## ONE DIMENSIONAL ROOT-FINDING

This chapter describes routines for finding roots of arbitrary one-dimensional functions. The library provides low level components for a variety of iterative solvers and convergence tests. These can be combined by the user to achieve the desired solution, with full access to the intermediate steps of the iteration. Each class of methods uses the same framework, so that you can switch between solvers at runtime without needing to recompile your program. Each instance of a solver keeps track of its own state, allowing the solvers to be used in multi-threaded programs.

The header file qsl\_roots.h contains prototypes for the root finding functions and related declarations.

### 36.1 Overview

One-dimensional root finding algorithms can be divided into two classes, *root bracketing* and *root polishing*. Algorithms which proceed by bracketing a root are guaranteed to converge. Bracketing algorithms begin with a bounded region known to contain a root. The size of this bounded region is reduced, iteratively, until it encloses the root to a desired tolerance. This provides a rigorous error estimate for the location of the root.

The technique of *root polishing* attempts to improve an initial guess to the root. These algorithms converge only if started "close enough" to a root, and sacrifice a rigorous error bound for speed. By approximating the behavior of a function in the vicinity of a root they attempt to find a higher order improvement of an initial guess. When the behavior of the function is compatible with the algorithm and a good initial guess is available a polishing algorithm can provide rapid convergence.

In GSL both types of algorithm are available in similar frameworks. The user provides a high-level driver for the algorithms, and the library provides the individual functions necessary for each of the steps. There are three main phases of the iteration. The steps are,

- initialize solver state, s, for algorithm T
- update s using the iteration T
- test s for convergence, and repeat iteration if necessary

The state for bracketing solvers is held in a  $gsl\_root\_fsolver$  struct. The updating procedure uses only function evaluations (not derivatives). The state for root polishing solvers is held in a  $gsl\_root\_fdfsolver$  struct. The updates require both the function and its derivative (hence the name fdf) to be supplied by the user.

## 36.2 Caveats

Note that root finding functions can only search for one root at a time. When there are several roots in the search area, the first root to be found will be returned; however it is difficult to predict which of the roots this will be. *In most cases, no error will be reported if you try to find a root in an area where there is more than one.* 

Care must be taken when a function may have a multiple root (such as  $f(x) = (x - x_0)^2$  or  $f(x) = (x - x_0)^3$ . It is not possible to use root-bracketing algorithms on even-multiplicity roots. For these algorithms the initial interval must contain a zero-crossing, where the function is negative at one end of the interval and positive at the other end. Roots with even-multiplicity do not cross zero, but only touch it instantaneously. Algorithms based on root bracketing will still work for odd-multiplicity roots (e.g. cubic, quintic, ...). Root polishing algorithms generally work with higher multiplicity roots, but at a reduced rate of convergence. In these cases the *Steffenson algorithm* can be used to accelerate the convergence of multiple roots.

While it is not absolutely required that f have a root within the search region, numerical root finding functions should not be used haphazardly to check for the *existence* of roots. There are better ways to do this. Because it is easy to create situations where numerical root finders can fail, it is a bad idea to throw a root finder at a function you do not know much about. In general it is best to examine the function visually by plotting before searching for a root.

# 36.3 Initializing the Solver

#### gsl\_root\_fsolver

This is a workspace for finding roots using methods which do not require derivatives.

### gsl\_root\_fdfsolver

This is a workspace for finding roots using methods which require derivatives.

```
gsl_root_fsolver * gsl_root_fsolver_alloc (const gsl_root_fsolver_type * T)
```

This function returns a pointer to a newly allocated instance of a solver of type T. For example, the following code creates an instance of a bisection solver:

```
const gsl_root_fsolver_type * T = gsl_root_fsolver_bisection;
gsl_root_fsolver * s = gsl_root_fsolver_alloc (T);
```

If there is insufficient memory to create the solver then the function returns a null pointer and the error handler is invoked with an error code of GSL ENOMEM.

```
gsl_root_fdfsolver * gsl_root_fdfsolver_alloc (const gsl_root_fdfsolver_type * T)
```

