradient is less than
the default value of the function tolerance.



Fitting finished
```

Compare results for non-coherent signal

Comparison of relative errors. Results of PSFE or FPSWF are correct, however FFT is affected by non-coherent signal considerably.

```
disp('SP-FFT errors (ppm):')
[tmp, ind] = max(DOspfft.A.v);
ferr  = (DOspfft.f.v(ind) - fnc)/fnc .* 1e6
Aerr  = (DOspfft.A.v(ind) - Anom)/Anom .* 1e6
pherr = (DOspfft.ph.v(ind) - phnom)/phnom .* 1e6

disp('PSFE errors:')
ferr  = (DOpsfe.f.v - fnc)/fnc .* 1e6
Aerr  = (DOpsfe.A.v - Anom)/Anom .* 1e6
pherr = (DOpsfe.ph.v - phnom)/phnom .* 1e6

disp('FPSWF errors:')
ferr  = (DOfpswf.f.v - fnc)/fnc .* 1e6
Aerr  = (DOfpswf.A.v - Anom)/Anom .* 1e6
pherr = (DOfpswf.ph.v - phnom)/phnom .* 1e6
```

```
SP-FFT errors (ppm):

ferr =

   -19.9996


Aerr =

    -2.8780


pherr =

   -4.3550e+05

PSFE errors:

ferr =
```

```
   -1.1368e-10


Aerr =

    3.8924e-07


pherr =

    3.3073e-04

FPSWF errors:

ferr =

   -1.1368e-10


Aerr =

   -3.2951e-07


pherr =

    1.4655e-08
```

Harmonically distorted signal.

In other cases a harmonic distortion can appear. Suppose a signal with second order harmonic of 10% amplitude as the main signal.

```
hadist_wave = Anom*sin(2*pi*fnom*timestamps + phnom) +
    0.1*Anom*sin(2*pi*fnom*2*timestamps + 2);
DI.y.v = hadist_wave;
DOspfft = qwtb('SP-FFT', DI);
DOpsfe = qwtb('PSFE', DI);
```

```
DOfpswf = qwtb('FPSWF', DI);
```

```
QWTB: no uncertainty calculation
QWTB: no uncertainty calculation
QWTB: no uncertainty calculation
Fitting started

Local minimum possible.

lsqnonlin stopped because the final change in the
   sum of squares relative to
its initial value is less than the default value of
    the function tolerance.



Fitting finished
```

Compare results for harmonically distorted signal.

Comparison of relative errors. PSFE or FPSWF are not affected by harmonic distortion, however FPSWF is not suitable.

```
disp('SP-FFT errors (ppm):')
[tmp, ind] = max(DOspfft.A.v);
ferr  = (DOspfft.f.v(ind) - fnom)/fnom .* 1e6
Aerr  = (DOspfft.A.v(ind) - Anom)/Anom .* 1e6
pherr = (DOspfft.ph.v(ind) - phnom)/phnom .* 1e6

disp('PSFE errors:')
ferr  = (DOpsfe.f.v - fnom)/fnom .* 1e6
Aerr  = (DOpsfe.A.v - Anom)/Anom .* 1e6
pherr = (DOpsfe.ph.v - phnom)/phnom .* 1e6

disp('FPSWF errors:')
ferr  = (DOfpswf.f.v - fnom)/fnom .* 1e6
Aerr  = (DOfpswf.A.v - Anom)/Anom .* 1e6
pherr = (DOfpswf.ph.v - phnom)/phnom .* 1e6
```

```
SP-FFT errors (ppm):
ferr =
     0

Aerr =
     0

pherr =
  -4.2920e+05
PSFE errors:
ferr =
  -2.2737e-10

Aerr =
   6.7212e-04

pherr =
    0.5311
FPSWF errors:
ferr =
   -0.7356
```

```
Aerr =

    0.1407


pherr =

  231.4552
```

Harmonically distorted, noisy, non-coherent signal.

In final test all distortions are put in a waveform and results are compared.

