HIntLib Manual

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1st November 2003

About This Document

To begin with, this document is a mess! It is supposed to document all the public interfaces provided by HIntLib. However, it is covering only about 10 % of them right now. It is also supposed to give examples of the usage of HIntLib, which at the moment it does not do at all.

This document refers to and is distributed with version 0.0.5 of HIntLib.

Contents

Chapter 1

Introduction

HINTLIB is a C++ library for high-dimensional numerical integration.

Chapter 2

Basic Types and Concepts

2.1 The Namespace HIntLib

All types, functions, and variables defined by HIntLib reside in the namespace `HIntLib`.

For reasons of conciseness, the namespace is never given explicitely in this document. However, the user should bear in mind that names like `u32` and `u64` in the next section are actually `HIntLib::u32` and `HIntLib::u64`, respectively.

2.2 Unsigned Numbers

Unsigned numbers play a major role in HINTLIB, since they are used for tasks as diverse as bit-maps or counting integrand evaluations.

The C++ language provides a number of unsigned types, however their size is not specified exactly. To ensure that the proper type is used in all situations, HINTLIB provides two typedefs: `u32` is the smallest unsigned integer type with at least 32 bits, `u64` the smallest type with at least 64 bits.

2.3 Counting Points

The type used by HINTLIB for counting points—for instance the number of allowed integrand evaluations, the number of abscissas of an interpolatory rule, or the current index in a low-discrepancy sequence—is `Index`.

`Index` is a typedef for either `u32` or `u64`, depending on the architecture. By default, HINTLIB uses 64 bits for `Index` if `unsigned long` has also at least 64 bits, assuming that the host computer has probably a 64-bit processor. If a different behavior is required, `Index` can be set to `u32` or `u64` by giving the options `--with-index=32` or `--with-index=64`, respectively, to `configure`. More information about configuring HINTLIB can be found in Appendix A.

2.4 Real Numbers

HINTLIB uses the type `real` for all real numbers.

By default, `real` is only a typedef for `double`. However, HINTLIB can be configured to use a different type to cope with increased precision or performance requirements. See Appendix A for details.

2.5 Points in $\mathbb{R}^s$

Points $\boldsymbol{x} \in \mathbb{R}^s$ are represented by C-style arrays of `real`s, i. e., a point $\boldsymbol{x}$ is usually passed to a function or method as `const real*`. This design seems rather low-level, but provides the most efficient implementation of this crucial data structure.

If the user needs to allocate memory for a point with a dimension not known at compile time, the datatype `Point` should be used. `Point` is a typedef for `Array<real>`, therefore it does not cause any memory or performance penalties compared to `new[]`. However, it is exception save and ensures that the memory allocated is freed even in the case of an exception.

2.6 Hypercubes $C_s \subset \mathbb{R}^s$

All integration routines implemented in HINTLIB work on hyper-rectangular domains. The concept of such a region $C_s = [r_1, t_1] \times \cdots \times [r_s, t_s] \subset \mathbb{R}^s$ is available as class `Hypercube`:

```
class Hypercube
{
public:
  explicit Hypercube (unsigned s);
  Hypercube (unsigned s, real r, real t);
  Hypercube (unsigned s, const real r [], const real t []);
```

Constructors are provided to create all kinds of `Hypercube`s. To be precise, $[0,1]^s$, $[r,t]^s$, and $[r_i, t_i]^s$ can be created directly by the constructors given above.

```
  Hypercube (const Hypercube &);
  Hypercube& operator= (const Hypercube&);
```

`Hypercube`s have value semantic, both copy-constructor and assignment are provided. Assignment can not be used to change the dimension of a `Hypercube`.

```
  Hypercube (Hypercube &, unsigned dim);
```

This constructor creates a new `Hypercube` by splitting a given one by halving it along the specified dimension. The newly constructed `Hypercube` is initialized to one half of the old cube, the `Hypercube` passed in as argument is set to the other half.

```
  unsigned int getDimension() const;
  real getVolume () const;
  const real* getCenter() const;
  const real* getWidth () const;
        real  getCenter (unsigned) const;
        real  getWidth  (unsigned) const;
        real  getUpperBound (unsigned) const;
        real  getLowerBound (unsigned) const;
        real  getDiameter (unsigned) const;
```

A large number of methods for querying all kind of information about a `Hypercube` are provided. Constant-time inline implementations are available for all these methods, so no overhead is introduced when `Hypercube`s are used.

```
  void set (unsigned dim, real a, real b);
```

Resets the lower and upper bound of the `Hypercube` for a certain dimension.

```
  void move (unsigend dim, real distance);
```

Moves the cube a certain distance in the given direction.

```
  void cutLeft  (unsigned dim);
  void cutRight (unsigned dim);
```

Halves the `Hypercube` along a certain coordinate axis and sets it either to the left or to the right part of itself.

```
};
```

The following function can be used for `Hypercube`s.

```
bool operator== (const Hypercube &) const;
bool operator!= (const Hypercube &) const;
bool isUnitCube () const;
```

Comparing cubes.

```
bool isPointInside (const Hypercube &, const real[]);
Hypercube::Location whereIsPoint (const Hypercube &, const real[]);
```

These functions determine whether a given point is inside a `Hypercube`. `isPointInside()` returns `true` or `false`, without any special treatment for borderline cases. `whereIsPoint()` returns `INSIDE`, `OUTSIDE`, or `BORDER`, depending on the position of the point. These three values are defined in the enumeration `Hypercube::Location`.

```
std::ostream& operator<< (std::ostream &, const Hypercube &);
```

Prints a readable version (lower and upper bounds) of the cube into an `ostream`.

2.7 Integrand Functions

All integrand functions have to implement the following, self-explanatory interface. The user basically provides an implementation for `operator()`, the method that evaluates the integrand for a given point $\boldsymbol{x} \in \mathbb{R}^s$.

```
class Integrand
{
public:
  explicit Integrand (unsigned s);
  virtual ~Integrand ();
  unsigned getDimension() const;

  virtual real operator() (const real []) = 0;
  virtual real derivative (const real [], unsigned d);
};
```

The constructor expects the dimensionality of the integrand as parameter.

Some cubature rules base their calculations not only on function values, but also on first partial derivatives. If such a rule is used, an implementation for `derivative()` has to be provided in addition to `operator()()`—the default implementation in `Integrand` merely throws `DerivativeNotSupported`.