This function returns a pointer to a newly allocated instance of a derivative-based solver of type T. For example, the following code creates an instance of a Newton-Raphson solver:

```
const gsl_root_fdfsolver_type * T = gsl_root_fdfsolver_newton;
gsl_root_fdfsolver * s = gsl_root_fdfsolver_alloc (T);
```

If there is insufficient memory to create the solver then the function returns a null pointer and the error handler is invoked with an error code of GSL\_ENOMEM.

```
int gsl_root_fsolver_set (gsl_root_fsolver * s, gsl_function * f, double x_lower, double x_upper)
```

This function initializes, or reinitializes, an existing solver s to use the function f and the initial search interval [x lower, x upper].

```
int gsl_root_fdfsolver_set (gsl_root_fdfsolver * s, gsl_function_fdf * fdf, double root)
```

This function initializes, or reinitializes, an existing solver s to use the function and derivative fdf and the initial guess root.

```
void gsl_root_fsolver_free (gsl_root_fsolver * s)
void gsl_root_fdfsolver_free (gsl_root_fdfsolver * s)
```

These functions free all the memory associated with the solver s.

```
const char * gsl_root_fsolver_name (const gsl_root_fsolver * s)
const char * gsl_root_fdfsolver_name (const gsl_root_fdfsolver * s)
```

These functions return a pointer to the name of the solver. For example:

```
printf ("s is a '%s' solver\n", gsl_root_fsolver_name (s));
```

would print something like s is a 'bisection' solver.

# 36.4 Providing the function to solve

You must provide a continuous function of one variable for the root finders to operate on, and, sometimes, its first derivative. In order to allow for general parameters the functions are defined by the following data types:

#### qsl function

This data type defines a general function with parameters.

```
double (* function) (double x, void * params)
```

this function should return the value f(x, params) for argument x and parameters params

```
void * params
```

a pointer to the parameters of the function

Here is an example for the general quadratic function,

$$f(x) = ax^2 + bx + c$$

with  $a=3,\,b=2,\,c=1.$  The following code defines a  $gsl\_function$  F which you could pass to a root finder as a function pointer:

```
struct my_f_params { double a; double b; double c; };

double
my_f (double x, void * p)
    {
        struct my_f_params * params = (struct my_f_params *)p;
        double a = (params->a);
        double b = (params->b);
        double c = (params->c);

        return (a * x + b) * x + c;
    }

gsl_function F;
struct my_f_params params = { 3.0, 2.0, 1.0 };

F.function = &my_f;
F.params = &params;
```

The function f(x) can be evaluated using the macro GSL\_FN\_EVAL(&F, x) defined in gsl\_math.h.

### gsl\_function\_fdf

This data type defines a general function with parameters and its first derivative.

```
double (* f) (double x, void * params)
```

this function should return the value of f(x, params) for argument x and parameters params

```
double (* df) (double x, void * params)
```

this function should return the value of the derivative of f with respect to x, f'(x, params), for argument x and parameters params

```
void (* fdf) (double x, void * params, double * f, double * df)
```

this function should set the values of the function f to f(x, params) and its derivative df to f'(x, params) for argument x and parameters params. This function provides an optimization of the separate functions for f(x) and f'(x)—it is always faster to compute the function and its derivative at the same time.

```
void * params
```

a pointer to the parameters of the function

Here is an example where  $f(x) = \exp(2x)$ :

```
double
my_f (double x, void * params)
   return exp (2 * x);
}
double
my_df (double x, void * params)
   return 2 * exp (2 * x);
}
void
my_fdf (double x, void * params,
        double * f, double * df)
   double t = \exp(2 * x);
   *f = t;
   *df = 2 * t; /* uses existing value */
}
gsl_function_fdf FDF;
FDF.f = &my_f;
FDF.df = \&my_df;
FDF.fdf = &my_fdf;
FDF.params = 0;
```

The function f(x) can be evaluated using the macro GSL\_FN\_FDF\_EVAL\_F (&FDF, x) and the derivative f'(x) can be evaluated using the macro GSL\_FN\_FDF\_EVAL\_DF (&FDF, x). Both the function y = f(x) and its derivative dy = f'(x) can be evaluated at the same time using the macro GSL\_FN\_FDF\_EVAL\_F\_DF (&FDF, x, y, dy). The macro stores f(x) in its y argument and f'(x) in its dy argument—both of these should be pointers to double.