```
err_wave = Anom*sin(2*pi*fnc*timestamps + phnom) + 0.1*
   Anom*sin(2*pi*fnc*2*timestamps + 2) + normrnd(0, 100
   e-6, size(ideal_wave));
DI.y.v = err_wave;
DOspfft = qwtb('SP-FFT', DI);
DOpsfe = qwtb('PSFE', DI);
DOfpswf = qwtb('FPSWF', DI);
```

```
QWTB: no uncertainty calculation
QWTB: no uncertainty calculation
QWTB: no uncertainty calculation
Fitting started

Local minimum possible.

lsqnonlin stopped because the final change in the
   sum of squares relative to
its initial value is less than the default value of
    the function tolerance.



Fitting finished
```

Compare results for harmonically distorted, noisy, non-coherent signal.

```
disp('SP-FFT errors (ppm):')
[tmp, ind] = max(DOspfft.A.v);
ferr  = (DOspfft.f.v(ind) - fnc)/fnc .* 1e6
Aerr  = (DOspfft.A.v(ind) - Anom)/Anom .* 1e6
pherr = (DOspfft.ph.v(ind) - phnom)/phnom .* 1e6

disp('PSFE errors:')
ferr  = (DOpsfe.f.v - fnc)/fnc .* 1e6
Aerr  = (DOpsfe.A.v - Anom)/Anom .* 1e6
pherr = (DOpsfe.ph.v - phnom)/phnom .* 1e6

disp('FPSWF errors:')
ferr  = (DOfpswf.f.v - fnc)/fnc .* 1e6
Aerr  = (DOfpswf.A.v - Anom)/Anom .* 1e6
pherr = (DOfpswf.ph.v - phnom)/phnom .* 1e6
```

```
SP-FFT errors (ppm):

ferr =

   -19.9996


Aerr =

    0.5539


pherr =

   -4.3550e+05

PSFE errors:

ferr =

    0.0094
```

```
Aerr =

    2.7791


pherr =

   -1.0151

FPSWF errors:

ferr =

   -0.7082


Aerr =

    3.1053


pherr =

  224.3897
```

Appendix D

INL – Integral Non-Linearity of ADC

Info file data

.id — INL

.name — Integral Non-Linearity of ADC

.desc — Calculates Integral Non-Linearity of an ADC. ADC has to sample sinewave, ADC codes are required.

.citation — Virosztek, T., Pálfi V., Renczes B., Kollár I., Balogh L., Sárhegyi A., Márkus J., Bilau Z. T., ADCTest project site: `http://www.mit.bme.hu/projects/adctest` 2000-2014

.remarks — Based on the ADCTest Toolbox v4.3, November 25, 2014.

.license — UNKNOWN

.requires

t — time series of sampled data

codes — Sampled values represented as ADC codes (not converted to voltage)

.returns

INL — INL

.providesGUF — no

.providesMCM — no

Example

Integral Non Linearity of ADC

Example for algorithm INL

INL is an algorithm for estimating Integral Non-Linearity of an ADC. ADC has to sample sinewave, ADC codes are required.

See also 'Virosztek, T., Pálfi V., Renczes B., Kollár I., Balogh L., Sárhegyi A., Márkus J., Bilau Z. T., ADCTest project site: `http://www.mit.bme.hu/projects/adctest` 2000-2014';

Contents

- Generate sample data
- Call algorithm

Generate sample data

Suppose a sine wave of nominal frequency 10 Hz and nominal amplitude 1 V is sampled by ADC with bit resolution of 4. First quantities `t` with time of samples and quantity `bits` with number of bits are prepared and put into input data structure `DI`.

```
DI = [];
DI.t.v=[0:1/1e4:1-1/1e4];
DI.bits.v = 4;
```

Waveform is constructed.

