

# Documentation of the C functions

## Weighted BACON algorithms

Tobias Schoch

University of Applied Sciences Northwestern Switzerland FHNW  
School of Business, Riggensbachstrasse 16, CH-4600 Olten  
`tobias.schoch@fhnw.ch`

April 8, 2021, version 0.2

---

## Contents

<b>1</b>	<b>Introduction</b>	<b>1</b>
<b>2</b>	<b>Exported functions</b>	<b>1</b>
<b>3</b>	<b>Error handling [<code>wbacon_error.c</code>]</b>	<b>6</b>
<b>4</b>	<b>wBACON [<code>wbacon.c</code>]</b>	<b>7</b>
<b>5</b>	<b>wBACON_reg [<code>wbacon_reg.c</code>]</b>	<b>15</b>
<b>6</b>	<b>Weighted least squares [<code>fitwls.c</code>]</b>	<b>26</b>
<b>7</b>	<b>Weighted quantile [<code>wquantile.c</code>]</b>	<b>28</b>
<b>8</b>	<b>Partial sorting [<code>partial_sort.c</code>]</b>	<b>33</b>

---

## 1 Introduction

In this report, we document the C functions underlying the `wbacon` R package. Only the following methods are exported:

- `wbacon` (BACON algorithm for multivariate outlier detection)
- `wbacon_reg` (BACON algorithm for robust linear regression)
- `wquantile` (weighted quantile)

All other functions are not exported, hence, they are not callable from R. The methodological details of the functions are discussed in the document “methods.pdf” (see package folder `doc`).

For ease of referencing, we use the following abbreviations.

**LAPACK:** Anderson, E., Z. Bai, C. Bischof, L. S. Blackford, J. Demmel, J. Dongarra, J. D. Croz, A. Greenbaum, S. Hammerling, A. McKenney, and D. Sorensen (1999). *LAPACK Users’ Guide*, 3rd ed., Philadelphia: Society for Industrial and Applied Mathematics (SIAM).

**BLAS:** Blackford, L. S., A. Petit, R. Pozo, K. Remington, R. C. Whaley, J. Demmel, J. Dongarra, I. Duff, S. Hammerling, G. Henry, M. Heroux, L. Kaufman, and A. Lumsdaine (2002). An updated set of basic linear algebra subprograms (BLAS), *ACM Transactions on Mathematical Software*, 28, 135–151.

**OpenMP:** OpenMP Architecture Review Board (2018). *OpenMP Application Program Interface Version 5.0*, URL <https://https://www.openmp.org>.

## 2 Exported functions

---

wbacon	<i>Weighted BACON algorithm for multivariate outlier detection</i>
--------	--

---

### Description

The function implements a weighted variant of Algorithm 3 of Billor et al. (2000). It calls a weighted variant of Algorithm 2 of Billor et al. (2000) to initialize the subset (see `initial_subset`).

### Usage

```
void wbacon(double *x, double *w, double *center, double *scatter, double *dist,
            int *n, int *p, double *alpha, int *subset, double *cutoff, int *maxiter,
            int *verbose, int *version2, int *collect, int *success)
```

### Arguments

<code>x</code>	data, double array[n, p].
<code>w</code>	sampling weights, double array[n].
<code>center</code>	center, double array[p].
<code>scatter</code>	scatter matrix, double array[p, p].
<code>dist</code>	distances, double array[n].
<code>n, p</code>	dimensions, [int].
<code>alpha</code>	tuning constant, [double], it defines the $1 - \alpha$ quantile of the chi-squared distribution.
<code>subset</code>	subset, int array[n]; with elements in the set $\{0, 1\}$ , where 1 signifies that the element is in the subset.
<code>cutoff</code>	cutoff threshold, [double], i.e. $1 - \alpha$ quantile of the chi-squared distribution.
<code>maxiter</code>	maximum number of iterations, [int].
<code>verbose</code>	toggle, [int], 1: verbose (i.e., the function prints detailed information to the console), 0: quiet.
<code>version2</code>	toggle, [int], defines the method to construct the initial subset: 1: “Version 2” of Billor et al. (2000) is used; 0: “Version 1” is used.
<code>collect</code>	size of the initial basic subset, [int].
<code>success</code>	indicator, [int], 1: algorithm converged, 0: failure of convergence.

## Details

The `subset` is implemented as an `int array[n]`. Elements in the subset are coded 1; otherwise 0. The function makes a copy, `w_cpy`, of the array `w` with sampling weights. This copy is used in the computations (e.g., `weightedmean`) and is modified such that `w_cpy[i] = 0.0` if `subset[i] == 0`.

See `methods.pdf` for more details.

## Dependencies

**internal:** `initial_location`, `initial_subset`, `mahalanobis`, `cutoffval`, and `wbacon_error`

**external:** `Rmath.h:qchisq`

## Value

On return, the following slots are overwritten:

<code>center</code>	estimated weighted coordinate-wise center
<code>scatter</code>	estimated lower triangular matrix of the weighted scatter matrix
<code>dist</code>	Mahalanobis distance
<code>subset0</code>	subset of outlier-free observations
<code>cutoff</code>	$1 - \alpha$ quantile of the chi-squared distribution
<code>maxiter</code>	number of iteration required
<code>success</code>	convergence or failure of convergence

## References

Billor N., Hadi A.S., Vellemann P.F. (2000). BACON: Blocked Adaptive Computationally efficient Outlier Nominators. *Computational Statistics and Data Analysis* 34, pp. 279-298.

Béguin C., Hulliger B. (2008). The BACON-EEM Algorithm for Multivariate Outlier Detection in Incomplete Survey Data. *Survey Methodology* 34, pp. 91-103.

---

<code>wbacon_reg</code>	<i>Weighted BACON algorithm for robust linear regression</i>
-------------------------	--

---

## Description

The function implements a weighted variant of the Algorithms 4 and 5 of Billor et al. (2000).