## 36.5 Search Bounds and Guesses

You provide either search bounds or an initial guess; this section explains how search bounds and guesses work and how function arguments control them.

A guess is simply an x value which is iterated until it is within the desired precision of a root. It takes the form of a double.

Search bounds are the endpoints of an interval which is iterated until the length of the interval is smaller than the requested precision. The interval is defined by two values, the lower limit and the upper limit. Whether the endpoints are intended to be included in the interval or not depends on the context in which the interval is used.

## 36.6 Iteration

The following functions drive the iteration of each algorithm. Each function performs one iteration to update the state of any solver of the corresponding type. The same functions work for all solvers so that different methods can be substituted at runtime without modifications to the code.

```
int gsl_root_fsolver_iterate (gsl_root_fsolver * s)
int gsl_root_fdfsolver_iterate (gsl_root_fdfsolver * s)
```

These functions perform a single iteration of the solver s. If the iteration encounters an unexpected problem then an error code will be returned.

```
GSL EBADFUNC
```

the iteration encountered a singular point where the function or its derivative evaluated to Inf or NaN.

```
GSL_EZERODIV
```

the derivative of the function vanished at the iteration point, preventing the algorithm from continuing without a division by zero.

The solver maintains a current best estimate of the root at all times. The bracketing solvers also keep track of the current best interval bounding the root. This information can be accessed with the following auxiliary functions,

```
double gsl_root_fsolver_root (const gsl_root_fsolver * s)
double gsl_root_fdfsolver_root (const gsl_root_fdfsolver * s)
```

These functions return the current estimate of the root for the solver s.

```
double gsl_root_fsolver_x_lower (const gsl_root_fsolver * s) double gsl_root_fsolver_x_upper (const gsl_root_fsolver * s)
```

These functions return the current bracketing interval for the solver s.

# 36.7 Search Stopping Parameters

A root finding procedure should stop when one of the following conditions is true:

- A root has been found to within the user-specified precision.
- A user-specified maximum number of iterations has been reached.
- An error has occurred.

The handling of these conditions is under user control. The functions below allow the user to test the precision of the current result in several standard ways.

```
int gsl_root_test_interval (double x_lower, double x_upper, double epsabs, double epsrel)
```

This function tests for the convergence of the interval [x\_lower, x\_upper] with absolute error epsabs and relative error epsrel. The test returns GSL\_SUCCESS if the following condition is achieved,

```
|a-b| < epsabs + epsrel \min(|a|, |b|)
```

when the interval x = [a, b] does not include the origin. If the interval includes the origin then  $\min(|a|, |b|)$  is replaced by zero (which is the minimum value of |x| over the interval). This ensures that the relative error is accurately estimated for roots close to the origin.

This condition on the interval also implies that any estimate of the root r in the interval satisfies the same condition with respect to the true root  $r^*$ ,

$$|r - r^*| < epsabs + epsrel r^*$$

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assuming that the true root  $r^*$  is contained within the interval.

### int gsl\_root\_test\_delta (double x1, double x0, double epsabs, double epsrel)

This function tests for the convergence of the sequence x0, x1 with absolute error epsabs and relative error epsabs. The test returns GSL\_SUCCESS if the following condition is achieved,

$$|x_1 - x_0| < epsabs + epsrel |x_1|$$

and returns GSL\_CONTINUE otherwise.

### int gsl\_root\_test\_residual (double f, double epsabs)

This function tests the residual value f against the absolute error bound epsabs. The test returns GSL\_SUCCESS if the following condition is achieved,

and returns GSL\_CONTINUE otherwise. This criterion is suitable for situations where the precise location of the root, x, is unimportant provided a value can be found where the residual, |f(x)|, is small enough.