2.8 Integral Estimate with Estimated Error

Another concept that arises quite naturally during the implementation of numerical integration routines is the combination of two `real` values, the first one representing the estimation Qf of an integral, the second one representing the estimated error Ef of this approximation. An object `EstErr` is used for implementing this concept. Even though this type is rather simple and has only a small number of convenience methods, the use of this class simplifies many integration routines and avoids bugs.

```
class EstErr
{
public:
  EstErr ();
  EstErr (real newEst, real newErr);

  real getEstimate() const;
  real getError()    const;
  real getRelError() const;

  void set (real newEst, real newErr);
  void setNoErr (real newEst);
  EstErr& operator+= (const EstErr &);
  EstErr& operator-= (const EstErr &);

  void scale (real a);
};
std::ostream& operator<< (std::ostream &, const EstErr &);
```

2.9 Integration Routines

All integration routines are subclasses of `Integrator`. This class provides a common interface for calling integration routines and defines a number of possible status codes that inform the user about the outcome of the calculation.

```
class Integrator
{
public:
  enum Status {
    ABS_ERROR_REACHED, // Estimated error <= reqAbsError
    REL_ERROR_REACHED, // Estimated error <= reqRelError
    MAX_EVAL_REACHED,  // Max integ evaluations reached
    ERROR,             // Other reason
  };
```

An `Integrator` returns one of these status codes if it has been able to derive a result.

```
  Integrator ();
```

An `Integrator` has only a normal constructor. Copy constructor and assignment are private.

```
  virtual
  Status integrate (Integrand &,
                    const Hypercube &,
                    Index maxEval,
                    real reqRelError, real reqAbsError,
                    EstErr &) = 0;
```

This pure virtual function is overwritten by subclasses of `Integrator` to provide the actual implementation of the integration routine. The integral and the integration error are estimated for a given integrand and a given hyper-rectangular domain. A requested relative or absolute error, or a maximum number of integrand evaluations has to be specified. The routine terminates when at least one of these three criteria is met. The returned `Status` reports which condition terminated the routine.

```
real operator() (Integrand &, const Hypercube &,
                 Index maxEval,
                 real reqRelError, real reqAbsError);
```

This convenience function calls `integrate()`, discards `Status` and the estimated error, and returns the estimate for the integral directly.

```
};
```

Chapter 3

Integration Routines

Chapter 4

Pseudo Random Number Generators

All `Integrator`s based on Monte Carlo or randomized QMC techniques require some source of random numbers, which is provided by the pseudo random number generators (PRNGs) described in this chapter. If a Monte Carlo routine does not produce the expected result, there is a good chance that the PRNG in use has some deficiency which surfaces in this specific calculation. Therefore, a number of PRNGs are provided to allow the user to choose.

4.1 General Concepts

This section describes the design issues considered during the implementation of the PRNG interface. You will probably need this information if you design your own PRNG or implement new Monte Carlo algorithms using one of the provided PRNGs. If you only want to use one of the existing PRNGs in combination with one of the existing `Integrator`s, you can skip this section and continue with the description of the various available PRNGs. You can also go directly to Section 4.4 which describes the Mersenne Twister, one of the best PRNGs available today.

4.1.1 Interface of PRNGs

A PRNG in the sense of HINTLIB is some class that provides the following interface:

```
class PRNGName
{
public:
   PRNGName (unsigned start = someDefault);
   void init (unsigned seed);

   typedef someType ReturnType;

   ReturnType  getMax() const;
   const real& getResolution() const;
   const real& getRange() const;

   ReturnType operator() ();
   int operator() (int max);
   real getReal();

   size_t getStateSize () const;
   void saveState (void *) const;
   void restoreState (const void *);
};
```

The constructor takes an `unsigned` with is used by `init()` to seed the state of the PRNG. Initializing two PRNGs of identical type with equal start values results in identical generated sequences. Implementations should try to guarantee that the sequences generated by different start values are non-overlapping for a long time. However, if this can actually be achieved by a PRNG depends on the implementation.

`operator()()` is used to get the next value from the generator. The return type of this function depends on the PRNG. Usually, it is `long`, `u32`, or `u64`. This type is available as `ReturnType`. The number returned by `operator()` is always larger or equal to 0 and less or equal to $m =$ `getMax()`. For a manual conversion to a real number, it is often useful to have $m+1$ and $1/(m+1)$ available, with can easily be obtained by `getRange()` and `getResolution()`, respectively.

`operator()(int max)` returns a random integer from $\{0, 1, 2, \ldots, max - 1\}$. Syntax and semantics of this method are exactly what the C++ Standard Template Library expects as a Random Number Generator object.

`getReal()` returns a random sample from the uniform distribution on $(0, 1)$. Implementations have to ensure that 0 and 1 are never returned.

`saveState()` and `restoreState()` allow to save and restore the state of the PRNG to/from some buffer in memory. `getStateSize()` gives the required size of this buffer in `char`s.

4.2 Linear Congruential Generators

Linear Congruential Generators (LCGs) produce pseudo random numbers by the simple recurrence

$$x_{n+1} = ax_n + c \bmod m.$$

Parameters a, c, and m have to be chosen obeying a number of constraints in order to make the sequence appear to be random. In addition to these theoretical constraints, the multiplication modulo m can be implemented efficiently only for certain values of m and a.

Detailed information on the construction of powerful LCGs and a detailed discussion of the proper choice of m, a, and c can be found in [9, Section 3.2.1].

4.2.1 LCGs with $m = 2^e$

LCGs with $m = 2^e$ can be implemented very efficiently on binary machines. However, the modulus leads to a number of caveats in the quality of the PRNG, most noteworthy that the lower order bits show a periodic pattern.

The choice of $c = 0$ leads to a slightly faster generator because the incrementation of x_n can be skipped. However, this marginal performance improvement is bought by restricting the period length to one fourth ($m/4$ instead of m) and invalidating half of the possible seed values (all x_n, and therefore x_0, have to be odd). An arbitrary odd value for c does not impose these restrictions. Therefore, the only two reasonable values for c are $c = 0$ (if efficiency is a premium) and $c = 1$, which allows a faster implementation than any other odd c and does not introduce any restrictions on the period length. The maximum period as described above is accomplished if and only if $a \bmod 4 = 1$ for c odd and $a \bmod 8 \in \{3, 5\}$ for $c = 0$ and $e > 3$.

Implementation

A special implementation making use of the optimizations possible for power-of-two modulus is provided as template `LCG_Pow2<>`:

```
template<typename T, T a, unsigned e, T c = T(1)>  // from lcg_pow2.h
class LCG_Pow2
{
```

```
public:
   LCG_Pow2 (unsigned start = 0, bool force = false);

   static const T A = a;
   static const T C = c;
   typedef T ReturnType;

   // other members common to all PRNGs
};
```

The first template parameter `typename T` must be an unsigned integral type, large enough to store e bits. The parameters a, e, and c of the LCG are provided as template parameters, allowing complete inlining and optimal code generation for all time-critical operations.