```
Anom = 1; fnom = 2; phnom = 0;
wvfrm = Anom*sin(2*pi*fnom*DI.t.v + phnom);
```

Next code values are calculated. It is simulated by quantization and scaling of the sampled waveform. In real measurement code values can be obtained directly from the ADC. Suppose ADC range is -1..1.

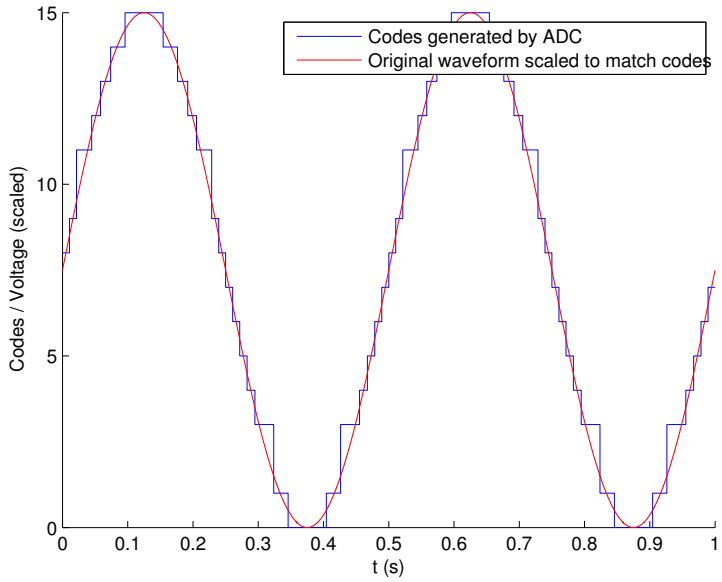
```
codes = wvfrm;
rmin = -1; rmax = 1;
levels = 2.^DI.bits.v - 1;
codes(codes<rmin) = rmin;
codes(codes>rmax) = rmax;
codes = round((codes-rmin)./2.*levels);
```

Now lets introduce ADC error. Instead of generating code 2 ADC erroneously generates code 3 and instead of 10 it generates 11.

```
codes(codes==2) = 3;
codes(codes==10) = 11;
codes = codes + min(codes);
```

Create quantity codes and plot a figure with sampled sine wave and codes.

```
DI.codes.v = codes;
figure
%plot(t, (y+1).*1/2.*levels, t, codes);
hold on
stairs(DI.t.v, codes);
wvfrm = (wvfrm + Anom).*levels./2;
plot(DI.t.v, wvfrm, '-r');
xlabel('t (s)')
ylabel('Codes / Voltage (scaled)');
legend('Codes generated by ADC','Original waveform
   scaled to match codes');
hold off
```



Call algorithm

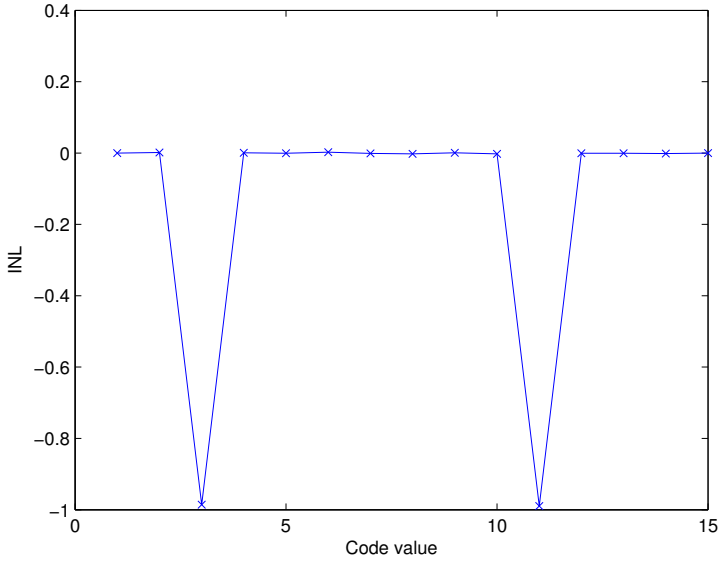
Apply INL algorithm to the input data DI.