## Usage

```
void wbacon_reg(double *x, double *y, double *w, double *resid, double *beta,
               int *subset0, double *dist, int *n, int *p, int *m, int *verbose,
               int *success, int *collect, double *alpha, int *maxiter)
```

## Arguments

<code>x</code>	design matrix, <code>double array[n, p]</code> .
<code>y</code>	response, <code>double array[n]</code> .
<code>w</code>	sampling weights, <code>double array[n]</code> .
<code>resid</code>	reiduals, <code>double array[n]</code> .
<code>subset0</code>	subset, <code>int array[n]</code> ; with elements in the set $\{0, 1\}$ , where 1 signifies that the element is in the subset.
<code>dist</code>	distances/ tis, <code>double array[n]</code> .
<code>n, p</code>	dimensions, <code>[int]</code> .
<code>m</code>	size of subset, <code>[int]</code> .
<code>verbose</code>	toggle, <code>[int]</code> , 1: verbose (i.e., the function prints detailed information to the console), 0: quiet.
<code>success</code>	1: successful termination; 0: error, did not converge, <code>[int]</code> .
<code>collect</code>	size of the initial basic subset, <code>[int]</code> .
<code>alpha</code>	cutoff threshold, <code>[double]</code> , i.e. $1 - \alpha$ quantile of the Student $t$ -distribution.
<code>maxiter</code>	maximum number of iterations, <code>[int]</code> .

## Details

The regression is computed in two steps. First, we call the weighted BACON algorithm for multivariate outlier detection (Algorithm 3, see [wbacon](#)) on the design matrix `x` (Note: the regression intercept, if there is one, must be dropped). As a result, we obtain `subset` and `m`, which are then used as an input to `wbacon_reg`.

The function `wbacon_reg` calls [initial\\_reg](#) to initialize the regression. Then, it calls [algorithm\\_4](#) and [algorithm\\_5](#).

See [methods.pdf](#) for more details.

## Dependencies

[initial\\_reg](#), [algorithm\\_4](#), and [algorithm\\_5](#)

## Value

On return, the following slots are overwritten:

<code>beta</code>	regression coefficients
<code>resid</code>	residuals
<code>dist</code>	distances/ tis
<code>subset0</code>	subset of outlier-free observations
<code>maxiter</code>	number of iteration required
<code>success</code>	convergence or failure of convergence
<code>x</code>	is overwritten with the QR factorization as returned by LAPACK: <code>dgeqls</code> , respectively, LAPACK: <code>dgeqrf</code>

## References

Billor N., Hadi A.S., Vellemann P.F. (2000). BACON: Blocked Adaptive Computationally efficient Outlier Nominators. *Computational Statistics and Data Analysis* 34, pp. 279-298.

---

wquantile

*Weighted quantile*

---

## Description

Weighted quantile.

## Usage

```
void wquantile(double *array, double *weights, int *n, double *prob,  
              double *result)
```

## Arguments

<code>array</code>	data, double array[n].
<code>weights</code>	sampling weights, double array[n].
<code>n</code>	dimension, int.
<code>prob</code>	probability that defines the quantile, double, such that $0 \leq \text{prob} \leq 1$ .
<code>result</code>	quantile, double.

## Details

- The function is based on a weighted version of the Select (FIND, quickselect) algorithm of C.A.R. Hoare with the Bentley and McIlroy (1993) 3-way partitioning scheme. For very small arrays, we use insertion sort.
- For equal weighting, i.e. when all elements in `weights` are equal, `wquantile` computes quantiles of type 2 in Hyndman and Fan (1996).
- (Weighted) Select (and Quicksort) is efficient for large arrays. But its overhead can be severe for small arrays; hence, we use insertion sort for small arrays; cf. Bentley and McIlroy (1993). The size threshold below which insertion sort is used can be specified by setting the macro `_n_quickselect` at compile time; see Sect. 7.

See `methods.pdf` for more details.

## Dependency

`wquantile_noalloc`

## Value

On return, `result` is overwritten with the weighted quantile.

## References

- Bentley, J.L. and D.M. McIlroy (1993). Engineering a Sort Function, *Software - Practice and Experience* 23, pp. 1249-1265.
- Hyndman, R.J. and Y. Fan (1996). Sample Quantiles in Statistical Packages, *The American Statistician* 50, pp. 361-365.

### 3 Error handling [wbacon\_error.c]

Error handling refers to the functions that operate on matrices, and which may fail (e.g., because of rank deficiency). These functions return a value of typedef enum [wbacon\\_error\\_type](#). The function [wbacon\\_error](#) can be called to return a human readable error message.

---

wbacon_error_type	<i>Error type</i> [typedef enum]
-------------------	----------------------------------

---

WBACON_ERROR_OK	no error.
WBACON_ERROR_RANK_DEFICIENT	matrix is rank deficient.
WBACON_ERROR_NOT_POSITIVE_DEFINITE	matrix is not positive definite.
WBACON_ERROR_TRIANG_MAT_SINGULAR	triangular matrix is singular.
WBACON_ERROR_CONVERGENCE_FAILURE	the algorithm did not converge
[WBACON_ERROR_COUNT]	error count. This is not an actual error; it is used for internal purposes.

---

wbacon_error	<i>Human readable error string</i>
--------------	------------------------------------

---

#### Description

Returns a human readable error string.

#### Usage

```
const char* wbacon_error(wbacon_error_type err)
```

#### Arguments

err                      error of typedef enum [[wbacon\\_error\\_type](#)].

#### Value

Returns a string with a human readable error message.

## 4 wBACON [wbacon.c]

To offer functions with a clean interface, most of the functions use the typedef struct `wbdata` and `workarray`.