The constructor takes an optional *start* argument, specifying the initial value of the generator. x_0 is set to *start* if c is odd, otherwise to $2 \cdot start + 1$, ensuring that the maximal possible period is achieved. The boolean argument *force* determines, if the constructor should perform a consistency check on the values a, c, m as described above. Since all three values are available at compile time, this check can usually be optimized away by the compiler and does not introduce any runtime overhead. Setting $force = true$ allows the construction of a degenerated LCGs with a period length less than m and $m/4$ for c odd and $c = 0$, respectively.

`init()` can be used to reinitialize the generator.

`operator()()` returns the current value x_n from $\{0, 1, \ldots, m-1\}$ if c is odd. If $c = 0$, then $x_n \in \{1, 5, 9, \ldots, m-3\}$ or $x_n \in \{3, 7, 11, \ldots, m-1\}$, depending on the set x_0 belongs to. `operator()(n)` returns $\lfloor n x_n / m \rfloor \in \{0, 1, \ldots, n-1\}$. `getReal()` returns $(x_n + 1/2)/m$ for c odd, and x_n/m for c even. Both results are strictly between 0 and 1.

Predefined LCGs of this type

A number of LCGs of this type are provided as `typedef`s. All these generators, including the comments provided here are taken from the spectral test result list in [9, Section 3.3.4]:

```
LCG_Pow2<u32,1103515245,32,12345> LCG_Pow2_Ansi_C;
```

The generator proposed in the ANSI C reference.

```
typedef LCG_Pow2<u64,1220703125,35,0> LCG_Pow2_Taussky_0;
typedef LCG_Pow2<u64,1220703125,35,1> LCG_Pow2_Taussky;
```

A reminder of the good old days when 35 bits was a common word size. It performs quite well in the spectral test, but requires 64 bit architecture. It is due to O. Taussky an is listed as line 11 of Knuth's spectral test result list.

```
typedef LCG_Pow2<u32,65539u,31,0> LCG_Pow2_RANDU_0
```

This is the infamous RANDU, one of the wort generators ever conceived. It has exceptionally bad values in the spectral test in dimensions 3, 4, 5, and 6 and therefore should have never be used. $a \bmod 4 = 3$, therefore this generator can only be used with $c = 0$, making it even worse. Line 12 in [9].

```
typedef LCG_Pow2<u32,1812433253,32,0> LCG_Pow2_BoroshNiederreiter_0;
typedef LCG_Pow2<u32,1812433253,32,1> LCG_Pow2_BoroshNiederreiter;
```

Borosh–Niederreiter multiplier for $m = 2^{32}$. Line 13.

```
typedef LCG_Pow2<u32,1566083941,32,0> LCG_Pow2_Waterman_0;
typedef LCG_Pow2<u32,1566083941,32,1> LCG_Pow2_Waterman;
```

Due to A. Waterman. Line 14.

```
typedef LCG_Pow2<u32,69069,32,0> LCG_Pow2_69069_0;
typedef LCG_Pow2<u32,69069,32,1> LCG_Pow2_69069;
```

Here is another famous one, probably due to its nice looking a. However, it also performs well in the spectral test. Line 15.

```
typedef LCG_Pow2<u32,1664525,32,0> LCG_Pow2_LavauxJanssens32_0;
typedef LCG_Pow2<u32,1664525,32,1> LCG_Pow2_LavauxJanssens32;
typedef LCG_Pow2<u64,31167285ull,48,0> LCG_Pow2_LavauxJanssens48_0;
typedef LCG_Pow2<u64,31167285ull,48,1> LCG_Pow2_LavauxJanssens48;
```

These two multipliers have been found by M. Lavaux and F. Janssens in a computer search for spectrally good multipliers having a very high μ_2. Lines 16 and 23.

```
typedef LCG_Pow2<u64,44485709377909ull,48,0> LCG_Pow2_Cray_0;
typedef LCG_Pow2<u64,44485709377909ull,48,1> LCG_Pow2_Cray;
```

The one with $c = 0$ is used in the Cray X-MP library. Line 22.

```
typedef LCG_Pow2<u64,636413622384679300 5ull,64,0> LCG_Pow2_Haynes_0;
typedef LCG_Pow2<u64,636413622384679300 5ull,64,1> LCG_Pow2_Haynes;
```

Finally, an excellent one for 64 bit numbers due to C. E. Haynes. Line 26.

4.2.2 LCGs with m prime and special multiplier

LCGs with a prime number modulus m have advantageous theoretical properties. If the multiplier a is chosen to be a primitive element modulo m, a period length of $m - 1$ (cycling through all values except 0) is obtained even for $c = 0$. The low-order bits are as random as the most significant bit.

The drawback is that a prime-number LCG with m close to the word size requires double-word and therefore slow arithmetic to calculate $x_{n+1} = ax_n \bmod m$. However, for m fitting in a signed integer variable and certain well-chosen a, there is an algorithm that allows the calculation of x_{n+1} from x_n using only ordinary integer arithmetic. This algorithm requires two constants $q = \lfloor m/a \rfloor$ and $r = m \bmod a$. It works if and only if r turns out to be less than q, which is less likely for increasing a.

Implementation

```
template<typename T, T a, T m>     //  from lcg_prim.h
class LCG_Prime
{
public:
   LCG_Prime (unsigned start = 0);

   typedef T ReturnType;

   static const T    A = a;
   static const T    M = m;
   static const T    C = 0;

   typedef T ReturnType;
   // other members common to all PRNGs
};
```

The first template parameter `typename T` must be a signed integral type, large enough to store m. The parameters a and m of the LCG are provided as template parameters, allowing complete inlining of all time-critical operations.

The constructor takes an optional *start* argument, specifying the initial value of the generator to $x_0 = start + 1$. `init()` can be used to reinitialize the generator. The constructor contains code for doing some consistency checks on `T`, a and m. These tests can be done at compile time, so no additional run time overhead is introduced.

`getMax()` returns the value x_n from $\{1, 2, \ldots, m-1\}$. `operator(n)` return $\lfloor nx_n/m \rfloor \in \{0, 1, \ldots, n-1\}$. `getReal()` returns x_n/m which is strictly between 0 and 1.

