

C++ Functions in Maxliklib Library

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Abstract

The functions in the maxliklib repository are described. Arguments and their definitions are specified, and dependencies of functions are stated.

Keywords: Maximization procedures, quadrature procedures, maximum likelihood

The maxliklib repository consists of C++ functions helpful in estimation related to maximum likelihood. The functions should be appropriate for C++11. Except if otherwise stated, functions rely on the Armadillo library (Sanderson & Curtin, 2016, 2018) at <http://arma.sourceforge.net>. The following functions are found in the library:

- `adapt.cpp`
- `adaptv.cpp`
- `cloglog.cpp`
- `cloglog1.cpp`
- `conjgrad.cpp`
- `cumlogit.cpp`
- `cumlogit1.cpp`
- `cumloglog.cpp`
- `cumloglog1.cpp`

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- `cumprobit.cpp`
- `cumprobit1.cpp`
- `genfact.cpp`
- `genprods.cpp`
- `gradascent.cpp`
- `gradlogit.cpp`
- `gradlogit1.cpp`
- `gradloglog.cpp`
- `gradloglog1.cpp`
- `gradprobit.cpp`
- `gradprobit1.cpp`
- `gumbel.cpp`
- `gumbel1.cpp`
- `hermcoeff.cpp`
- `hermpoly.cpp`
- `hermpw.cpp`
- `logistic.cpp`
- `logistic1.cpp`
- `logit.cpp`
- `logit1.cpp`
- `logmean.cpp`
- `logmean1.cpp`
- `lw.cpp`
- `lwm.cpp`
- `maxflvvar.cpp`

- maxf2vvar.cpp
- maxlin2.cpp
- maxlin.cpp
- multlogit.cpp
- multlogit1.cpp
- modit.cpp
- normal.cpp
- normal1.cpp
- nrv.cpp
- probit.cpp
- probit1.cpp
- rebound.cpp

Distributions of Sums of Independent Multinomial Variables

The functions in this section implement a modified and generalized version of the Lord-Wingsky algorithm (Lord & Wingsky, 1984; Thissen et al., 1995). The numerical procedures and their rationale are discussed in lw.pdf.

lw.cpp

The function lw.cpp finds the probability mass function of the sum S of mutually independent Bernoulli random variables X_j , $0 \leq j < n$. The function declaration is

vec lw(double & c, vec & p).

The vector p has dimension n and has positive elements that are less than 1. For $0 \leq j < n$, the probability that $X_j = 1$ is element j of p . The variable c is normally a small positive number used as in lw.pdf to remove very small probabilities from consideration in order to speed computation. If c is not positive, then the modified Lord-Wingsky algorithm used by lw.cpp reduces to the conventional algorithm. The probability mass function is provided by lw , a vector with $n + 1$ elements. For $0 \leq k \leq n$, element k of lw is the probability that $S = k$.

lwm.cpp

The function `lwm.cpp` finds the probability mass function of the sum S of n mutually independent random variables X_j , $0 \leq j < n$ with integer values from 0 to $I_j - 1$ for an integer $I_j > 1$. The function declaration is

vec lwm(double & cc, int & n, vec p[]).

The array p of vectors has n members. For $0 \leq j < n$, member j of p is the vector $p[j]$ with I_j nonnegative elements. The sum of these elements is 1, and element k , $0 \leq k < I_j$, of $p[j]$ is the probability that $X_j = k$. The probability mass function is provided by lwm , a vector with $K = 1 + \sum_{j=1}^n (I_j - 1)$ elements. Element k of lwm , $0 \leq k < K$, is the probability that $S = k$. The variable c is normally a small positive number used as in `lw.pdf` to remove very small probabilities from consideration in order to speed computation. If c is not positive, then the modified algorithm used by `lwm.cpp` reduces to the conventional generalization of the Lord-Wingersky algorithm to sums of independent multinomial variables.

Tools for Line Searches

The functions in this section facilitate line searches during function maximization. Throughout discussions in this section and in Functions related to the Newton-Raphson algorithm and Functions Related to Gradient Methods, the theoretical background is provided in `convergence.pdf`. For some positive integer p and nonempty open convex set O of p -dimensional vectors, a continuously differentiable real function $f.value$ on O is to be maximized by an iterative algorithm with a starting value in O . It is assumed that, for some real a , the set A of members of O at which $f.value$ is at least a is closed and bounded, and the sets A_0 of members of O at which $f.value$ exceeds a is nonempty. The function $f.value$ is assumed to be strictly pseudoconcave on A_0 . The starting values for algorithms are assumed to be in A_0 . The convention is adopted that $f.value$ has value NaN at any p -dimensional vector not in O .

modit.cpp

The function `modit.cpp` truncates an iteration to conform to limits on step size and bounds in the case of a real function of one variable with a unique critical point and a limit of $-\infty$ as the absolute value of the function argument approaches ∞ . The function declaration is

*double modit(const double & eta, const double & alpha0, const double & alpha1,
const double & stepmax, const double & lower, const double & upper).*

Here *eta* is a positive multiplier less than 1, *alpha0* is the previous location, *alpha1* is the proposed new location, *stepmax* is the positive limit on step size, *lower* is the lower bound, and *upper* is the upper bound. It is assumed that *alpha0* and *alpha1* are different. The function returns a value *modit* that is normally *alpha1*; however, if *alpha1* exceeds *alpha0*, then *modit* is truncated above so that it does not exceed the minimum of *alpha0+stepmax* and *alpha0+eta(upper-alpha0)*, while if *alpha1* is less than *alpha0*, then *modit* is truncated below so that it is at least the maximum of *alpha0-stepmax* and *alpha0+eta(lower-alpha0)*.

rebound.cpp

The function `rebound.cpp` updates the lower and upper bounds for maximization of a differentiable real function on the real line with a unique critical point and a limit of $-\infty$ as the absolute value of the function argument approaches ∞ . The function declaration is

```
void rebound(const double & y,const double & der,double & lower,double & upper).
```

Here *y* is the current location, *der* is the function derivative at *y*, *lower* is the lower bound, and *upper* is the upper bound. It is assumed that *der* is not 0. If *der* is positive, *lower* is changed to *y*. If *der* is negative, *upper* is changed to *y*.