<code>wbdata</code>	<i>Data</i> [typedef struct]
<code>n</code>	dimension.
<code>p</code>	dimension.
<code>x</code>	pointer to data, <code>double array[n,p]</code> .
<code>w</code>	pointer to weight, <code>double array[n]</code> .
<code>dist</code>	pointer to distance, <code>double array[n]</code> .

<code>workarray</code>	<i>Work arrays</i> [typedef struct]
<code>iarray</code>	pointer to work array, <code>int array[n]</code> .
<code>work_n</code>	pointer to work array, <code>double array[n]</code> .
<code>work_np</code>	pointer to work array, <code>double array[n, p]</code> .
<code>work_pp</code>	pointer to work array, <code>double array[pp]</code> .
<code>work_2n</code>	pointer to work array, <code>double array[2n]</code> .



## Internal functions

---

<code>initial_location</code>	<i>Internal function</i>
-------------------------------	--------------------------

---

### Description

Computes the initial location: either version “v1” or “v2” or Billor et al. (2000).

### Usage

```
static wbacon_error_type initial_location(wbdata *dat, workarray *work,  
    double* restrict select_weight, double* restrict center,  
    double* restrict scatter, int* version2)
```

### Arguments

<code>dat</code>	data, typedef struct <a href="#">wbdata</a> .
<code>work</code>	work array, typedef struct <a href="#">workarray</a> .
<code>select_weight</code>	weight that indicates membership of an observation in the sample (=1.0), otherwise 0.0, <code>array[n]</code> .
<code>center</code>	center, <code>double array[p]</code> .
<code>scatter</code>	scatter matrix, <code>double array[p, p]</code> .
<code>version2</code>	toggle, <code>[int]</code> , defines the method to construct the initial subset: 1: “Version 2” of Billor et al. (2000) is used; 0: “Version 1” is used.

### Dependency

[wquantile\\_noalloc](#), [euclidean\\_norm2](#), and [mahalanobis](#)

### Value

The function returns a [wbacon\\_error\\_type](#): the return value is either `WBACON_ERROR_OK` (i.e., no error) or the error handed over by [mahalanobis](#).

See [methods.pdf](#) for the details.

On return, the following slots are overwritten:

`center`  
`scatter`

---

<code>initial_subset</code>	<i>Internal function</i>
-----------------------------	--------------------------

---

## Description

Computes the initial subset. This is a weighted variant of Algorithm 2 of Billor et al. (2000).

## Usage

```
static wbacon_error_type initial_subset(wbdata *dat, workarray *work,
double* restrict select_weight, double* restrict center,
double* restrict scatter, int* restrict subset,
int* restrict subssize, int *verbose, int *collect)
```

## Arguments

<code>dat</code>	data, typedef struct <a href="#">wbdata</a> .
<code>work</code>	work array, typedef struct <a href="#">workarray</a> .
<code>select_weight</code>	weight that indicates membership of an observation in the sample (=1.0), otherwise 0.0, <code>array[n]</code> .
<code>center</code>	center, <code>double array[p]</code> .
<code>scatter</code>	scatter matrix, <code>double array[p, p]</code> .
<code>subset</code>	subset, <code>int array[n]</code> ; with elements in the set $\{0,1\}$ , where 1 signifies that the element is in the subset.
<code>subssize</code>	size of <code>subset</code> , <code>[int]</code> .
<code>verbose</code>	toggle, <code>[int]</code> , 1: verbose (i.e., the function prints detailed information to the console), 0: quiet.
<code>collect</code>	size of the initial basic subset, <code>[int]</code> .

## Dependency

[scatter\\_w](#)

## Value

The function returns a [wbacon\\_error\\_type](#): the return value is either `WBACON_ERROR_OK` (i.e., no error) or the error handed over by [check\\_matrix\\_fullrank](#).

On return, the following slots are overwritten:

<code>dat-&gt;w</code>	elements in the initial subset have $w_i = 1$ , else $w_i = 0$
<code>subset</code>	subset
<code>subssize</code>	size of the subset

**Description**

Computes the Mahalanobis distance of the  $x_i$ 's; see `methods.pdf` for the details.

**Usage**

```
static inline wbacon_error_type mahalanobis(wbdata *dat, workarray *work,
      double* restrict select_weight, double* restrict center,
      double* restrict scatter)
```

**Arguments**

<code>dat</code>	data, typedef struct <code>wbdata</code> .
<code>work</code>	work array, typedef struct <code>workarray</code> .
<code>select_weight</code>	weight that indicates membership of an observation in the sample (=1.0), otherwise 0.0, <code>array[n]</code> .
<code>center</code>	center, double array[p].
<code>scatter</code>	scatter matrix, double array[p, p].

**Details**

The function's loop over the columns of the data matrix is parallelized using the OpenMP preprocessor directive

```
#pragma omp parallel for if(n > OMP_MIN_SIZE)
```

where `OMP_MIN_SIZE` is of size 100 000 , and `n` and is the number of rows. The inner loop over the `n` rows is equipped with the directive `#pragma omp simd` to tell the compiler that we demand SIMD vectorization.

**Dependencies**

**internal:** `mean_scatter_w`

**external:** LAPACK:dtrsm and LAPACK:dpotrf

**Value**

The function returns a `wbacon_error_type`: the return value is either `WBACON_ERROR_OK` (i.e., no error) or `WBACON_ERROR_RANK_DEFICIENT`.

On return, `dat->dist` is overwritten with the Mahalanobis distance.

---

`scatter_w`

*Internal function*

---

## Description

Computes the weighted scatter matrix.

## Usage

```
static inline void scatter_w(wbdata *dat, double* restrict work,  
    double* restrict select_weight, double* restrict center,  
    double* restrict scatter)
```

## Arguments

<code>dat</code>	data, typedef struct <code>wbdata</code> .
<code>work_np</code>	work array, double array[n, p].
<code>select_weight</code>	weight that indicates membership of an observation in the sample (=1.0), otherwise 0.0, array[n].
<code>center</code>	center, double array[p].
<code>scatter</code>	scatter matrix, double array[p, p].