Predefined LCGs of this type

A number of LCGs of this type are provided as `typedef`s. All these generators, including the comments provided here, are taken from the Spectral Test result list in [9, Section 3.3.4]:

```
typedef LCG_Prime<long, 7*7*7*7*7, (1ul << 31) - 1> LCG_Prime_IMSL;
```

This generator is know is the "Minimum Standard Generator" and has been one of the main generators in the popular IMSL subroutine library since 1971. The multiplier $a = 7^5 = 16807$ is due to Lewis, Goodman, and Millers and the main reason for its continued use that a^2 is less than the modulus m, hence fast algorithms for calculating $ax \bmod m$ have been available for quite some time. However, the following multipliers perform better in the spectral test and allow for the same efficient implementation. Line 19 in [9].

```
typedef LCG_Prime<long, 48271, (1ul << 31) - 1> LCG_Prime_Fishman;
```

The best multipliers for $m = 2^{31} - 1$ (a Mersenne Prime) allowing this implementation technique. Due to G. S. Fishman. Line 20.

```
typedef LCG_Prime<long, 40692, (1ul << 31) - 249> LCG_Prime_Lecuyer;
```

Another good one, due to P. L'Ecuyer, for a slightly smaller prime modulus. Line 21.

4.3 Combined LCGs

Two LCGs x_n and y_n can be combined to a new generator by simply using

$$z_n := x_n - y_n \bmod m$$

where m is the larger one of the moduli of x_n and y_n (see [9, Section 3.2.2]).

Implementation

```
template<typename T, T a1, T m1, T a2, T m2>
class LCG_Combined
{
public:
   LCG_Combined (unsigned start = 0);
   typedef T ReturnType;
   // other members common to all PRNGs
};
```

The first template parameter `typename T` must be a signed integral type, large enough to store m_1 and m_2. The parameters a_1, a_2, m_1 and m_2 define the LCGs to be used.

Predefined LCGs of this type

A `typedef` exists for the following combined LCG: It is taken from the spectral test result list in [9, Section 3.3.4]:

```
typedef LCG_Combined<long,
   48271, (1ul << 31) - 1,
   40692, (1ul << 31) - 249> LCG_Combined_Lecuyer;
```

This generator is based on two prime-modulus LCGs discussed in Section 4.2.2 and has a period length of $(2^{31}-1)(2^{31}-249)$. The spectral test results can be found in line 24 of Knuth's Spectral Test result list in [9, Section 3.3.4]

4.4 Mersenne Twister

The Mersenne Twister PRNG was proposed by M. Matsumoto and T. Nishimura in [10]. It has a period of $2^{19937}-1$ (a Mersenne Prime), produces a sequence that is 623-dimensionally equidistributed, has passed many stringent tests, including the *die-hard test* of G. Marsaglia and the *load-test* of P. Hellekalek and S. Wegenkittl, and has no known weaknesses. Therefore, it is considered to be one of the best PRNGs available today.

A number of open source implementations are publicly available, most noteworthy the original implementation of Takuji Nishimura in C, an optimized C version due to S. Cokus, and a Mersenne Twister source-forge project maintained by R. J. Wagner. The implementation contained in this library is compatible to each of them, including initialization. At least on my computer, it is also faster than any of the other implementations.

```
class MersenneTwister    // from mersennetwister.h
{
public:
   MersenneTwister (u32 start = 4357u);
   void init (unsigned = 4357u);
   void initCokus (unsigned start = 4357u);

   typedef u32 ReturnType;

   // other members common to all PRNGs
};
```

Three different initialization routines are available: `init()` is compatible with the original code of Nishimura, as well as Wagner's `MTRand` class. It used the LCG $x_0 = start$, $x_{n+1} = 69069x_n + 1$ to seed the state of the generator. Each 32-bit integer in `MersenneTwisters`'s state array is seeded by combining the most significant 16 bits of two values of this LCG.

`initCokus()` is compatible with Cokus' implementation. It uses the LCG $x_0 = start|1$, $x_{n+1} = 69069x_n$ to seed the state array. Therefore, $start$-values $2n$ and $2n+1$ result in the same initialization. Use this initialization routine only for compatibility reasons.

The constructor uses `init()` to initialize the state array. Non of these initializers guarantees that the sequences resulting form two different start values are non-overlapping. If you know a method for seeding `MersenneTwister` in away that allows the construction of n different non-overlapping sequence with a length of at least m, please let me know!

4.5 The Built-In Random Number Generator

Every C and C++ implementation provides a built-in PRNG available through the C library functions `rand()` and `srand()`. The following class from `builtinprng.h` provides an interface to this facility that is compatible with HIntLib.

```
class BuiltInPRNG      // from builtinprng.h
{
public:
   BuiltInPRNG (unsigned start = 0);
   ~BuiltInPRNG ();

   typedef int ReturnType;

   // other members common to all PRNGs
};
```

`operator()` is just a call to `rand()`, `seed()` a call to `srand()`. The implementation ensures that only one instance of `BuiltInPRNG` exists at the same time.

Chapter 5

Low Discrepancy Sequences

Chapter 6

Interpolatory Cubature Rules

Cubature rules are the basic building block of most adaptive integration routines. These algorithms use a certain basic rule

$$\mathrm{Q}_n f := \sum_{i=1}^{n} w_i f(\boldsymbol{x}_i)$$

with a fixed number n of abscissas which is applied to subregions of the initial integration domain. The final result is obtained by combining the transformed rules for each subregion to a copy rule for the whole integration domain.

A good cubature rule is crucial for the performance of every adaptive algorithm. Primarily, the cubature rule must provide two methods for the adaptive integration routine:

- The cubature rule must give good approximations $\mathrm{Q}_n f$ of $\mathrm{I} f$, while requiring a low number of integrand evaluations n.
- The cubature rules must support some method for estimating the integration error $|\mathrm{Q}_n f - \mathrm{I} f|$. The actual value of this estimation is not important. The required property is that a high estimated error is reported if and only if the actual integration error is large.

The second functionality (error estimation) is usually implemented based on the first one: two cubature rules $\mathrm{Q}^{(1)}_{n^{(1)}}$ and $\mathrm{Q}^{(2)}_{n^{(2)}}$ of different degree of accuracy are used. We assume that $\deg \mathrm{Q}^{(1)} > \deg \mathrm{Q}^{(2)}$, which will usually result in $n^{(2)}$ being significantly smaller than $n^{(1)}$. If these two rules are applied to the same integrand, the integration error $\left|\mathrm{Q}^{(1)} f - \mathrm{I} f\right|$ can be expected to be less than the difference $\mathrm{E} f := \left|\mathrm{Q}^{(1)} f - \mathrm{Q}^{(2)} f\right|$ of both estimations, i. e.

$$\left|\mathrm{Q}^{(1)} f - \mathrm{Q}^{(2)} f\right| \geq \left|\mathrm{Q}^{(1)} f - \mathrm{I} f\right| .$$

When $n^{(2)}$ is significantly smaller than $n^{(1)}$, this error estimation comes at little additional cost ($n^{(1)} + n^{(2)}$ instead of $n^{(1)}$ integrand evaluations). In some cases, the rule $\mathrm{Q}^{(2)}$ uses a subset of the abscissas of $\mathrm{Q}^{(1)}$. In this case, error estimation does not require any additional integrand evaluation, and $\mathrm{Q}^{(1)}$-$\mathrm{Q}^{(2)}$ is called an *Embedded Rule*.