Functions related to the Newton-Raphson algorithm

In this section, functions are discussed that are related to the Newton-Raphson algorithm. It should be noted that references to function values, gradients, and Hessian matrices do not address computational methods. In fact, the function values, gradients, and Hessian matrices employed may be approximations derived by numerical differentiation or large-sample approximations. In this section, *f.value* is assumed to be twice continuously differentiable.

maxlin2.cpp

The function `maxlin2.cpp` performs a line search based on the Newton-Raphson algorithm. The gradient of *f.value* is *f.grad*. The Hessian matrix of *f.value* is *f.hess*. The function declaration is

```
maxf2v maxlin2(const paramnr & nrparams, const vec & v,  
maxf2v & vary0, function<f2v(vec)>f).
```

The struct *maxf2v* has the definition

```
struct maxf2v{vec locmax; double max; vec grad; mat hess;};
```

The struct *paramnr* has the definition

```
struct paramnr{int maxit; int maxits; double eta; double gamma1; double gamma2;
double kappa; double tol;};
```

The struct *f2v* has the definition

```
struct f2v{double value; vec grad;};
```

The gradient of *f.value* is *f.grad*. The Hessian matrix is *f.hess*. Parameters used are defined in *nrparams*. The maximum number of primary iterations used in *nrv.cpp* is *nrparams.maxit*. The maximum number of secondary iterations per main iteration used in the line search is *nrparams.maxits*. The maximum fraction of a step toward a boundary is *nrparams.eta*. For secondary iterations, the improvement check is *nrparams.gamma1* < 1. The value of *nrparams.gamma2* is used in *nrv.cpp* to ensure that the direction of *v* is satisfactory. The largest permitted step length is *nrparams.kappa* > 0. The convergence criterion for primary iterations is *nrparams.tol*.

Information concerning the starting point of the line search is in *vy0*, while *v* provides the starting direction. The initial location is *vy0.locmax*, the value of *f.value* at *vy0.locmax* is *vy0.max*, the gradient of *f.value* at *vy0.locmax* is *vy0.grad*, and the Hessian matrix of *f.value* at *vy0.locmax* is *vy0.hess*. It is assumed that the inner product of *v* and *vy0.grad* is positive. The returned value includes the approximate location *maxlin2.locmax* of the maximum value of *f.value* at a point on the ray with origin *vy0.locmax* that has direction *v*. In addition, *maxlin2.max* is the value of *f.value* at *maxlin2.locmax*, *maxlin2.grad* is the gradient of *f.value* at *maxlin2.locmax*, and *maxlin2.hess* is the Hessian matrix of *f.value* at *maxlin2.locmax*.

The function *maxlin2.cpp* uses *maxf2vvar.cpp*, *modit.cpp*, and *rebound.cpp*.

maxf2vvar.cpp

The function *maxf2vvar.cpp* is used to combine information on a location and on a functions value, gradient, and Hessian matrix at the location. The function *maxf2vvar.cpp* has declaration

```
maxf2v maxf2vvar(const vec & y,const f2v & fy);
```

The structs *f2v* and *maxf2v* are defined as in *maxlin2.cpp*. The returned value *maxf2vvar.locmax* is *y*, while *maxf2vvar.max* is the value of *f.value* at *y*, *maxf2vvar.gad* is the gradient of *f.value* at *y*, and *maxf2vvar.hess* is the Hessian matrix of *f.value* at *y*.

nrv.cpp

The function *nrv.cpp* applies a modified version of the Newton-Raphson algorithm to maximization of *f.value*. The function *nrv.cpp* has declaration

```
maxf2v nrv(const paramnr & nrparams, const vec & start, function<f2v(vec)> f).
```

The structs *f2v*, *maxf2v*, and *paramnr* are defined as in *maxlin2.cpp* and *maxf2vvar.cpp*. In *convergence.pdf*, γ_1 corresponds to *nrparams.gamma1*, γ_2 corresponds to *nrparams.gamma2*, and κ corresponds to *nrparams.kappa*. The starting vector *start* must be in *O*. Iterations cease once the value of *f.value* increases by less than *nrparams.tol* after a primary iteration.

The function *nrv.cpp* uses *maxf2vvar.cpp*, *maxlin2.cpp*, *modit.cpp*, and *rebound.cpp*.

Functions Related to Gradient Methods

In this section, functions are considered based on gradient-based methods.

conjgrad.cpp

The function *conjgrad.cpp* implements a conjugate gradient algorithm for maximization of *f.value*. The function declaration is

```
maxf1v conjgrad(const paramga & gaparams,  
const vec & start, const function<f1v(vec)> f).
```

The definition of *maxf1v* is

```
struct maxf1v{vec locmax; double max; vec grad;};.
```

The definition of *paramga* is

```
struct paramga{int maxit; int maxits; function<double(vec)> c; double eta;  
double gamma1; double gamma2; double kappa; double tol;};.
```

The definition of *f1v* is

```
struct f1v{double value; vec grad;};.
```

The starting vector is *start*. The maximum number of main iterations is *gaparams.maxit*. The maximum number of secondary iterations per main iteration is *gaparams.maxits*. The function *gaparams.c* specifies the step size for numerical differentiation of the gradient *f.grad* of *f.value*. It must be the case that, for any vector

y in the domain of $f.value$, $y+c(y)$ is also in that domain. The maximum fraction of a step toward a boundary is $gaparams.eta$. In `convergence.pdf`, γ_1 corresponds to $gaparams.gamma1$, γ_2 corresponds to $gaparams.gamma2$, and κ corresponds to $gaparams.kappa$. Iterations cease once the value of $f.value$ increases by less than $gaparams.tol$ after a primary iteration.