```
DO = qwtb('INL', DI);
```

```
QWTB: no uncertainty calculation
```

Plot results of integral non-linearity. One can clearly observe defects on codes 3 and 11.

```
figure
plot(DO.INL.v, '-x');
xlabel('Code value')
ylabel('INL')
```


0.4
0.2
0
−0.2
−0.4
−0.6
−0.8
−1
INL
0
5
10
15
Code value

Appendix E

PSFE – Phase Sensitive Frequency Estimator

Info file data

.id — PSFE

.name — Phase Sensitive Frequency Estimator

.desc — An algorithm for estimating the frequency, amplitude, and phase of the fundamental component in harmonically distorted waveforms. The algorithm minimizes the phase difference between the sine model and the sampled waveform by effectively minimizing the influence of the harmonic components. It uses a three-parameter sine-fitting algorithm for all phase calculations. The resulting estimates show up to two orders of magnitude smaller sensitivity to harmonic distortions than the results of the four-parameter sine fitting algorithm.

.citation — Lapuh, R., "Estimating the Fundamental Component of Harmonically Distorted Signals From Noncoherently Sampled Data," Instrumentation and Measurement, IEEE Transactions on , vol.64, no.6, pp.1419,1424, June 2015, doi: 10.1109/TIM.2015.2401211, URL: `http://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&arnumber=7061456&isnumber=7104190`

.remarks — Very small errors, effective for harmonically distorted signals.

.license — UNKNOWN

.requires

t — time series of sampled data

y — sampled values

.returns

f — Frequency of main signal component
A — Amplitude of main signal component
ph — Phase of main signal component

.providesGUF — no

.providesMCM — no

Example

Phase Sensitive Frequency Estimator

Example for algorithm PSFE.

PSFE is an algorithm for estimating the frequency, amplitude, and phase of the fundamental component in harmonically distorted waveforms. The algorithm minimizes the phase difference between the sine model and the sampled waveform by effectively minimizing the influence of the harmonic components. It uses a three-parameter sine-fitting algorithm for all phase calculations. The resulting estimates show up to two orders of magnitude smaller sensitivity to harmonic distortions than the results of the four-parameter sine fitting algorithm.

See also Lapuh, R., "Estimating the Fundamental Component of Harmonically Distorted Signals From Noncoherently Sampled Data," Instrumentation and Measurement, IEEE Transactions on , vol.64, no.6, pp.1419,1424, June 2015, doi: 10.1109/TIM.2015.2401211, URL: `http://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&arnumber=7061456&isnumber=7104190'`

Contents

- Generate sample data
- Call algorithm
- Display results

Generate sample data

Two quantities are prepared: `t` and `y`, representing 1 second of sinus waveform of nominal frequency 100 Hz, nominal amplitude 1 V and nominal phase 1 rad, sampled at sampling frequency 10 kHz.

```
DI = [];
Anom = 1; fnom = 100; phnom = 1;
DI.t.v = [0:1/1e4:1-1/1e4];
DI.y.v = Anom*sin(2*pi*fnom*DI.t.v + phnom);
```

Add noise:

```
DI.y.v = DI.y.v + normrnd(0, 1e-3, size(DI.y.v));
```

Call algorithm

Use QWTB to apply algorithm PSFE to data DI.

```
DO = qwtb('PSFE', DI);
```

```
QWTB: no uncertainty calculation
```

Display results

Results is the amplitude, frequency and phase of sampled waveform.