One of the most complete collections of techniques, as well as theoretical results available for the construction of cubature rules is Stroud's monograph [16]. Even though this book is more than 30 years old, it has not been superseded by anything comparable.

6.1 Implementation

This section describes the objects that are used for implementing cubature rules.

6.1.1 Class `CubatureRule`

All implemented cubature rules are subclasses of a single base class `CubatureRule`. An object of this type is created for a given dimension s and can be used for estimating the integral of various integrands on various hyperrectangular regions with this dimension.

```
class CubatureRule
{
   CubatureRule();
   virtual ~CubatureRule();
```

The constructor of subclasses is primarily used for initializing all dimension-depending constants and to reserve extra memory that may be required for a fast evaluation of the rule. The destructor has to clean up this extra memory.

```
   virtual real eval (Integrand &, const Hypercube &) = 0;
```

This pure virtual function has to be implemented by subclasses of `CubatureRule` to provide the actual implementation of the cubature rule. The cubature rule is applied to a given integrand and a hyper-rectangular region.

```
   virtual unsigned getDimension()      const = 0;
   virtual Index    getNumPoints()      const = 0;
   virtual unsigned getDegree()         const = 0;
   virtual bool     isAllPointsInside() const = 0;
   virtual real     getSumAbsWeight()   const = 0;
};
```

These methods can be used by algorithms to query basic information about a rule. Knowing the number of abscissas of the rule (`getNumPoints()`) is particularly important, because it allows algorithms to decide how often they can apply the rule until the number of available integrand evaluations is exhausted.

`getDimension()` returns the dimension of the rule, `getDegree()` its polynomial degree. `isAllPointsInsied()` is `true` if and only if all abscissas are inside the `Hypercube` the rule is applied to. Finally, `getSumAbsWeight()` returns the sum of the absolute weights, i. e.

$$\sum_{i=1}^{n} |w_i| \,.$$

`CubatureRules` cannot be assigned or copied.

6.1.2 Class `EmbeddedRule`

Class `EmbeddedRule` is a subclass of `CubatureRule` with the additional features of giving error estimations.

```
class EmbeddedRule : public CubatureRule
{
public:
   EmbeddedRule();

   virtual unsigned evalError
      (Integrand &, const Hypercube &, EstErr &ee) = 0;
```

This method is similar to `eval()` of `CubatureRule`. The difference is that, instead returning a `real`, an object of type `EstErr` (Section 2.8) is updated. The `unsigned` returned by `evalError()` suggests a split-direction for subsequent subdivision steps.

```
    virtual real eval (Integrand &, Hypercube &);
```

`EmbeddedRule` contains an implementation of the abstract method `CubatureRule::eval()`. It simply calls `evalError()`, discards the estimation of the error and returns the estimation for the integral as result.

```
};
```

6.1.3 Factories for Cubature Rules

A `CubatureRule` can only be applied to integration problems of a certain dimension which cannot be changed after the `CubatureRule` is created. Often one needs to specify a certain type of cubature rule, without determining the dimension. This can be accomplished by using a `CubatureRuleFactory`.

```
class CubatureRuleFactory
{
public:
   CubatureRuleFactory();
   virtual ~CubatureRuleFactory();
   virtual CubatureRule* create (unsigned) = 0;
   virtual CubatureRuleFactory* clone() const = 0;
};

class EmbeddedRuleFactory : public CubatureRuleFactory
{
public:
   EmbeddedRuleFactory();
   virtual ~EmbeddedRuleFactory();
   virtual EmbeddedRule* create (unsigned) = 0;
   virtual EmbeddedRuleFactory* clone() const = 0;
};
```

A `CubatureRuleFactory` creates `CubatureRule`s of a certain type. A call to `create()` returns a new `CubatureRule` for the specified dimension allocated on the free store. The user is responsible for `delete`ing it if it is not used anymore.

`CubatureRuleFactory`s cannot be copied or assigned. There is a `clone()` method which creates a copy, allocated on free store. In general, `CubatureRuleFactories` are always allocated on the free store.

`EmbeddedRuleFactory` is a subclass of `CubatureRuleFactory`, creating `EmbeddedRules`.

6.1.4 Pseudo Embedded Rules

For embedded rules, it is easy to implement `EmbeddedRule` directly. However, if a rule with error estimation is to be assembled from two unrelated rules, the following class can be used. Its constructor takes two `CubatureRuleFactories` in its constructor, and implements all other required methods by appropriately forwarding the calls.

```
class PseudoEmbeddedRule : public EmbeddedRule
{
public:
   PseudoEmbeddedRule (
      unsigned dimension,
      CubatureRuleFactory *fac1,
      CubatureRuleFactory *fac2);
```

```
    // All pure virtual functions inherited from EmbeddedRule
    // are implemented
};
```

The constructor of `PseudoEmbeddedRule` expects the dimension of the rule, together with two pointers to `CubatureRuleFactory`s, which are used for creating the `CubatureRules` the new `EmbeddedRule` is based upon.

```
class PseudoEmbeddedRuleFactory : public EmbeddedRuleFactory
{
public:
   PseudoEmbeddedRuleFactory (CubatureRuleFactory *fac1,
                              CubatureRuleFactory *fac2);

   virtual PseudoEmbeddedRuleFactory* clone() const;
   virtual PseudoEmbeddedRule* create (unsigned dim);
};
```

There is also an `EmbeddedRuleFactory` available which creates `PseudoEmbeddedRules`. Its constructor takes two pointers to `CubatureRuleFactories`. These factories are not `cloned` by the constructor, but `deleted` by the destructor of `PseudoEmbeddedRuleFactory`.

6.2 Implemented Cubature Rules

An abundant number of different cubature rules for multi-dimensional integration can be found in the literature. The most comprehensive collection of rules has been compiled by Stroud in [16], which covers most cubature rules known in 1971. This work was continued by Cools in [2], a collection of literature references published under the title *"Monomial Cubature Rules since* 'Stroud' ".

From all the cubature rules referenced in these collections, only those with the following properties have been implemented:

- Only rules for the hypercube C_s have been considered
- The article presenting the rule must contain all information for actually implementing the rule

Most cubature rules referenced in [16] and [2] with the stated properties have been implemented. The following sections will discuss these rules in detail.