The function `conjgrad.cpp` uses `maxflvvar.cpp`, `maxlin.cpp`, `modit.cpp`, and `rebound.cpp`.

gradascent.cpp

The function `gradascent.cpp` uses a gradient-ascent algorithm for maximization of $f.value$. The function declaration for `gradient.cpp` is

```
maxflv gradascent(const paramga & gaparams,  
const vec & start, const function<flv(vec)> f).
```

The definitions of `gaparams`, `paramga`, `flv`, and f are the same as in `conjgrad.cpp`, and `maxflvvar.cpp`, `maxlin.cpp`, `modit.cpp`, and `rebound.cpp` are used.

maxflvvar.cpp

The function `maxflvvar.cpp` is used to combine information on a location and on a functions value and gradient at the location. The function `maxflvvar.cpp` has declaration

```
maxflv maxflvvar(const vec & y,const flv & fy).
```

The structs `flv` and `maxflv` are defined as in `conjgrad.cpp`. The returned value `maxflvvar.locmax` is y , while `maxflvvar.max` is the value of $f.value$ at y and `maxflvar.gad` is the gradient of $f.value$ at y .

maxlin.cpp

The function `maxlin.cpp` uses numerical differentiation to provide an approximate Newton-Raphson procedure for a line search. The function declaration is

```
maxflv maxlin(const paramga & gaparams, const vec & v,  
maxflv & vary0, function<flv(vec)>f).
```

The structs `maxflv`, `paramga`, and `flv` are defined as in `conjgrad.cpp`. The functions `maxflvvar.cpp`, `modit.cpp`, and `rebound.cpp` are all used.

Log-likelihood Components

In this section, components of log-likelihood functions are provided. For a positive integer n and an observation i , $0 \leq i < n$, positive integers r_i and q_i are given. The component of the log likelihood for observation i involves the predicted random vector \mathbf{Y}_i in a nonempty subset \mathcal{Y}_i of r_i -dimensional vectors and the q_i by p predicting matrix \mathbf{X}_i in a nonempty set \mathcal{X}_i . For some positive real numbers w_i , $0 \leq i < n$, and some real functions v_i on \mathcal{Y}_i , the log-likelihood function under study has the form

$$\ell(\gamma) = \sum_{i=0}^{n-1} w_i(\mathbf{Y}_i)[v_i(\mathbf{Y}_i) + \ell_i(\mathbf{X}_i\gamma; \mathbf{Y}_i)] \quad (1)$$

for γ in O . For $0 \leq i < n$, w_i is a sampling weight associated with observation i . For a nonempty open convex set O_i of q_i -dimensional vectors, $\ell_i(\cdot; \mathbf{y})$ is a twice continuously differentiable real function on O_i for all \mathbf{y} in \mathcal{Y}_i . For any γ in O and \mathbf{X} in \mathcal{X}_i , $\mathbf{X}\gamma$ is in O_i . If \mathcal{Y}_i is finite or countably infinite and β is in O_i , then 1 is the sum of the $\exp(v_i(\mathbf{y}) + \ell_i(\beta; \mathbf{y}))$ over \mathbf{y} in \mathcal{Y}_i and some random vector \mathbf{Y} equals \mathbf{y} with probability $\exp(v_i(\mathbf{y}) + \ell_i(\beta; \mathbf{y}))$ for each \mathbf{y} in \mathcal{Y}_i . If \mathcal{Y}_i is a convex set with a nonempty interior and β is in O_i , then the integral of $\exp(v_i(\mathbf{y}) + \ell_i(\beta; \mathbf{y}))$ over \mathbf{y} in \mathcal{Y}_i is 1 and a continuous random vector \mathbf{Y}_i has density $\exp(v_i(\mathbf{y}) + \ell_i(\beta; \mathbf{y}))$ at \mathbf{y} in \mathcal{Y}_i . The gradient function of $\ell_i(\cdot; \mathbf{y})$ is $\nabla \ell_i(\cdot; \mathbf{y})$ and the corresponding Hessian matrix is $\nabla^2 \ell_i(\cdot; \mathbf{y})$. It follows that the gradient of ℓ at γ is

$$\nabla \ell(\gamma) = \sum_{i=0}^{n-1} w_i \mathbf{X}_i^T \nabla \ell_i(\mathbf{X}_i\gamma; \mathbf{Y}_i), \quad (2)$$

and the Hessian matrix of ℓ at γ is

$$\nabla^2 \ell(\gamma) = \sum_{i=0}^{n-1} w_i \mathbf{X}_i^T \nabla^2 \ell_i(\mathbf{X}_i\gamma; \mathbf{Y}_i) \mathbf{X}_i. \quad (3)$$

Many standard cases of $\ell_i(\cdot; \mathbf{y})$ exist, some of which are examined in the literature on survival analysis (Cox, 1972; Kalbfleisch & Prentice, 2002), generalized linear models (McCullagh & Nelder, 1989), multivariate analysis (Anderson, 2003), and discrete choice (McFadden, 1973). It should be noted that names for models are somewhat variable in different references, especially for graded and cumulative cases. The following C++ functions are employed for common examples. The structs `flv` and `f2v` are defined as in `maxlin2.cpp` and `maxlin.cpp`. Unless otherwise noted, $v_i(\mathbf{y})$ is equal to 0 for all \mathbf{y} in \mathcal{Y}_i .