# 36.8 Root Bracketing Algorithms

The root bracketing algorithms described in this section require an initial interval which is guaranteed to contain a root—if a and b are the endpoints of the interval then f(a) must differ in sign from f(b). This ensures that the function crosses zero at least once in the interval. If a valid initial interval is used then these algorithm cannot fail, provided the function is well-behaved.

Note that a bracketing algorithm cannot find roots of even degree, since these do not cross the x-axis.

#### gsl\_root\_fsolver\_type

### gsl\_root\_fsolver\_bisection

The *bisection algorithm* is the simplest method of bracketing the roots of a function. It is the slowest algorithm provided by the library, with linear convergence.

On each iteration, the interval is bisected and the value of the function at the midpoint is calculated. The sign of this value is used to determine which half of the interval does not contain a root. That half is discarded to give a new, smaller interval containing the root. This procedure can be continued indefinitely until the interval is sufficiently small.

At any time the current estimate of the root is taken as the midpoint of the interval.

#### qsl root fsolver falsepos

The *false position algorithm* is a method of finding roots based on linear interpolation. Its convergence is linear, but it is usually faster than bisection.

On each iteration a line is drawn between the endpoints (a, f(a)) and (b, f(b)) and the point where this line crosses the x-axis taken as a "midpoint". The value of the function at this point is calculated and its sign is used to determine which side of the interval does not contain a root. That side is discarded to give a new, smaller interval containing the root. This procedure can be continued indefinitely until the interval is sufficiently small.

The best estimate of the root is taken from the linear interpolation of the interval on the current iteration.

### gsl\_root\_fsolver\_brent

The *Brent-Dekker method* (referred to here as *Brent's method*) combines an interpolation strategy with the bisection algorithm. This produces a fast algorithm which is still robust.

On each iteration Brent's method approximates the function using an interpolating curve. On the first iteration this is a linear interpolation of the two endpoints. For subsequent iterations the algorithm uses an inverse quadratic fit to the last three points, for higher accuracy. The intercept of the interpolating curve with the x-axis is taken as a guess for the root. If it lies within the bounds of the current interval then the interpolating point is accepted, and used to generate a smaller interval. If the interpolating point is not accepted then the algorithm falls back to an ordinary bisection step.

The best estimate of the root is taken from the most recent interpolation or bisection.

# 36.9 Root Finding Algorithms using Derivatives

The root polishing algorithms described in this section require an initial guess for the location of the root. There is no absolute guarantee of convergence—the function must be suitable for this technique and the initial guess must be sufficiently close to the root for it to work. When these conditions are satisfied then convergence is quadratic.

These algorithms make use of both the function and its derivative.

#### gsl\_root\_fdfsolver\_newton

Newton's Method is the standard root-polishing algorithm. The algorithm begins with an initial guess for the location of the root. On each iteration, a line tangent to the function f is drawn at that position. The point where this line crosses the x-axis becomes the new guess. The iteration is defined by the following sequence,

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

Newton's method converges quadratically for single roots, and linearly for multiple roots.

### gsl\_root\_fdfsolver\_secant

The *secant method* is a simplified version of Newton's method which does not require the computation of the derivative on every step.

On its first iteration the algorithm begins with Newton's method, using the derivative to compute a first step,

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$

Subsequent iterations avoid the evaluation of the derivative by replacing it with a numerical estimate, the slope of the line through the previous two points,

$$x_{i+1} = x_i - \frac{f(x_i)}{f'_{est}}$$
 where  $f'_{est} = \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}$ 

When the derivative does not change significantly in the vicinity of the root the secant method gives a useful saving. Asymptotically the secant method is faster than Newton's method whenever the cost of evaluating the derivative is more than 0.44 times the cost of evaluating the function itself. As with all methods of computing a numerical derivative the estimate can suffer from cancellation errors if the separation of the points becomes too small.

On single roots, the method has a convergence of order  $(1 + \sqrt{5})/2$  (approximately 1.62). It converges linearly for multiple roots.