## Details

The weighted `scatter` matrix is computed without (re-) computing the `center`.

The function's loop over the columns of the data matrix is parallelized using the OpenMP preprocessor directive

```
#pragma omp parallel for if(n > OMP_MIN_SIZE)
```

where `OMP_MIN_SIZE` is of size 100 000 and `n` is the number of rows. The inner loop over the `n` rows is equipped with the directive `#pragma omp simd` to tell the compiler that we demand SIMD vectorization.

## Dependency

BLAS:dsyrk

## Value

On return, `scatter` is overwritten with the lower triangular matrix of the weighted scatter matrix.

**Description**

Computes the weighted scatter matrix.

**Usage**

```
static inline void mean_scatter_w(wbdata *dat, double* restrict select_weight,
    double* restrict work_n, double* restrict work_np, double* restrict center,
    double* restrict scatter)
```

**Arguments**

<code>dat</code>	data, typedef struct <a href="#">wbdata</a> .
<code>select_weight</code>	weight that indicates membership of an observation in the sample (=1.0), otherwise 0.0, <code>array[n]</code> .
<code>work_n</code>	work array, <code>double array[n]</code> .
<code>work_np</code>	work array, <code>double array[n, p]</code> .
<code>center</code>	center, <code>double array[p]</code> .
<code>scatter</code>	scatter matrix, <code>double array[p, p]</code> .

**Details**

The function's loop over the columns of the data matrix is parallelized using the OpenMP preprocessor directive

```
#pragma omp parallel for if(n > OMP_MIN_SIZE)
```

where `OMP_MIN_SIZE` is of size 100 000 and `n` is the number of rows. The inner loop over the `n` rows is equipped with the directive `#pragma omp simd` to tell the compiler that we demand SIMD vectorization.

**Dependency**

BLAS:dsyrk

**Value**

On return, `scatter` and `mean` are overwritten with, respectively, the lower triangular matrix of the weighted scatter matrix and the weighted coordinate-wise mean.

---

euclidean\_norm2

*Internal function*

---

### Description

Computes the squared Euclidean norm  $\|\mathbf{x} - \mathbf{c}\|_2^2$ , where  $\mathbf{c}$  denotes the center.

### Usage

```
static inline void euclidean_norm2(wbdata *dat, double* restrict work_np,  
    double* restrict center)
```

### Arguments

`dat` data, typedef struct `wbdata`.  
`work_np` work array, double array[n, p].  
`center` center, double array[p].

### Details

The implementation follows closely S. Hammarling's `dnrm2` function in LAPACK, which uses a onepass algorithm. The algorithm incorporates some form of scaling to prevent underflows. Higham (2002, p. 507 and 571) shows that the return value of the function can only overflow if  $\|\mathbf{x}\|_2$  exceeds the largest storable double value. See also Hanson and Hopkins (2017).

### Value

On return, `dat->dist` is overwritten with the Euclidean norm.

### References

Hanson, R.J., and T. Hopkins (2017). Remark on Algorithm 539: A Modern Fortran Reference Implementation for Carefully Computing the Euclidean Norm, *ACM Transactions on Mathematical Software* 44, Article 24.  
Higham, N.J. (2002). *Accuracy and Stability of Numerical Algorithms*, 2nd ed., Philadelphia: Society for Industrial and Applied Mathematics.

---

check\_matrix\_fullrank

*Internal function*

---

### Description

Check whether the array/ matrix `x` has full rank.

### Usage

```
static wbacon_error_type check_matrix_fullrank(double* restrict x, int p)
```

## Arguments

x                    data, double array[p, p].  
p                    dimension, [int].

## Details

See `methods.pdf` for the details.

## Dependency

LAPACK:dpotrf

## Value

The function returns a instance of `wbacon_error_type`:

- `WBACON_ERROR_OK` (i.e., no error),
- `WBACON_ERROR_NOT_POSITIVE_DEFINITE` or
- `WBACON_ERROR_RANK_DEFICIENT`.

---

<code>cutoffval</code>	<i>Internal function</i>
------------------------	--------------------------

---

## Description

Computes the correction factor used in the determination of the chi-squared quantile criterion; see `methods.pdf` for the details.

## Usage

```
static inline double cutoffval(int n, int k, int p)
```

## Arguments

k                    subset size, [int].  
n, p                  dimensions, [int].

## Value

Returns the correction factor.

## 5 wBACON\_reg [wbacon\_reg.c]

To offer functions with a clean interface, most of the functions use the typedef structs `regdata` (see `regdata.h`), `estimate`, and `workarray`.

---

wbdata	<i>Data</i> [typedef struct]
<hr/>	
<code>n</code>	dimension.
<code>p</code>	dimension.
<code>x</code>	pointer to the design matrix, <code>double array[n,p]</code> .
<code>wx</code>	pointer to a copy of the design matrix, <code>double array[n,p]</code> .
<code>y</code>	pointer to the response, <code>double array[n]</code> .
<code>wy</code>	pointer to a copy of the response, <code>double array[n]</code> .
<code>w</code>	pointer to the sampling weights, <code>double array[n]</code> .
<code>w_sqrt</code>	pointer to the square root of sampling weights, <code>double array[n]</code> .

**Note.** All slots of the instances of the typedef struct `regdata` are considered immutable, with one exception: `wx` and `wy` will be modified.

---

<code>estimate</code>	<i>Estimates</i> [typedef struct]
<hr/>	
<code>sigma</code>	regression scale, <code>double</code> .
<code>weight</code>	pointer to the weights, <code>double array[n]</code> .
<code>resid</code>	pointer to the residuals, <code>double array[n]</code> .
<code>beta</code>	pointer to the regression coefficient, <code>double array[p]</code> .
<code>dist</code>	pointer to the distances, <code>double array[n]</code> .
<code>L</code>	pointer to the Cholesky factor, <code>double array[p,p]</code> .
<code>xty</code>	pointer to $X^T y$ , <code>double array[p]</code> .