The class name of the rules is always given in the section name. There is always a constructor of the form *`classname`*`(unsigned dim)`, and a `Cubature/EmbeddedRuleFactory` can be created using the static member function *`classname`*`::getFactory()`.

6.2.1 Midpoint Rule (`Rule1Midpoint`)

Degree 1, Fully Symmetric with $1 = O(1)$ point, equal-weight formula. For $s \geq 1$.

C_s:1-1 in [16].

Abscissas	w_i
$(0, \ldots, 0)$	V

This is the simplest possible integration formula. It consists of a single point in the center of C_s. The single weight w_1 is V, making this formula not only a positive-, but also an equal-weight formula. However, the degree is 1, so nothing but linear functions are integrated exactly.

6.2.2 Product Trapezoidal Rule (`Rule1Trapezoidal`)

Degree 1, Fully Symmetric with $2^s = O(2^s)$ points, equal-weight formula. For $s \geq 1$.
C_s:1-2 in [16].

Abscissas	w_i
$(\pm 1, \ldots, \pm 1)$	$\frac{1}{2^s} V$

This is the tensor product formula of the 1-dimensional trapezoidal rule

$$\int_a^b f(x)\,dx \approx \frac{f(a)+f(b)}{2}.$$

6.2.3 "Simplex" Rule (`Rule2Simplex`) due to Stroud

Degree 2, Non-symmetric with $s+1 = O(s)$ points, equal-weight formula. For $s \geq 1$.
[14] and C_s:2-1 in [16].

The integration nodes of this formula are the vertices of an s-dimensional regular simplex. The tricky part is to rotate it to make it fit into the cube for any possible dimension s.

6.2.4 A Degree 2 Rule due to Thacher (`Rule2Thacher`)

Degree 2, Non-symmetric with $2s+1 = O(s)$ points, $\frac{1}{V}\sum_{i=1}^{n} |w_i| = O(s)$. For $s \geq 1$.
[17] and C_s:2-2 in [16].

Abscissas	w_i
$(2r, \ldots, 2r)$	V
$(1, r, \ldots, r)_{\mathrm{S}}$	$-rV$
$(-1, r, \ldots, r)_{\mathrm{S}}$	rV

with $r = \frac{\sqrt{3}}{6}$.

6.2.5 A Degree 2 Rule due to Ionesu (`Rule2Ionescu`)

Degree 2, Non-symmetric with 4 integrand and 2 derivative evaluations. Only for $s = 2$.
[8] and C_2:2-1 in [16].

Abscissas	w_i
$(-1, -1)$	$\frac{1}{4} V$
$(1, -1)$	$\frac{1}{12} V$
$(-1, 1)$	$\frac{1}{12} V$
$(1, 1)$	$\frac{7}{12} V$
$\frac{\partial}{\partial x}(1, 1)$	$-\frac{1}{3} V$
$\frac{\partial}{\partial y}(1, 1)$	$-\frac{1}{3} V$

In addition to integrand values (`Integrand::operator()()`), this rule uses derivatives of the integrand function to estimate the integral. Therefore, the integrand function has to define `Integrand::derivative()`.

6.2.6 "Octahedron" Rule due to Stroud (`Rule3Octahedron`)

Degree 3, Non-symmetric with $2s = O(s)$ points, equal-weight formula. For $s \geq 1$.
[14] and C_s:3-1 in [16].
The integration nodes of this formula are the vertices of an s-dimensional regular octahedron. The tricky part is to rotate the octahedron such that it fits into the cube for any possible dimension s.

6.2.7 `Rule3Cross`

Degree 3, Fully Symmetric with $2s = O(s)$ points, equal-weight formula. For $s \geq 1$.
C_s:3-2 in [16].

Abscissas	w_i
$(\sqrt{\frac{s}{3}}, 0, \ldots, 0)_{\mathrm{FS}}$	$\frac{1}{2s}V$

For $s > 3$ all abscissas are outside C_s.

6.2.8 A Degree 3 Rule due to Tyler (`Rule3Tyler`)

Degree 3, Fully symmetric with $2s + 1 = O(s)$ points, $\frac{1}{V}\sum_{i=1}^{n} |w_i| = O(s)$. For $s \geq 1$.
[18] and C_s:2-3 in [16].

Abscissas	w_i	
$(0, \ldots, 0)$	W_1	
$(1, 0, \ldots, 0)_{\mathrm{FS}}$	W_2	with $W_1 = \frac{3-s}{3}V$ and $W_2 = \frac{1}{6}V$.

The weight W_1 is negative for $s > 3$. For $s = 3$ the weight W_1 becomes 0, thus, the rule has actually only 6 instead of 7 abscissas. However, this optimization is not implemented at the moment.

6.2.9 Product Gauss Rule of Degree 3 (`Rule3Gauss`)

Degree 3, Fully symmetric with $2^s = O(2^s)$ points, equal-weight formula. For $s \geq 1$.
C_s:2-4 in [16].

Abscissas	w_i	
$(\alpha, \ldots, \alpha)_{\mathrm{FS}}$	$\frac{1}{2^s}V$	with $\alpha = \frac{1}{\sqrt{3}}$.

This is the tensor product formula of the 1-dimensional 2-point degree 3 Gauss formula

$$\int_0^1 f(x)\,dx \approx \frac{f(-\frac{1}{\sqrt{3}}) + f(-\frac{1}{\sqrt{3}})}{2}.$$

6.2.10 A Degree 3 Rule due to Ewing (`Rule3Ewing`)

Degree 3, Fully symmetric with $2^s + 1 = O(s^s)$ points, positive-weight formula. For $s \geq 1$.
[4] and C_s:3-5 in [16].

Abscissas	w_i	
$(0, \ldots, 0)$	W_1	
$(\pm 1, \ldots, \pm 1)$	W_2	with $W_1 = \frac{2}{3}V$ and $W_2 = \frac{1}{3\cdot 2^s}V$.

Most points are at the border of C_s.

6.2.11 A Degree 5 Rule due to Hammer and Stroud (`Rule5Hammer`)

Degree 5, Fully symmetric with $2s^2+1 = O(s^2)$ points, $\frac{1}{V}\sum_{i=1}^{n}|w_i| = O(s^2)$. For $s \geq 2$.

[7] and C_s:5-2 in [16].