```
f = DO.f.v
A = DO.A.v
ph = DO.ph.v
```

```
f =

   100.0000


A =

    1.0000
```

```
ph =

    1.0000
```

Errors of estimation in parts per milion:

```
ferrppm = (DO.f.v - fnom)/fnom .* 1e6
Aerrppm = (DO.A.v - Anom)/Anom .* 1e6
pherrppm = (DO.ph.v - phnom)/phnom .* 1e6
```

```
ferrppm =

    0.1322


Aerrppm =

   -10.1106


pherrppm =

   -34.9097
```

Appendix F

FPSWF – Four Parameter Sine Wave Fitting

Info file data

.id — FPSWF

.name — Four Parameter Sine Wave Fit

.desc — Fits a sine wave to the recorded data by means of least squares using 4 parameter model. Different functions are used when run in MATLAB or GNU Octave.

.citation —

.remarks — Algorithm is very sensitive to distortion. Algorithm requires good estimate of frequency.

.license —

.requires

t — Time series of sampled data
y — Sampled values

.returns

f — Frequency of main signal component
A — Amplitude of main signal component
ph — Phase of main signal component
O — Offset of signal

.providesGUF — no

.providesMCM — no

Example

Four parameter sine wave fitting

Example for algorithm FPSWF.

FPSWF is an algorithm for estimating the frequency, amplitude, and phase of the sine waveform. The algorithm use least squares method. Algorithm requires good estimate of frequency.

Contents

Generate sample data

Two quantities are prepared: t and y, representing 1 second of sinus waveform of nominal frequency 1 kHz, nominal amplitude 1 V, nominal phase 1 rad and offset 1 V sampled at sampling frequency 10 kHz.

```
DI = [];
Anom = 2; fnom = 100; phnom = 1; Onom = 0.2;
DI.t.v = [0:1/1e4:1-1/1e4];
DI.y.v = Anom*sin(2*pi*fnom*DI.t.v + phnom) + Onom;
```

Lets make an estimate of frequency 0.2 percent higher than nominal value:

```
DI.f.v = 100.2;
```

Call algorithm

Use QWTB to apply algorithm FPSWF to data DI.

```
CS.verbose = 1;
DO = qwtb('FPSWF', DI, CS);
```

```
QWTB: no uncertainty calculation
Fitting started

Local minimum found.

Optimization completed because the size of the
    gradient is less than
the default value of the function tolerance.



Fitting finished
```

Display results

Results is the amplitude, frequency and phase of sampled waveform.

```
A = DO.A.v
f = DO.f.v
ph = DO.ph.v
O = DO.O.v
```

```
A =

    2.0000


f =

  100.0000


ph =

    1.0000
```

```
O =

    -0.2000
```

Errors of estimation in parts per milion:

```
Aerrppm = (DO.A.v - Anom)/Anom .* 1e6
ferrppm = (DO.f.v - fnom)/fnom .* 1e6
pherrppm = (DO.ph.v - phnom)/phnom .* 1e6
Oerrppm = (DO.O.v - Onom)/Onom .* 1e6
```

```
Aerrppm =

    4.8894e-07


ferrppm =

   -1.4211e-10


pherrppm =

    1.7542e-08


Oerrppm =

   -2.0000e+06
```

Appendix G

SP-FFT – Spectrum by means of Fast Fourier Transform

Info file data

.id — SP-FFT

.name — Spectrum by means of Fast Fourier Transform

.desc — Calculates frequency and phase spectrum by means of Fast Fourier Transform algorithm. Result is normalized.

.citation —

.remarks —

.license —

.requires

y — Sampled values
fs — Sampling frequency

.returns

f — Frequency series
A — Amplitude series
ph — Phase series

.providesGUF — no

.providesMCM — no

Example

Signal Spectrum by means of Fast fourier transform

Example for algorithm SP-FFT.

Calculates frequency and phase spectrum by means of Fast Fourier Transform algorithm. Result is normalized.

Contents

Generate sample data

Two quantities are prepared: y and fs, representing 1 second of signal containing 5 harmonic components and one inter-harmonic component. Main signal component has nominal frequency 1 kHz, nominal amplitude 2 V, nominal phase 1 rad and offset 1 V sampled at sampling frequency 10 kHz.