**Note.** The slots of the typedef struct `estimate` reflect the data and parameters of the model fit at the current stage. The instance `est` of `estimate` is updated iteratively.



---

<code>workarray</code>	<i>Work arrays</i> [typedef struct]
------------------------	-------------------------------------

---

<code>lwork</code>	determines the size of the array <code>dgles_work</code> , [int];
<code>iarray</code>	pointer to work array, <code>int array[n]</code> .
<code>work_n</code>	pointer to work array, <code>double array[n]</code> .
<code>work_np</code>	pointer to work array, <code>double array[np]</code> .
<code>work_pp</code>	pointer to work array, <code>double array[pp]</code> .
<code>degels_work</code>	pointer to <code>double array[lwork]</code> ; this array is required by LAPACK:dgels.

**Note.** The slots of the typedef struct `workarray` are not (and should not be) used to reference data over different function calls.

## Internal functions

---

<code>initial_reg</code>	<i>Internal function</i>
--------------------------	--------------------------

---

### Description

Initializes the least squares estimate.

### Usage

```
static wbacon_error_type initial_reg(regdata *dat, workarray *work,
    estimate *est, int* restrict subset, int *m, int *verbose)
```

### Arguments

<code>dat</code>	regression data, typedef struct <a href="#">regdata</a> .
<code>work</code>	work array, typedef struct <a href="#">workarray</a> .
<code>est</code>	estimates, typedef struct <a href="#">estimate</a> .
<code>subset</code>	subset, <code>int array[n]</code> ; with elements in the set $\{0,1\}$ , where 1 signifies that the element is in the subset.
<code>m</code>	size of the subset, [int].
<code>verbose</code>	toggle, [int], 1: verbose (i.e., the function prints detailed information to the console), 0: quiet.

## Details

The function's loop over the columns of the data matrix is parallelized using the OpenMP preprocessor directive

```
#pragma omp parallel for if(n > REG_OMP_MIN_SIZE)
```

where `REG_OMP_MIN_SIZE` is of size 1 000 000 and `n` is the number of rows and columns.

See `methods.pdf` for more details.

## Dependencies

`fitwls`, `psort_array`, and `compute_ti`

## Value

The function returns a `wbacon_error_type`: the return value is either `WBACON_ERROR_OK` (i.e., no error) or `WBACON_ERROR_RANK_DEFICIENT`.

On return, the following slots are overwritten:

<code>est-&gt;sigma</code>	regression scale
<code>est-&gt;resid</code>	residuals
<code>est-&gt;beta</code>	regression coefficients
<code>est-&gt;dist</code>	distances/ $t_i$ 's
<code>subset</code>	initial subset
<code>m</code>	size of <code>subset1</code>

---

<code>algorithm_4</code>	<i>Internal function</i>
--------------------------	--------------------------

---

## Description

Computes a weighted variant of Algorithm 4 of Billor et al. (2000).

## Usage

```
static wbacon_error_type algorithm_4(regdata *dat, workarray *work,  
    estimate *est, int* restrict subset0, int* restrict subset1, int *m,  
    int *verbose, int *collect)
```

## Arguments

<code>dat</code>	regression data, typedef struct <code>regdata</code> .
<code>work</code>	work array, typedef struct <code>workarray</code> .
<code>est</code>	estimates, typedef struct <code>estimate</code> .
<code>subset0</code>	subset, int array[n]; with elements in the set {0,1}, where 1 signifies that the element is in the subset.

<code>subset1</code>	subset, <code>int array[n]</code> ; with elements in the set $\{0,1\}$ , where 1 signifies that the element is in the subset.
<code>m</code>	size of the subset, <code>[int]</code> .
<code>verbose</code>	toggle, <code>[int]</code> , 1: verbose (i.e., the function prints detailed information to the console), 0: quiet.
<code>collect</code>	size of the initial basic subset, <code>[int]</code> .

## Details

See `methods.pdf` for more details.

## Dependencies

**internal:** `update_chol_xty`, `cholesky_reg`, `compute_ti`, and `select_subset`

**external:** BLAS: `dgemv`

## Value

The function returns a `wbacon_error_type` either `WBACON_ERROR_OK` (i.e., no error) or the error handed over by

- `update_chol_xty` or
- `compute_ti`.

On return, the following slots are overwritten:

<code>est-&gt;sigma</code>	regression scale
<code>est-&gt;resid</code>	residuals
<code>est-&gt;beta</code>	regression coefficients
<code>est-&gt;dist</code>	distances/ $t_i$ 's
<code>subset1</code>	final subset of Algorithm 4
<code>m</code>	size of <code>subset1</code>

---

<code>algorithm_5</code>	<i>Internal function</i>
--------------------------	--------------------------

---

## Description

Computes a weighted variant of Algorithm 5 of Billor et al. (2000).

## Usage

```
static wbacon_error_type algorithm_5(regdata *dat, workarray *work,
    estimate *est, int* restrict subset0, int* restrict subset1,
    double *alpha, int *m, int *maxiter, int *verbose)
```

## Arguments

<code>dat</code>	regression data, typedef struct <code>regdata</code> .
<code>work</code>	work array, typedef struct <code>workarray</code> .
<code>est</code>	estimates, typedef struct <code>estimate</code> .
<code>subset0</code>	subset, <code>int array[n]</code> ; with elements in the set $\{0,1\}$ , where 1 signifies that the element is in the subset.
<code>subset1</code>	subset, <code>int array[n]</code> ; with elements in the set $\{0,1\}$ , where 1 signifies that the element is in the subset.
<code>alpha</code>	defines the $1 - \alpha$ quantile of the Student $t$ -distribution.
<code>m</code>	size of the subset, <code>[int]</code> .
<code>maxiter</code>	maximum number of iterations, <code>[int]</code> .
<code>verbose</code>	toggle, <code>[int]</code> , 1: verbose (i.e., the function prints detailed information to the console), 0: quiet.