Abscissas	w_i
$(0,\ldots,0)$	W_0
$(\sqrt{\frac{3}{5}},0,\ldots,0)_{\mathrm{FS}}$	$W_{\alpha,1}$
$(\sqrt{\frac{3}{5}},\sqrt{\frac{3}{5}},0,\ldots,0)_{\mathrm{FS}}$	$W_{\alpha,2}$

6.2.12 A Degree 5 Rule due to Stroud (`Rule5Stroud`)

Degree 5, Symmetric with $3s^2+3s+1 = O(s^2)$ points, $\frac{1}{V}\sum_{i=1}^{n}|w_i| = O(s^2)$. For $s \geq 2$.

[15] and C_s:5-3 in [16].

Abscissas	w_i
$(0,\ldots,0)$	W_0
$(\alpha,\alpha,0,\ldots,0)_{\mathrm{S}}$	$W_{\alpha,2}$
$(-\alpha,-\alpha,0,\ldots,0)_{\mathrm{S}}$	$W_{\alpha,2}$
$(\alpha,0,\ldots,0)_{\mathrm{FS}}$	$W_{\alpha,1}$
$(\beta,-\gamma,0,\ldots,0)_{\mathrm{S}}$	$W_{\beta+\gamma}$
$(-\beta,\gamma,0,\ldots,0)_{\mathrm{S}}$	$W_{\beta+\gamma}$
$(\beta,0,\ldots,0)_{\mathrm{FS}}$	$W_{\beta,\gamma}$
$(\gamma,0,\ldots,0)_{\mathrm{FS}}$	$W_{\beta,\gamma}$

with $\alpha = \sqrt{\frac{7}{15}}$, $\beta = \sqrt{\frac{7+\sqrt{24}}{15}}$, and $\gamma = \sqrt{\frac{7-\sqrt{24}}{15}}$.

6.2.13 A Degree 7 Rule due to Phillips (`Rule7Phillips`)

Degree 7, Fully symmetric with $\frac{4}{3}s^3 - 2s^2 + \frac{14}{3}s + 1 = O(s^3)$ points, $\frac{1}{V}\sum_{i=1}^{n}|w_i| = O(s^3)$. For $s \geq 5$.

[12, 3] and C_s:7-1 in [16].

Abscissas	w_i
$(0,\ldots,0)$	W_0
$(1,0,\ldots,0)_{\mathrm{FS}}$	W_α
$(\beta_s,0,\ldots,0)_{\mathrm{FS}}$	W_β
$(\sqrt{\frac{3}{5}},\sqrt{\frac{3}{5}},0,\ldots,0)_{\mathrm{FS}}$	W_γ
$(\sqrt{\frac{3}{5}},\sqrt{\frac{3}{5}},\sqrt{\frac{3}{5}},0,\ldots,0)_{\mathrm{FS}}$	W_δ

This formula is proposed in [12]. In [3] Dobrodeev proposes a 7th-degree formula with the same basic structure. He presents the formulas for abscissas and weights without showing how these results have been obtained. Even though the notation used by Dobrodeev is significantly different, it turns out that both formulas are actually identical. Due to the fact that Dobrodeev's paper does not contain a derivation and was published three years after Phillips' paper, this formula will be referred to as Rule Phillips and not as Rule Dobrodeev in HINTLIB.

6.2.14 A Degree 9 Rule due to Stenger (`Rule9Stenger`)

Degree 9, Fully symmetric with $\frac{4}{3}s^4 - \frac{20}{3}s^3 + \frac{56}{3}s^2 - \frac{28}{3}s + 4 = O(s^4)$ points, $\frac{1}{V}\sum_{i=1}^{n}|w_i| = O(s^4)$. For $s \geq 4$.

[13] and C_s:9-1 in [16].

Abscissas	w_i
$(0,\ldots,0)$	W_0
$(\alpha,0,\ldots,0)_{\mathrm{FS}}$	W_α
$(\beta,0,\ldots,0)_{\mathrm{FS}}$	W_β
$(\alpha,\alpha,0,\ldots,0)_{\mathrm{FS}}$	$W_{2\alpha}$
$(\beta,\beta,0,\ldots,0)_{\mathrm{FS}}$	$W_{2\beta}$
$(\alpha,\beta,0,\ldots,0)_{\mathrm{FS}}$	$W_{\alpha\beta}$
$(\beta,\beta,\beta,0,\ldots,0)_{\mathrm{FS}}$	$W_{3\beta}$
$(\alpha,\alpha,\alpha,\alpha,0,\ldots,0)_{\mathrm{FS}}$	$W_{4\alpha}$
$(\beta,\beta,\beta,\beta,0,\ldots,0)_{\mathrm{FS}}$	$W_{4\beta}$

with $\alpha = \frac{5}{9} + \sqrt{\frac{50}{567}}$, $\beta = \frac{5}{9} - \sqrt{\frac{50}{567}}$.

6.2.15 An Embedded Degree 7 Rule Due to Genz and Malik (`Rule75GenzMalik`)

Degree 7, Fully symmetric with $2^s + 2s^2 + 2s + 1 = O(2^s)$ points,
$\frac{1}{V}\sum_{i=1}^{n}|w_i| = O(s^2)$. For $s \geq 2$. [5].

Abscissas	w_i	w_i'
$(0,\ldots,0)$	W_0	W_0'
$(\alpha,0,\ldots,0)_{\mathrm{FS}}$	W_α	W_α'
$(\beta,0,\ldots,0)_{\mathrm{FS}}$	W_β	W_β'
$(\beta,\beta,0,\ldots,0)_{\mathrm{FS}}$	$W_{2\beta}$	$W_{2\beta}'$
$(\gamma,\ldots,\gamma)_{\mathrm{FS}}$	W_δ	

with $\alpha = \sqrt{\frac{9}{70}}$, $\beta = \sqrt{\frac{9}{10}}$, and $\gamma = \sqrt{\frac{9}{19}}$.

This cubature rule is proposed by Genz and Malik in [5]. It is special in various ways: To begin with, this rule contains an embedded degree 5 rule, which uses a subset of the abscissas of the degree 7 rule, so no additional integrand evaluations are required to evaluate it. Therefore, `Rule75GenzMalik` is a subclass not only of `CubatureRule`, but also of `EmbeddedRule`.

The abscissas of the rule do not depend on the dimension s, which simplifies the implementation of this rule. Even though the number of abscissas increases exponentially with the dimension s, the number of abscissas for dimensions $s \leq 11$ is small compared to other degree 7 rules. However, the probably most important feature of this rule is the low sum of its absolute weights, which makes its results extraordinarily stable.