cloglog.cpp

The function `cloglog.cpp` computes the function value, gradient, and Hessian matrix associated with a complementary log-log transformation. Let G be the cumulative distribution function with $G(y) = 1 - \exp(-\exp(y))$ for real y . Thus G is

the cumulative distribution function of $-Y$ if Y has a standard Gumbel distribution with distribution function $\exp(-\exp(-y))$ at real y . The inverse function G^{-1} of G is the complementary log-log transformation with $G^{-1}(x) = \log(-\log(1-x))$ for real x such that $0 < x < 1$. In this case, $r_i = 1$, \mathcal{Y}_i is the set of one-dimensional vectors \mathbf{y} such that $y(0)$ is 0 or 1, $q_i = 1$, O_i is the set of all one-dimensional vectors. For β in O_i and \mathbf{y} in \mathcal{Y}_i , $\ell_i(\beta; \mathbf{y}) = \log(1 - G(\beta(0)))$ if $y(0) = 0$, and $\ell_i(\beta; \mathbf{y}) = \log(G(\beta(0)))$ if $y(0) = 1$. The function declaration is

f2v cloglog(ivec & y, vec & beta).

The function *cloglog.value* is $\ell_i(\beta; \mathbf{y})$ if y is \mathbf{y} and *beta* is β .

cloglog1.cpp

The function *cloglog1.cpp* computes the function value and gradient associated with a complementary log-log transformation. The definitions of r_i , q_i , O_i , \mathcal{Y}_i , and $\ell_i(\beta; \mathbf{y})$ are the same as in *cloglog.cpp*. The function declaration is

f1v cloglog1(ivec & y, vec & beta).

The function *cloglog1.value* is $\ell_i(\beta; \mathbf{y})$ if y is \mathbf{y} and *beta* is β .

cumlogit.cpp

The function *cumlogit.cpp* computes the function value, gradient, and Hessian matrix associated with a cumulative logit transformation. Let L be the distribution function of a standard logistic random variable, so that $L(y) = 1/[1 + \exp(-y)]$ for real y and the inverse function L^{-1} of L is the logit transformation with $L^{-1}(x) = \log(x/(1-x))$ for real x such that $0 < x < 1$. In this case, $r_i = 1$, $q_i \geq 1$, \mathcal{Y}_i is the set of one-dimensional vectors \mathbf{y} such that $y(0)$ is a nonnegative integer no greater than q_i , $q_i = n_i - 1$, and O_i is the set of all vectors of dimension q_i . For β in O_i and \mathbf{y} in \mathcal{Y}_i ,

$$\ell_i(\beta; \mathbf{y}) = \begin{cases} \log(1 - L(\beta(y(0)))), & y(0) = 0, \\ \log(1 - L(\beta(y(0)))) + \sum_{i=0}^{y(0)-1} \log(L(\beta(i))), & 0 < y(0) < q_i, \\ \sum_{i=0}^{y(0)-1} \log(L(\beta(i))), & y(0) = nqi. \end{cases} \quad (4)$$

The function declaration is

f2v cumlogit(ivec & y, vec & beta).

The function *cumlogit.value* is $\ell_i(\beta; \mathbf{y})$ if y is \mathbf{y} and *beta* is β .

cumlogit1.cpp

The function `cumlogit1.cpp` computes the function value and gradient associated with a cumulative logit transformation. As in `cumlogit.cpp`, r_i , q_i , O_i , and \mathcal{Y}_i are defined as in `cumlogit.cpp`, and Equation 4 holds for β in O_i and \mathbf{y} in \mathcal{Y}_i . The function declaration is

f1v cumlogit1(ivec & y, vec & beta).

The function `cumlogit1.value` is $\ell_i(\beta; y)$ if y is \mathbf{y} and `beta` is β .

cumloglog.cpp

The function `cumloglog.cpp` computes the function value, gradient, and Hessian matrix associated with a cumulative complementary log-log transformation. Define G as in `cloglog.cpp`. Then r_i , q_i , O_i , and \mathcal{Y}_i are defined as in `cumlogit.cpp`, and, for β in O_i and \mathbf{y} in \mathcal{Y}_i ,

$$\ell_i(\beta; \mathbf{y}) = \begin{cases} \log(1 - G(\beta(y(0)))), & y(0) = 0, \\ \log[1 - G(\beta(y(0)))] + \sum_{i=0}^{y(0)-1} \log(G(\beta(i))), & 0 < y(0) < q_i, \\ \sum_{i=0}^{y(0)-1} \log(1 - G(\beta(i))), & y(0) = q_i - . \end{cases} \quad (5)$$

The function declaration is

f2v cumloglog(ivec & y, vec & beta).

The function `cumloglog.value` is $\ell_i(\beta; \mathbf{y})$ if y is \mathbf{y} and `beta` is β . If $n = 2$, then `cumloglog.cpp` and `cloglog.cpp` yield the same result.

cumloglog1.cpp

The function `cumloglog1.cpp` computes the function value and gradient associated with a cumulative log-log transformation. Here r_i , q_i , O_i , and \mathcal{Y}_i are defined as in `cumlogit.cpp`. As in `cloglog.cpp`, Equation 5 holds for β in O_i and \mathbf{y} in \mathcal{Y}_i . The function declaration is

f1v cumloglog1(ivec & y, vec & beta).