#### gsl root fdfsolver steffenson

The Steffenson Method<sup>1</sup> provides the fastest convergence of all the routines. It combines the basic Newton algorithm with an Aitken "delta-squared" acceleration. If the Newton iterates are  $x_i$  then the acceleration procedure generates a new sequence  $R_i$ ,

$$R_i = x_i - \frac{(x_{i+1} - x_i)^2}{(x_{i+2} - 2x_{i+1} + x_i)}$$

which converges faster than the original sequence under reasonable conditions. The new sequence requires three terms before it can produce its first value so the method returns accelerated values on the second and subsequent iterations. On the first iteration it returns the ordinary Newton estimate. The Newton iterate is also returned if the denominator of the acceleration term ever becomes zero.

As with all acceleration procedures this method can become unstable if the function is not well-behaved.

# 36.10 Examples

For any root finding algorithm we need to prepare the function to be solved. For this example we will use the general quadratic equation described earlier. We first need a header file (demo\_fn.h) to define the function parameters,

We place the function definitions in a separate file (demo\_fn.c),

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<sup>&</sup>lt;sup>1</sup> J.F. Steffensen (1873–1961). The spelling used in the name of the function is slightly incorrect, but has been preserved to avoid incompatibility.

The first program uses the function solver  $gsl\_root\_fsolver\_brent$  for Brent's method and the general quadratic defined above to solve the following equation,

$$x^2 - 5 = 0$$

with solution  $x = \sqrt{5} = 2.236068...$ 

```
#include <stdio.h>
#include <gsl/gsl_errno.h>
#include <gsl/gsl_math.h>
#include <gsl/gsl_roots.h>
#include "demo_fn.h"
#include "demo_fn.c"
int
main (void)
  int status;
  int iter = 0, max_iter = 100;
  const gsl_root_fsolver_type *T;
  gsl_root_fsolver *s;
  double r = 0, r_expected = sqrt (5.0);
  double x_{lo} = 0.0, x_{hi} = 5.0;
  gsl_function F;
  struct quadratic_params params = {1.0, 0.0, -5.0};
  F.function = &quadratic;
  F.params = &params;
  T = gsl_root_fsolver_brent;
  s = gsl_root_fsolver_alloc (T);
  gsl_root_fsolver_set (s, &F, x_lo, x_hi);
  printf ("using %s method\n",
         gsl_root_fsolver_name (s));
  printf ("%5s [%9s, %9s] %9s %10s %9s\n",
          "iter", "lower", "upper", "root",
```

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```
"err", "err(est)");
do
  {
    iter++;
    status = gsl_root_fsolver_iterate (s);
    r = gsl_root_fsolver_root (s);
    x_lo = gsl_root_fsolver_x_lower (s);
    x_hi = gsl_root_fsolver_x_upper (s);
    status = gsl_root_test_interval (x_lo, x_hi,
                                      0, 0.001);
    if (status == GSL_SUCCESS)
     printf ("Converged:\n");
    printf ("%5d [%.7f, %.7f] %.7f %+.7f %.7f\n",
            iter, x_lo, x_hi,
            r, r - r_expected,
            x_hi - x_lo);
while (status == GSL_CONTINUE && iter < max_iter);</pre>
gsl_root_fsolver_free (s);
return status;
```

Here are the results of the iterations:

```
$ ./a.out
using brent method
iter [ lower, upper] root err err(est)
    1 [1.0000000, 5.0000000] 1.0000000 -1.2360680 4.0000000
    2 [1.0000000, 3.0000000] 3.0000000 +0.7639320 2.0000000
    3 [2.0000000, 3.0000000] 2.0000000 -0.2360680 1.0000000
    4 [2.2000000, 3.0000000] 2.2000000 -0.0360680 0.8000000
    5 [2.2000000, 2.2366300] 2.2366300 +0.0005621 0.0366300

Converged:
    6 [2.2360634, 2.2366300] 2.2360634 -0.0000046 0.0005666
```

If the program is modified to use the bisection solver instead of Brent's method, by changing  $gsl\_root\_fsolver\_brent$  to  $gsl\_root\_fsolver\_bisection$  the slower convergence of the Bisection method can be observed:

```
$ ./a.out
using bisection method
iter [ lower, upper] root err err(est)
    1 [0.0000000, 2.5000000] 1.2500000 -0.9860680 2.5000000
    2 [1.2500000, 2.5000000] 1.8750000 -0.3610680 1.2500000
    3 [1.8750000, 2.5000000] 2.1875000 -0.0485680 0.6250000
    4 [2.1875000, 2.5000000] 2.3437500 +0.1076820 0.3125000
    5 [2.1875000, 2.3437500] 2.2656250 +0.0295570 0.1562500
    6 [2.1875000, 2.2656250] 2.2265625 -0.0095055 0.0781250
    7 [2.2265625, 2.2656250] 2.2460938 +0.0100258 0.0390625
    8 [2.2265625, 2.2460938] 2.2363281 +0.0002601 0.0195312
    9 [2.2265625, 2.2363281] 2.2314453 -0.0046227 0.0097656
```

(continues on next page)

```
10 [2.2314453, 2.2363281] 2.2338867 -0.0021813 0.0048828
11 [2.2338867, 2.2363281] 2.2351074 -0.0009606 0.0024414
Converged:
12 [2.2351074, 2.2363281] 2.2357178 -0.0003502 0.0012207
```

The next program solves the same function using a derivative solver instead.

```
#include <stdio.h>
#include <gsl/gsl_errno.h>
#include <gs1/gs1_math.h>
#include <gsl/gsl_roots.h>
#include "demo_fn.h"
#include "demo_fn.c"
int
main (void)
  int status;
  int iter = 0, max_iter = 100;
  const gsl_root_fdfsolver_type *T;
 gsl_root_fdfsolver *s;
  double x0, x = 5.0, r_expected = sqrt (5.0);
  gsl_function_fdf FDF;
  struct quadratic_params params = {1.0, 0.0, -5.0};
 FDF.f = &quadratic;
 FDF.df = &quadratic_deriv;
 FDF.fdf = &quadratic_fdf;
 FDF.params = &params;
  T = gsl_root_fdfsolver_newton;
  s = gsl_root_fdfsolver_alloc (T);
  gsl_root_fdfsolver_set (s, &FDF, x);
  printf ("using %s method\n",
         gsl_root_fdfsolver_name (s));
  printf ("%-5s %10s %10s %10s\n",
          "iter", "root", "err", "err(est)");
  do
      iter++;
     status = gsl_root_fdfsolver_iterate (s);
      x0 = x;
      x = gsl_root_fdfsolver_root (s);
      status = qsl_root_test_delta (x, x0, 0, 1e-3);
      if (status == GSL_SUCCESS)
       printf ("Converged:\n");
      printf ("%5d %10.7f %+10.7f %10.7f\n",
             iter, x, x - r_expected, x - x0);
  while (status == GSL_CONTINUE && iter < max_iter);</pre>
  gsl_root_fdfsolver_free (s);
```

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```
return status;
}
```

Here are the results for Newton's method:

```
$ ./a.out
using newton method
iter root err err(est)

1 3.0000000 +0.7639320 -2.0000000
2 2.3333333 +0.0972654 -0.6666667
3 2.2380952 +0.0020273 -0.0952381
Converged:
4 2.2360689 +0.0000009 -0.0020263
```

Note that the error can be estimated more accurately by taking the difference between the current iterate and next iterate rather than the previous iterate. The other derivative solvers can be investigated by changing  $gsl\_root\_fdfsolver\_newton$  to  $gsl\_root\_fdfsolver\_secant$  or  $gsl\_root\_fdfsolver\_steffenson$ .

# 36.11 References and Further Reading

For information on the Brent-Dekker algorithm see the following two papers,

- R. P. Brent, "An algorithm with guaranteed convergence for finding a zero of a function", *Computer Journal*, 14 (1971) 422–425
- J. C. P. Bus and T. J. Dekker, "Two Efficient Algorithms with Guaranteed Convergence for Finding a Zero of a Function", *ACM Transactions of Mathematical Software*, Vol.: 1 No.: 4 (1975) 330–345