## Details

See `methods.pdf` for more details.

## Dependencies

**internal:** `fitwls` and `compute_ti`

**external:** `Rmath.h:qt`

## Value

The function returns a `wbacon_error_type`: the return value is either the error handed over by `compute_ti` or

- `WBACON_ERROR_OK` (i.e., no error) or
- `WBACON_ERROR_CONVERGENCE_FAILURE` if it does not converge in `maxiter` iterations.

On return, the following slots are overwritten:

<code>est-&gt;sigma</code>	regression scale
<code>est-&gt;resid</code>	residuals
<code>est-&gt;beta</code>	regression coefficients
<code>est-&gt;dist</code>	distances/ $t_i$ 's
<code>subset1</code>	final subset of outlier-free data
<code>m</code>	size of <code>subset1</code>
<code>maxiter</code>	number of iterations required

---

select\_subset

*Internal function*

---

### Description

Selects the smallest  $1..m$  observations in **x** into the **subset**.

### Usage

```
static void select_subset(double* restrict x, int* restrict iarray,  
    int* restrict subset, int *m, int *n)
```

### Arguments

<b>x</b>	data, double array[n].
<b>iarray</b>	work array, int array[n].
<b>subset</b>	subset, int array[n]; with elements in the set $\{0,1\}$ , where 1 signifies that the element is in the subset.
<b>m</b>	size of the subset, [int].

### Details

The function calls [psort\\_array](#) to (partially) sort the elements of **x** in ascending order. Then, the smallest  $m$  observations are selected into **subset**.

### Value

On return, **subset** is overwritten with the generated subset.

---

compute\_ti

*Internal function*

---

### Description

Compute the  $t_i$ 's (**tis**) of Billor et al. (2000, p. 288).

### Usage

```
static wbacon_error_type compute_ti(regdata *dat, workarray *work,  
    estimate *est, int* restrict subset, int *m, double* restrict tis)
```

## Arguments

<code>dat</code>	regression data, typedef struct <a href="#">regdata</a> .
<code>work</code>	work array, typedef struct <a href="#">workarray</a> .
<code>est</code>	estimates, typedef struct <a href="#">estimate</a> .
<code>subset</code>	subset, <code>int array[n]</code> ; with elements in the set $\{0,1\}$ , where 1 signifies that the element is in the subset.
<code>m</code>	size of the subset, <code>[int]</code> .
<code>tis</code>	double array[n].

## Details

The function calls [hat\\_matrix](#) to compute the diagonal elements of the “hat” matrix and computes the regression scale. Then, it computes the  $t_i$ ’s.

## Dependency

[hat\\_matrix](#)

## Value

The function’s loop over the columns of the hat matrix is parallelized using the OpenMP preprocessor directive

```
#pragma omp parallel for if(n > REG_OMP_MIN_SIZE)
```

where `REG_OMP_MIN_SIZE` is of size 1 000 000 and `n` is the number of rows and columns.

The function returns a [wbacon\\_error\\_type](#): the return value is either `WBACON_ERROR_OK` (i.e., no error) or the error handed over by [hat\\_matrix](#).

On return, `tis` is overwritten with the computed  $t_i$ ’s.

---

<code>cholesky_reg</code>
---------------------------

---

*Internal function*

## Description

Compute the least squares estimate using the Cholesky factor  $L$  and the matrix  $X^T y$ .

## Usage

```
static inline void cholesky_reg(double *L, double *x, double *xty,  
    double *beta, int *n, int *p)
```

## Arguments

L	Cholesky factor, double array[p,p].
x	data, double array[n].
xy	$X^T y$ double array[p].
beta	regression coefficients double array[p].
n	dimension.
p	dimension.

## Value

On return, **beta** is overwritten with the updated least squares estimate.

---

hat_matrix	<i>Internal function</i>
------------	--------------------------

---

## Description

Computes the diagonal elements of the extended “hat” matrix.

## Usage

```
static inline wbacon_error_type hat_matrix(regdata *dat, workarray *work,  
double* restrict L, double* restrict hat)
```

## Arguments

dat	regression data, typedef struct <a href="#">regdata</a> .
work	work array, typedef struct <a href="#">workarray</a> .
L	Cholesky factor, double array[p,p].
hat	hat matrix, double array[n].

## Details

The diagonal elements of the “hat” matrix are computed for the observations in the subset. For the elements not in the subset, an “extended hat” matrix is computed.

## Value

The function returns a [wbacon\\_error\\_type](#): the return value is either WBACON\_ERROR\_OK (i.e., no error) or WBACON\_ERROR\_TRIANG\_MAT\_SINGULAR when the triangular matrix is singular.

On return, **hat** is overwritten with the diagonal elements of the “hat” matrix.

---

update_chol_xty	<i>Internal function</i>
-----------------	--------------------------

---

## Description

The function up- and downdates the Cholesky factor  $L$  and the matrix product by comparing the two sets `subset0` and `subset1`.

## Usage

```
static wbacon_error_type update_chol_xty(regdata *dat, workarray *work,  
    estimate *est, int* restrict subset0, int* restrict subset1, int *verbose)
```

## Arguments

<code>dat</code>	regression data, typedef struct <a href="#">regdata</a> .
<code>work</code>	work array, typedef struct <a href="#">workarray</a> .
<code>est</code>	estimates, typedef struct <a href="#">estimate</a> .
<code>subset0</code>	subset, <code>int array[n]</code> ; with elements in the set $\{0,1\}$ , where 1 signifies that the element is in the subset.
<code>subset1</code>	subset, <code>int array[n]</code> ; with elements in the set $\{0,1\}$ , where 1 signifies that the element is in the subset.
<code>m</code>	size of the <code>subset1</code> , <code>[int]</code> .
<code>verbose</code>	toggle, <code>[int]</code> , 1: verbose (i.e., the function prints detailed information to the console), 0: quiet.