The function `cumloglog1.value` is $\ell_i(\beta; \mathbf{y})$ if y is \mathbf{y} and `beta` is β . If $q_i = 1$, then `cumloglog1.cpp` and `cloglog1.cpp` yield the same result.

cumprobit.cpp

The function `cumprobit.cpp` computes the function value, gradient, and Hessian matrix associated with a cumulative probit transformation. Let Φ be the cumulative distribution function of the standard normal distribution with expectation 0

and variance 1, so that the inverse function Φ^{-1} defined on the interval $(0, 1)$ is the probit transformation. In this case, r_i , q_i , O_i , and \mathcal{Y}_i are defined as in `cumlogit.cpp`, and, for β in O_i and \mathbf{y} in \mathcal{Y}_i ,

$$\ell_i(\beta; \mathbf{y}) = \begin{cases} \log[1 - \Phi(\beta(y(0)))], & y(0) = 0, \\ \log(1 - \Phi(\beta(y(0)))) + \sum_{i=0}^{y(0)-1} \log(\Phi(\beta(i))), & 0 < y(0) < q_i, \\ \sum_{i=0}^{y(0)-1} \log(\Phi(\beta(i))), & y(0) = q_i. \end{cases} \quad (6)$$

The function declaration is

f2v cumprobit(ivec & y, vec & beta).

The function *cumprobit.value* is $\ell_i(\beta; \mathbf{y})$ if \mathbf{y} is \mathbf{y} and *beta* is β .

cumprobit1.cpp

The function `cumprobit1.cpp` computes the function value and gradient associated with a cumulative probit transformation. Definitions of r_i , q_i , \mathcal{Y}_i , and $\ell_i(\beta; \mathbf{y})$ are the same as in `cumprobit.cpp`. The function declaration is

f1v cumprobit1(ivec & y, vec & beta).

The function *cumprobit1.value* is $\ell_i(\beta; \mathbf{y})$ if \mathbf{y} is \mathbf{y} and *beta* is β .

gradlogit.cpp

The function `gradlogit.cpp` computes the function value, gradient, and Hessian matrix associated with a graded logit transformation. Define L as in `cumlogit.cpp`. Then $r_i = 1$, $q_i \geq 1$, O_i is the set of all vectors of dimension q_i with strictly increasing elements, \mathcal{Y}_i is the set of one-dimensional vectors \mathbf{y} with $y(0)$ a nonnegative integer no greater than q_i , and, for β in O_i and \mathbf{y} in \mathcal{Y}_i ,

$$\ell_i(\beta; \mathbf{y}) = \begin{cases} \log(L(\beta(y(0)))) & y(0) = 0, \\ \log(L(\beta(y(0))) - L(\beta(y(0) - 1))), & 0 < y(0) < q_i, \\ \log[1 - L(\beta(y(0) - 1))], & y(0) = q_i. \end{cases} \quad (7)$$

The function declaration is

f2v gradlogit(ivec & y, vec & beta).

The function *gradlogit.value* is $\ell_i(\beta; \mathbf{y})$ if \mathbf{y} is \mathbf{y} and *beta* is β . If $q_i = 1$, then `cumlogit.cpp` and `gradlogit.cpp` yield the same result.

gradlogit1.cpp

The function `gradlogit1.cpp` computes the function value and gradient associated with a graded logit transformation. Here r_i , q_i , O_i , \mathcal{Y}_i , and $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ are defined as in `gradlogit.cpp`. The function declaration is

f1v gradlogit1(ivec & y, vec & beta).

The function `gradlogit1.value` is $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ if y is \mathbf{y} and `beta` is $\boldsymbol{\beta}$. If $q_i = 1$, then `gradlogit1.cpp` and `cumlogit1.cpp` yield the same result.

gradloglog.cpp

The function `gradloglog.cpp` computes the function value, gradient, and Hessian matrix associated with a graded complementary log-log transformation. Define G as in `cloglog.cpp`. Then $r_i = 1$, $q_i \geq 1$, O_i is the set of all vectors of dimension q_i with strictly increasing elements, \mathcal{Y}_i is the set of one-dimensional vectors \mathbf{y} with $y(0)$ a nonnegative integer no greater than q_i , and, for $\boldsymbol{\beta}$ in O_i and \mathbf{y} in \mathcal{Y}_i ,

$$\ell_i(\boldsymbol{\beta}; \mathbf{y}) = \begin{cases} \log(G(\boldsymbol{\beta}(y(0)))) & y(0) = 0, \\ \log(G(\boldsymbol{\beta}(y(0))) - G(\boldsymbol{\beta}(y(0) - 1))), & 0 < y(0) < q_i, \\ \log[1 - G(\boldsymbol{\beta}(y(0) - 1))], & y(0) = q_i. \end{cases} \quad (8)$$

The function declaration is

f2v gradloglog(ivec & y, vec & beta).

The function `gradloglog.value` is $\ell_i(\boldsymbol{\beta}; y)$ if y is \mathbf{y} and `beta` is $\boldsymbol{\beta}$. If $q_i = 2$, then `gradloglog.cpp` and `cloglog.cpp` yield the same result.

gradloglog1.cpp

The function `gradloglog1.cpp` computes the function value and gradient associated with a graded complementary log-log transformation. Here r_i , q_i , O_i , \mathcal{Y}_i , and $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ are defined as in `gradloglog.cpp`. The function declaration is

f1v gradloglog1(ivec & y, vec & beta).

The function `gradloglog1.value` is $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ if y is \mathbf{y} and `beta` is $\boldsymbol{\beta}$. If $q_i = 1$, then `gradloglog1.cpp` and `cloglog1.cpp` yield the same result.

gradprobit.cpp

The function `gradprobit.cpp` computes the function value, gradient, and Hessian matrix associated with a graded probit transformation. Define Φ as in `cumprobit.cpp`. Then $r_i = 1$, $q_i \geq 1$, O_i is the set of all vectors of dimension q_i with strictly

increasing elements, \mathcal{Y}_i is the set of one-dimensional vectors \mathbf{y} with $y(0)$ a nonnegative integer no greater than q_i , and, for β in O_i and \mathbf{y} in \mathcal{Y}_i ,

$$\ell_i(\beta; \mathbf{y}) = \begin{cases} \log(\Phi(\beta(y(0)))) & y(0) = 0, \\ \log(\Phi(\beta(y(0))) - \Phi(\beta(y(0) - 1))), & 0 < y(0) < q_i, \\ \log[1 - \Phi(\beta(y(0) - 1))], & y(0) = q_i. \end{cases} \quad (9)$$

The function declaration is

f2v gradprobit(ivec & y, vec & beta).