```
DI = [];
fsnom = 1e4; Anom = 2; fnom = 100; phnom = 1; Onom =
    0.2;
t = [0:1/fsnom:1-1/fsnom];
DI.y.v = Anom*sin(2*pi*fnom*t + phnom);
for i = 2:45
        DI.y.v = DI.y.v + Anom./i*sin(2*pi*fnom*i*t +
    phnom + i - 1);
end
DI.y.v = DI.y.v + 1*sin(2*pi*fnom*1.456*t + phnom);
DI.fs.v = fsnom;
```

Call algorithm

Use QWTB to apply algorithm SP-FFT to data DI.

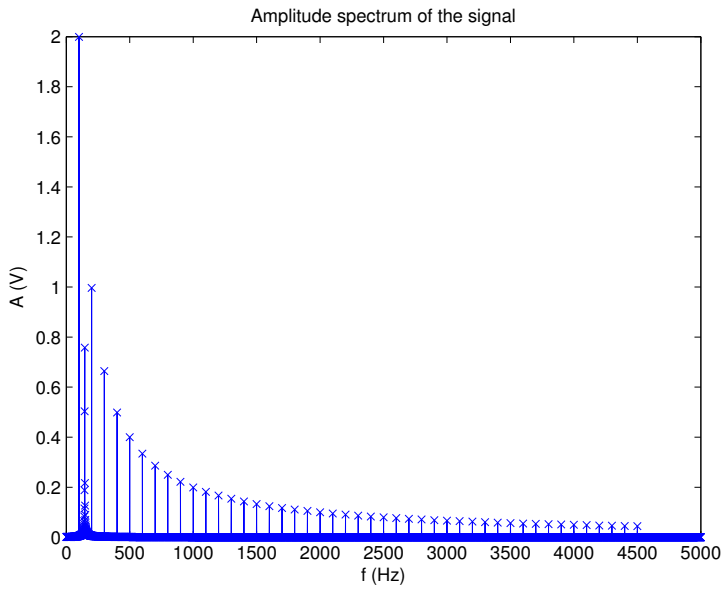
```
DO = qwtb('SP-FFT', DI);
```

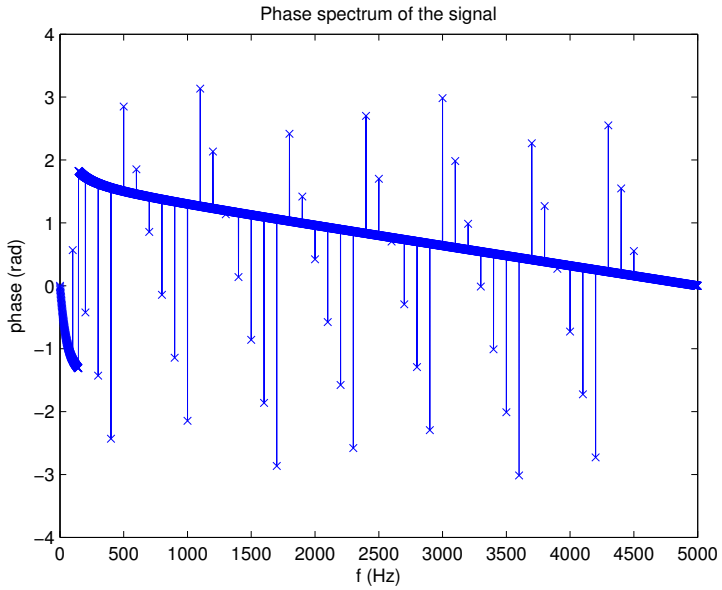
```
QWTB: no uncertainty calculation
```

Display results

Results is the amplitude and phase spectrum.

```
figure
plot(DO.f.v, DO.A.v, '-x')
xlabel('f (Hz)'); ylabel('A (V)'); title('Amplitude
    spectrum of the signal');
figure
plot(DO.f.v, DO.ph.v, '-x')
xlabel('f (Hz)'); ylabel('phase (rad)'); title('Phase
    spectrum of the signal');
```




Phase spectrum of the signal
phase (rad)
f (Hz)
4
3
2
1
0
−1
−2
−3
−4
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000