## Details

The function `update_chol_xty` compares the sets `subset0` and `subset1`. For all elements that are in `subset0` but not in `subset1`, it calls [chol\\_downdate](#). For all elements that are not in `subset0` but in `subset1`, it calls [chol\\_update](#).

## Value

The function returns a [wbacon\\_error\\_type](#): the return value is either `WBACON_ERROR_OK` (i.e., no error) or the error handed over by [chol\\_downdate](#).

On return, `L` and `xty` are overwritten with their updated values.



---

chol_update	<i>Internal function</i>
-------------	--------------------------

---

### Description

Rank-one update of the Cholesky factor.

### Usage

```
static inline void chol_update(double* restrict L, double* restrict u, int p)
```

### Arguments

L	Cholesky factor, double array[p,p].
u	rank-one update for L, double array[p].
p	dimension.

### Details

This function computes a one rank-one update of the Cholesky factor.

### Value

On return, L is overwritten by its updated value.

---

chol_downdate	<i>Internal function</i>
---------------	--------------------------

---

### Description

Rank-one downdate of the Cholesky factor.

### Usage

```
static inline wbacon_error_type chol_downdate(double* restrict L,  
double* restrict u, int p)
```

### Arguments

L	Cholesky factor, double array[p,p].
u	rank-one downdate for L, double array[p].
p	dimension.

### Details

This function computes a one rank-one downdate of the Cholesky factor. The attempt to downdate may break down if the Cholesky factor becomes/is not positive definite. In this case, an error is returned.

**Value**

The function returns a `wbacon_error_type`: the return value is either `WBACON_ERROR_OK` (i.e., no error) or `WBACON_ERROR_RANK_DEFICIENT`.

On return, `L` is overwritten by its downdated value.

## 6 Weighted least squares [fitwls.c]

---

fitwls

*Weighted least squares*

---

### Description

Returns the least squares estimate, the matrices Q and R of the QR factorization, the estimate of regression scale, and the residuals of a weighted linear regression.

### Usage

```
int fitwls(regdata *dat, estimate* est, int* restrict subset,
           double* restrict work_dgels, int lwork)
```

### Arguments

<code>dat</code>	regression data, typedef struct <a href="#">regdata</a> .
<code>est</code>	estimates, typedef struct <a href="#">estimate</a> .
<code>subset</code>	subset, <code>int array[n]</code> ; with elements in the set $\{0, 1\}$ , where 1 signifies that the element is in the subset.
<code>work_dgels</code>	work array, <code>double array[lwork]</code> .
<code>lwork</code>	dimension of array <code>work</code> , <code>[int]</code> ; if <code>lwork&lt;1</code> , the function determines and returns the optimal

### Details

The regression coefficients are computed with the LAPACK:dgels subroutine using a QR factorization of the weighted design matrix.

The function's loop over the columns of the hat matrix is parallelized using the OpenMP preprocessor directive

```
#pragma omp parallel for if(n > FITLS_OMP_MIN_SIZE)
```

where `FITWLS_OMP_MIN_SIZE` is of size 1 000 000 and `n` is the number of rows.

### Dependencies

LAPACK:dgels and BLAS:dgemv

### Value

The function `fitwls` returns its status `info`; if successful, `info=0`; otherwise the computation failed. On return, the following slots of `struct estimate est` are overwritten:

<code>beta</code>	regression coefficients
<code>sigma</code>	regression scale
<code>resid</code>	residuals

and, the following slots of `struct regdata dat` are overwritten:

`wx`                    the QR factorization as returned by the subroutine `LAPACK:dgeqrf`

## 7 Weighted quantile [wquantile.c]

The following functions are documented in this section:

- [wquantile\\_noalloc](#)
- [wselect0](#)
- some internal functions

The source file `wquantile.c` defines two macros:

`_n_quickselect`      threshold to switch from insertion sort to a weighted variant of the Select (FIND, quickselect) algorithm, default: 40 (i.e., for samples smaller than 40, insertion sort is used).

`_n_ninther`      threshold for choosing the pivotal element, default: 50; for samples smaller than 50, the pivot is chosen by the median-of-three; for larger samples, Tukey's ninther is used.

(Weighted) quicksort/ Select(FIND, quickselect) method is efficient for large arrays. But its overhead can be severe for small arrays; hence, we use insertion sort for small arrays; cf. Bentley and McIlroy (1993). We have determined the numerical values by a series of benchmark tests with [Google benchmark](#) on an ordinary laptop computer (Intel i7 8th generation).

---

<code>wquantile_noalloc</code>	<i>Weighted quantile without memory allocation</i>
--------------------------------	--

---

### Description

The same as `wquantile` but without memory allocation.

### Usage

```
void wquantile_noalloc(double *array, double *weights, double *work, int *n,
    double *prob, double *result)
```

### Arguments

<code>array</code>	data, double array[n].
<code>weights</code>	sampling weights, double array[n].
<code>workwork</code>	work array, double array[2*n].
<code>n</code>	dimension, [int].
<code>prob</code>	probability that defines the quantile, such that $0 \leq \text{prob} \leq 1$ , [double].
<code>result</code>	quantile, [double].

### Details

See [wquantile](#).

## Dependencies

[wselect0](#) and [wquant0](#)

## Value

On return, `result` is overwritten with the weighted quantile.