The function *gradprobit.value* is $\ell_i(\beta; y)$ if y is \mathbf{y} and *beta* is β . If $q_i = 1$, then *cumprobit.cpp* and *gradprobit.cpp* yield the same result.

gradprobit1.cpp

The function *gradprobit1.cpp* computes the function value and gradient associated with a graded probit transformation. Here r_i , q_i , O_i , \mathcal{Y}_i , and $\ell_i(\beta; \mathbf{y})$ are defined as in *gradprobit.cpp*. The function declaration is

f1v gradprobit1(ivec & y, vec & beta).

The function *gradprobit1.value* is $\ell_i(\beta; \mathbf{y})$ if y is \mathbf{y} and *beta* is β . If $q_i = 1$, then *cumprobit1.cpp* and *gradprobit1.cpp* yield the same result.

gumbel.cpp

The function *gumbel.cpp* computes the function value, gradient, and Hessian matrix associated with the distribution of a random variable with the distribution of $\beta(0) + \beta(1)Z$, where Z has a standard Gumbel distribution such that $Z \leq z$ is $\exp(-\exp(-z))$ for real z (*cloglog.cpp*), $\beta(0)$ is a real constant, and $\beta(1)$ is a positive real constant. The corresponding log-likelihood component is

$$\ell_i(\beta; \mathbf{y}) = \log(\beta(1)) - \beta(0) - \beta(1)y(0) - \exp(-\beta(0) - \beta(1)y(0)), \quad (10)$$

where $r_i = 1$, \mathcal{Y}_i is the set of one-dimensional vectors \mathbf{y} , $q_i = 2$, and O_i is the set of all two-dimensional vectors β with $\beta(1)$ positive. The function declaration is

f2v gumbel(vec & y, vec & beta).

The function *gumbel.value* is $\ell_i(\beta; \mathbf{y})$ if y is \mathbf{y} and *beta* is β .

gumbel1.cpp

The function `gumbel1.cpp` computes the function value and gradient associated with the Gumbel log-likelihood component defined by Equation 10. Here r_i , \mathcal{Y}_i , q_i , and O_i are defined as in `gumbel.cpp`. The function declaration is

f1v gumbel1(vec & y, vec & beta).

The function `gumbel1.value` is $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ if y is \mathbf{y} and $beta$ is $\boldsymbol{\beta}$.

logistic.cpp

The function `logistic.cpp` computes the function value, gradient, and Hessian matrix associated with the distribution of $\beta(0) + \beta(1)Z$, where Z has a standard logistic distribution (`cumlogit.cpp`). $\beta(0)$ is a real constant, and $\beta(1)$ is a positive real constant. In this case, $r_i = 1$, \mathcal{Y}_i , q_i , and O_i are defined as in `gumbel.cpp`. For $\boldsymbol{\beta}$ in O_i and \mathbf{y} in \mathcal{Y}_i ,

$$\ell_i(\boldsymbol{\beta}; \mathbf{y}) = \log(\beta(1)) + \log(L(\beta(0) + \beta(1)y(0))[1.0 - L(\beta(0) + \beta(1)y(0))]). \quad (11)$$

The function declaration is

f2v logistic(vec & y, vec & beta).

The function `logistic.value` is $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ if y is \mathbf{y} and $beta$ is $\boldsymbol{\beta}$.

logistic1.cpp

The function `logistic1.cpp` computes the function value and gradient associated with the log-likelihood component defined by Equation 11. Define r_i , \mathcal{Y}_i , q_i , O_i , and $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ as in `logistic.cpp`. The function declaration is

f1v logistic1(vec & y, vec & beta).

The function `logistic1.value` is $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ if y is \mathbf{y} and $beta$ is $\boldsymbol{\beta}$.

logit.cpp

The function `logit.cpp` computes the function value, gradient, and Hessian matrix associated with a logit transformation. Define L as in `cumlogit.cpp`. In this case, $r_i = 1$, \mathcal{Y}_i is the set of one-dimensional vectors \mathbf{y} such that $y(0)$ is 0 or 1, $q_i = 1$, and O_i is the set of all one-dimensional vectors. For $\boldsymbol{\beta}$ in O_i and \mathbf{y} in \mathcal{Y}_i , $\ell_i(\boldsymbol{\beta}; \mathbf{y}) = \log(1 - L(\beta(0)))$ if $y(0) = 0$, and $\ell_i(\boldsymbol{\beta}; \mathbf{y}) = \log(L(\beta(0)))$ if $y(0) = 1$. The function declaration is

f2v logit(ivec & y, vec & beta).

The function *logit.value* is $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ if *y* is \mathbf{y} and *beta* is $\boldsymbol{\beta}$. Use of *cumlogit.cpp* or *gradlogit.cpp* for $q_i = 1$ gives the same result as use of *logit.cpp*.

logit1.cpp

The function *logit1.cpp* computes the function value and gradient associated with a logit transformation. Define r_i , \mathcal{Y}_i , q_i , O_i , and $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ as in *logit.cpp*. The function declaration is

f1v logit1(ivec & y, vec & beta).

The function *logit1.value* is $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ if *y* is \mathbf{y} and *beta* is $\boldsymbol{\beta}$. If $q_i = 2$, use of *cumlogit1.cpp* or *gradlogit1.cpp* yields the same result as use of *logit1.cpp*.

logmean.cpp

The function *logmean.cpp* computes the function value, gradient, and Hessian matrix associated with a log-mean transformation for a Poisson random variable. In this case, $r_i = 1$, \mathcal{Y}_i is the set of one-dimensional vectors \mathbf{y} such that $y(0)$ is a nonnegative integer, $q_i = 1$, O_i is the set of all one-dimensional vectors, and $v_i(\mathbf{y}) = -\log([y(0)]!)$ for \mathbf{y} in \mathcal{Y}_i . For $\boldsymbol{\beta}$ in O_i and \mathbf{y} in \mathcal{Y}_i , $\ell_i(\boldsymbol{\beta}; \mathbf{y}) = y(0)\beta(0) - \exp(\beta(0))$. The function declaration is

f2v logmean(ivec & y, vec & beta).

The function *logmean.value* is $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ if *y* is \mathbf{y} and *beta* is $\boldsymbol{\beta}$.

logmean1.cpp

The function *logmean1.cpp* computes the function value and gradient associated with a log-mean transformation for a Poisson random variable. Define r_i , \mathcal{Y}_i , q_i , O_i , v_i , and $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ as in *logmean.cpp*. The function declaration is

f1v logmean1(ivec & y, vec & beta).

The function *logmean1.value* is $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ if *y* is \mathbf{y} and *beta* is $\boldsymbol{\beta}$.

multlogit.cpp

The function *multlogit.cpp* computes the function value, gradient, and Hessian matrix associated with a multinomial logit transformation. In this case, $r_i = 1$, \mathcal{Y}_i is the set of one-dimensional vectors \mathbf{y} such that $y(0)$ is a nonnegative integer no

greater than $q_i \geq 1$, and O_i is the set of all q_i -dimensional vectors. Let $\mathbf{0}_1$ be the one-dimensional vector with the single element 0. For β in O_i and \mathbf{y} in \mathcal{Y}_i ,

$$\ell_i(\beta; \mathbf{y}) = \begin{cases} -\log \left(1 + \sum_{k=0}^{q_i-1} \exp(\beta(k)) \right), & \mathbf{y} = \mathbf{0}_1, \\ \beta(y(0) - 1) + \ell_i(\beta; \mathbf{0}_1), & y(0) > 0. \end{cases} \quad (12)$$

The function declaration is

f2v multlogit(ivec & y, vec & beta).

The function *multlogit.value* is $\ell_i(\beta; \mathbf{y})$ if *y* is \mathbf{y} and *beta* is β . If $n_i = 2$, use of *multlogit.cpp* gives the same result as use of *multlogit1.cpp*.

multlogit1.cpp

The function *multlogit1.cpp* computes the function value and gradient associated with a multinomial logit transformation. Define r_i , \mathcal{Y}_i , q_i , O_i , and $\ell_i(\beta; \mathbf{y})$ as in *multlogit.cpp*. The function declaration is

f1v multlogit1(ivec & y, vec & beta).

The function *multlogit1.value* is $\ell_i(\beta; \mathbf{y})$ if *y* is \mathbf{y} and *beta* is β . If $n_i = 2$, use of *logit1.cpp* yields the same result as use of *multlogit1.cpp*.

normal.cpp

The function *normal.cpp* computes the function value, gradient, and Hessian matrix associated with the distribution of $\beta(0) + \beta(1)Z$, where Z has a standard normal distribution. In this case, $r_i = 1$, \mathcal{Y}_i , q_i , and O_i are defined as in *gumbel.cpp*, while $v_i(\mathbf{y}) = -0.5 \log(2\pi)$. For β in O_i and \mathbf{y} in \mathcal{Y}_i ,

$$\ell_i(\beta; \mathbf{y}) = \log(\beta(1)) - (\beta(0) + \beta(1)y(0))^2/2. \quad (13)$$

The function declaration is

f2v normal(vec & y, vec & beta).

The function *normal.value* is $\ell_i(\beta; \mathbf{y})$ if *y* is \mathbf{y} and *beta* is β .

normal1.cpp

The function *normal1.cpp* computes the function value and gradient associated with the log-likelihood component defined by Equation 13. Define r_i , \mathcal{Y}_i , q_i , O_i , v_i , and $\ell_i(\beta; \mathbf{y})$ as in *normal.cpp*. The function declaration is

flv normal1(*vec & y, vec & beta*).

The function *normal1.value* is $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ if *y* is \mathbf{y} and *beta* is $\boldsymbol{\beta}$.

probit.cpp

The function *probit.cpp* computes the function value, gradient, and Hessian matrix associated with a logit transformation. Define Φ as in *cumprobit.cpp*. In this case, $r_i = 1$, \mathcal{Y}_i is the set of one-dimensional vectors \mathbf{y} such that $y(0)$ is 0 or 1, $q_i = 1$, and O_i is the set of all one-dimensional vectors. For $\boldsymbol{\beta}$ in O_i and \mathbf{y} in \mathcal{Y}_i , $\ell_i(\boldsymbol{\beta}; \mathbf{y}) = \log(1 - \Phi(\beta(0)))$ if $y(0) = 0$, and $\ell_i(\boldsymbol{\beta}; \mathbf{y}) = \log(\Phi(\beta(0)))$ if $y(0) = 1$. The function declaration is

f2v probit(*ivec & y, vec & beta*).

The function *probit.value* is $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ if *y* is \mathbf{y} and *beta* is $\boldsymbol{\beta}$. Use of *cumprobit.cpp* or *gradprobit.cpp* in the case of $q_i = 1$ gives the same result as use of *probit.cpp*.

probit1.cpp

The function *probit1.cpp* computes the function value and gradient associated with a probit transformation. Define r_i , \mathcal{Y}_i , q_i , O_i , and $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ as in *probit.cpp*. The function declaration is

flv probit1(*ivec & y, vec & beta*).