---

<code>wselect0</code>	<i>Selection of the <math>k</math>-th largest element (<math>k</math>-th order statistic)</i>
-----------------------	---

---

## Description

Returns the  $k$ -th largest element ( $k$ -th order statistic); sampling weights allowed.

## Usage

```
void wselect0(double *array, double *weights, int lo, int hi, int k)
```

## Arguments

<code>array</code>	data, double array[lo..hi].
<code>weights</code>	sampling weights, double array[n].
<code>lo</code>	lower boundary of arrays, [int].
<code>hi</code>	upper boundary of arrays, [int].
<code>k</code>	$k$ -th largest element, such that $lo \leq k \leq hi$ , [int].

## Details

See [wquantile](#).

## Dependency

[partition\\_3way](#)

## Value

On return, element `array[k]` is in its final sorted position; `weights` is sorted along with `array`.

---

`insertionselect`

*Internal function*

---

### Description

Computes the weighted quantile by sorting all elements in `array` in ascending order (using insertion sort). For small arrays, this can be considerably faster than quicksort.

### Usage

```
double insertionselect(double *array, double *weights, int lo, int hi,
    double prob)
```

### Arguments

<code>array</code>	data, <code>double array[n]</code> .
<code>weights</code>	sampling weights, <code>double array[n]</code> .
<code>lo</code>	lower boundary of arrays, <code>[int]</code> .
<code>hi</code>	upper boundary of arrays, <code>[int]</code> .
<code>prob</code>	probability that defines the quantile, <code>double</code> , such that $0 \leq \text{prob} \leq 1$ .

### Dependency

[swap2](#)

### Value

On return, element `array[k]` is in its final sorted position; `weights` is sorted along with `array`.

## Internal functions

---

wquant0

*Internal function*

---

### Description

Workhorse function that computes the weighted quantile recursively; see [wquantile](#).

### Usage

```
void wquant0(double *array, double *weights, double sum_w, int lo, int hi,
             double prob, double *result)
```

### Dependencies

[insertionselect](#) and [partition\\_3way](#)

---

partition\_3way

*Internal function*

---

### Description

3-way partitioning scheme of Bentley and McIlroy's (1993) with weights.

### Usage

```
void partition_3way(double *array, double *weights, int lo, int hi, int *i,
                   int *j)
```

### Dependency

[swap2](#)

### References

Bentley, J.L. and D.M. McIlroy (1993). Engineering a Sort Function, *Software - Practice and Experience* 23, pp. 1249-1265.



---

choose_pivot	<i>Internal function</i>
--------------	--------------------------

---

### Description

Choose pivotal element: for arrays of size  $< \_n\_ninther$ , the median of three is taken as pivotal element, otherwise Tukey's ninther is used; see e.g. Bentley and McIlroy (1993).

### Usage

```
static inline int choose_pivot(double *array, int lo, int hi)
```

### Dependency

[med3](#)

### References

Bentley, J.L. and D.M. McIlroy (1993). Engineering a Sort Function, *Software - Practice and Experience* 23, pp. 1249-1265.

---

swap2	<i>Internal function</i>
-------	--------------------------

---

### Description

Two elements in `array` are swapped (and the corresponding elements in array `weights` are also swapped).

### Usage

```
static inline void swap2(double *array, double *weights, int i, int j)
```

---

med3	<i>Internal function</i>
------	--------------------------

---

### Description

Median-of-three (but without swaps); see e.g. Sedgewick (1997, Chap. 7.5).

### Usage

```
static inline double med3(double *array, int i, int j, int k)
```

### References

Sedgewick, R. (1997). *Algorithms in C, Parts 1-4, Fundamentals, Data Structures, Sorting, and Searching*, Addison-Wesley Longman Publishing Co., Inc., 3rd ed.

## 8 Partial sorting [partial\_sort.c]

---

`psort_array`

*Partially sort an array with index*

---

### Description

Partially sorts array `x` in ascending order; the accompanying `int` array (called `index`) is sorted along with the array.

### Usage

```
void psort_array(double *x, int *index, int n, int k)
```

### Arguments

<code>x</code>	data, <code>double</code> array[n].
<code>index</code>	<code>index</code> , <code>int</code> array[n]; the array will be overwritten.
<code>n</code>	dimension, [int].
<code>k</code>	value that determines the upper array boundary of <code>x[0..k]</code> , where $k \leq n$ , [int].

### Details

This function is a wrapper for the function [partial\\_sort\\_with\\_index](#).

The function takes care of generating the array `index`. The elements of this array will set up to be `0..(n-1)`.

### Dependency

[partial\\_sort\\_with\\_index](#)

### Value

On return, the array `x[0..k]` is partially sorted in ascending order; the array `index[0..k]` is sorted along with `x[0..k]`.

### Internal functions

Most of the internal functions which are called from [psort\\_array](#) are identical with the internal functions of [wselect0](#). Therefore, we do not document separately.

---

`partial_sort_with_index`

*Internal function*

---

## Description

Partially sorts a array `x` in ascending order; the accompanying `int` array (called `index`) is sorted along with the array.

## Usage

```
void partial_sort_with_index(double *x, int *index, int *lo, int *hi, int *k)
```

## Arguments

<code>x</code>	data, <code>double</code> array [ <code>lo..hi</code> ].
<code>index</code>	<code>index</code> , <code>int</code> array [ <code>lo..hi</code> ]; the array will be overwritten.
<code>lo, hi</code>	indices, [ <code>int</code> ], usually <code>lo = 0</code> and <code>hi = n - 1</code> .
<code>k</code>	an [ <code>int</code> ] in <code>lo..hi</code> ; determines the <code>k</code> -th largest element up to which <code>x</code> is to be sorted.

## Details

The array `index` must be generated by the caller.

## Value

On return, the elements `lo..k` in the array `x[lo..hi]` are partially sorted in ascending order; the array `index[lo..k]` is sorted along with `x[lo..k]`.