The function *probit1.value* is $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ if *y* is \mathbf{y} and *beta* is $\boldsymbol{\beta}$. If $n_i = 2$, use of *cumprobit1.cpp* or *gradprobit1.cpp* yields the same result as use of *probit1.cpp*.

Integration Tools

The functions in this section aid in cases in which integration is required.

adapt.cpp

The function *adapt.cpp* provides a linear transformation of a set of real quadrature points and adjusts the corresponding weights for each point. The linear transformation has the form $L(x) = a + bx$ for x real, where a is a real number and b is a positive real number. The linear transformation is applied to each quadrature point and the weights are multiplied by b . The function declaration is

pw adapt(*double & loc, double & scale, pw & pws*).

The struct *pw* has the definition

```
struct pw{vec points; vec weights;};
```

The variable *loc* is *a* and the variable *scale* is *b*. The original points are provided by *pws.points*, and the original positive weights are given by *pws.weights*. The transformed points are *adapt.points*, and the transformed weights are *adapt.weights*. If *scale* is not positive, then *adapt* is set equal to *pws*. The number of elements in *pws.points*, *pws.weights*, *adapt.points*, and *adapt.weights* is the same.

adaptv.cpp

The function *adaptv.cpp* provides a linear transformation of a set of *D*-dimensional quadrature points and adjusts the corresponding weights for each point, where *D* is a positive integer. The linear transformation has the form $L(\mathbf{x}) = \mathbf{a} + \mathbf{B}\mathbf{x}$ for the *D*-dimensional vector \mathbf{x} , where \mathbf{a} is a *D*-dimensional vector and \mathbf{B} is a *D* by *D* lower triangular matrix. The linear transformation is applied to each quadrature point and the weights are multiplied by the determinant of \mathbf{B} . The function declaration is

```
pwv adapt(vec & loc, mat & lt, pwv & pws).
```

The struct *pwv* has the definition

```
struct pwv{mat points; vec weights;};
```

The variable *loc* is \mathbf{a} and the variable *lt* is \mathbf{B} . The original points are provided by *pws.points*, and the original positive weights are in *pws.weights*. The transformed points are in *adaptv.points*, and the transformed weights are in *adaptv.weights*. If any diagonal element of *lt* is not positive, then *adaptv* is set equal to *pws*. The number of elements in *pws.weights* and *adaptv.weights* is the same and is the same as both the number of columns in *adaptv.points* and the number of columns in *pws.points*. The number of rows in *adaptv.points* is equal to the number of rows in *pws.points*.

genfact.cpp

For a vector *sizes* of positive integers, the function *genfact.cpp* generates all vectors *i* of nonnegative integers with the same number of elements as *sizes* such that each element of *i* is less than the corresponding element of *sizes*. The function declaration is

```
imat genfact(ivec & sizes).
```

The columns of *genfact* are the possible vectors *i*. For example, if the elements of *sizes* are 2 and 3, then Column 0 of *genfact* has elements 0 and 0, and Column 1

has elements 1 and 0. In all, *sizes* has 6 columns, and Column 5 has elements 1 and 2.

genprods.cpp

The function `genprods.cpp` generates a collection of quadrature points and quadrature weights for a multivariate integral from quadrature weights and quadrature points for a univariate integral. The function declaration is

pwv genprods(imat & indices, pw pws []).

The struct *pw* is defined as in `adapt.cpp`, and the struct *pwv* is defined as in `adaptv.cpp`. Consider the case of Q quadrature points for a multidimensional integral on the space of D -dimensional vectors, where Q and D are positive integers. Then *genprods.points* has Q columns and *genprods.weights* has Q elements. The matrix *genprods.points* has D rows. The array *pws* has D members. For $0 \leq d < D$, *pws[d].points* and *pws[d].weights* have $m(d) > 1$ members, and the members of *pws[d].weights* are positive. The matrix *indices* specifies the quadrature vectors and quadrature weights to construct from *pws*. If *indices* has p columns, $0 \leq k < p$, and $0 \leq d < D$, then row d and column k of *indices* is nonnegative and less than $m(d)$ and the corresponding row and column of *genprods.points* is *pws[d].points(indices(d,k))*. Element k of *genprods.weights* is the product of *pws[d].weights(indices(d,k))* for $0 \leq d < D$.

hermcoeff.cpp

The function `hermcoeff.cpp` finds the coefficients of a Hermite polynomial of a given order. The function declaration is

vec hermcoeff(int & n).

The integer variable n is the nonnegative order. The vector *hermcoeff* has $n+1$ elements. The polynomial is $H_n(x) = \sum_{i=0}^n \alpha_i x^{n-i}$ for real x , and element i of *hermcoeff* is α_i . For example, if n is 2, then the elements of *hermcoeff* are 1, 0, and -1 .

hermpoly.cpp

The function `hermpoly.cpp` evaluates the Hermite polynomials up to a given order at a specified real value. The function declaration is

vec hermpoly(int &n, double & x).

The order is the nonnegative integer variable n , and the real value is x . The vector *hermpoly* has $n+1$ elements. For $0 \leq k \leq n$, element k of *hermpoly* is the value of H_k at x .

hermpw.cpp

The function *hermpw.cpp* uses the algorithm of Golub and Welsch (1969) to find the quadrature points and quadrature weights for Gauss-Hermite quadrature. The function declaration is

pw hermpw(int & n).

The struct *hermpw* has vector elements *hermpw.points* and *hermpw.weights*. The number of quadrature points is n . The ordered quadrature points are in *hermpw.points*. The corresponding weights are in *hermpw.weights*.

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