This cubature rule is only a special case of a family of cubature rules developed by Genz and Malik in [6]. In this article a complete theory of a family of cubature rules $R^{(m,s)}$ of degree $2m+1$ for arbitrary dimensions s and $1 \leq m \leq 6$ is developed, with the rule given here corresponding to $R^{(3,s)}$. This family is fully embedded, i. e., the abscissas of $R^{(m-1,s)}$ are a subset of the abscissas of $R^{(m,s)}$, allowing the construction of efficient embedded cubature rules of degree $3, 5, \ldots, 13$. Even though Cools and Haegemans [1] have tackled the resulting equations for weights and abscissas with a computer algebra systems and achieved significant simplifications, especially for the generation of the abscissa set, this general family has been considered as too complicated for an implementation.

Chapter 7

Algebraic Structures

Digital nets and sequences, as well as other number theoretic constructions for low discrepancy sequences are based on algebraic structures like finite rings and fields, as well as polynomials and vector spaces based thereupon.

This chapter describes the classes available in HIntLib for performing arithmetic in these structures.

7.1 Concepts

Algebraic structures share concepts, not interfaces, because the basic operations are usually very simple and require inlining to be executed sufficiently fast. Most algebraic structures implement one or more the the following concepts.

7.1.1 Basic Features

An algebraic structure in the sense of HIntLib is a class encapsulating the features of some (number theoretical) algebraic structure. The methods provided by these classes perform the algebraic operations available in this structure (e. g. adding two values), while the data members of such a class contain all the information for actually performing these calculations. This data may consist of nothing (e. g. for normal integer arithmetic) up to tables used for performing algebraic operations based on table lookups.

Algebraic structures have normal value semantic: they always have a copy constructor, which creates a deep, independent copy of the original structure. On the other hand, copying algebraic structures is always cheap (i. e. they can be passed by value instead of by reference). Some algebraic structure may use techniques like reference counting to achieve this.

The following features are shared by all algebraic structures A:

```
class A
{
public:
   typedef _ type;
   typedef _ algebra_category;
   typedef _ polynomial_category;

   unsigned size() const;
   type element(unsigned i) const;
   unsigned index(const type&) const;

   void print(std::ostream &, const type&);
```

```
    void printShort(std::ostream &, const type&);
    void printSuffix(std::ostream &);
};
```

Each algebraic structure A has a typedef `type`, specifying the type of the elements $x \in A$. It can be assumed that `operator==()`, `operator=()` and a copy constructor are defined for `type`. `type` must have value semantic, i. e. assigning it or passing it to a copy constructor should result in a copy that is independent of the original.

`size()` returns the number of distinct elements in the structure—or 0 if A is infinite.

`element()` allows to enumerate the elements of A. For finite structures, `element(0)`, ...,`element(size()-1)` produce all elements. `index()` is the reverse operation of `element()`. `index(element(`i`))` is always equal to i for $i = 0, \ldots, \#A - 1$.

`print()` prints an element on the given `ostream`. `printShort()` does the same, however suppressing extra information like a modulus, which makes the result fit for use, for instance, as a coefficient of a polynomial. `printSuffix()` prints the information that is left out by `printShort()`.

`algebra_category` declares which operations can be performed in A. It can be used by template functions to decide which features are available. The following values are valid. Each of them is described in one of the following sections.

```
struct group_tag {};
struct ring_tag      : public group_tag {};
struct domain_tag    : public ring_tag {};
struct ufd_tag       : public domain_tag {};
struct euclidean_tag : public ufd_tag {};
struct field_tag     : public euclidean_tag {};
struct cyclic_tag    : public field_tag {};

struct vectorspace_tag : public group_tag {};
```

`polynomial_category` declares if the the elements of A are polynomials. It can be defined as one of the following two types:

```
struct nopolynomial_tag {};
struct polynomial_tag : public nopolynomial_tag {};
```

7.1.2 Abelian Groups

The simplest algebraic concept used in HIntLib is an Abelian group (or just group). It is shared by algebraic structures like rings, fields or vector spaces. A group has only a single operation $\oplus$, which is associative and commutative. There is also a neutral element denoted as "zero" or 0, and for each element $a \in A$, a negative (denoted as $-a$) can be found, such that $a \oplus -a = 0$.

In addition to the basic features listed in Section 7.1.1, each group provides the following methods:

```
class A
{
public:
    typedef group_tag algebra_category;

    type zero() const;

    bool is0(const type&) const;

    type  add  (const type&, const type&) const;
```

Method	Equivalent code
`addTo(a,b)`	`a = add(a,b)`
`negate(a)`	`a = neg(a)`
`sub(a,b)`	`add(a,neg(b))`
`subFrom(a,b)`	`a = sub(a,b)`

`times(a,k)`	`type t = zero();`
	`for (unsigned i = 0; i<k; ++i) addTo(t, a);`
	`return t;`

`is0(a)`	`a == zero()`

Table 7.1: Derived group operations

```
   type& addTo(      type&, const type&) const;

   type  neg   (const type&) const;
   type& negate(      type&) const;

   type  sub    (const type&, const type&) const;
   type& subFrom(      type&, const type&) const;

   type times(const type&, unsigned k) const;
};
```

`zero()` returns the neutral element, `add(a,b)` returns $a \oplus b$, and `neg(`a`)` gives $-a$, the additive inverse of a in $(A, \oplus)$. The other methods could be implemented based on these three, according to Table 7.1. However, optimized versions can usually be provided.

7.1.3 Rings

When we say ring, we always mean commutative rings with identity, i. e. an algebraic structure A with two binary operations $\oplus$ and $\otimes$ such that $(A, \oplus)$ forms an Abelian group, $(A, \otimes)$ is a commutative semi-group with a neutral element denoted as 1 or "one", and the distributive law holds.

In addition to the features of groups listed in Section 7.1.2, each ring provides the following methods:

```
class A
{
public:
   typedef ring_tag algebra_category;

   type one() const;

   bool is1(const type&) const;

   type  mul  (const type&, const type&) const;
   type& mulBy(      type&, const type&) const;

   type power(const type&, unsigned k) const;
};
```

`one()` returns the neutral element for $\otimes$ and `mul(`a`,`b`)` returns $a \otimes b$. The other methods could be implemented based on these two, according to Table 7.2. However, optimized versions can usually be provided.

Method	Equivalent code
`mulBy(a,b)`	`a = mul(a,b)`

`power(a,k)`	`type t = one();`
	`for (unsigned i=0; i<k; ++i) mulBy(t, a);`
	`return t;`

`is1(a)`	`a == one()`

Table 7.2: Derived ring operations

7.1.4 Integral Domains

An integral domain is a ring as described in the previous section, which has no zero divisors, i. e. the product of two non-zero elements is never zero. Domains do not provide any additional member functions compared to normal rings. However, they declare their property by setting `algebra_category` appropriately.

```
class A
{
public:
   typedef domain_tag algebra_category;
};
```

7.1.5 Unique Factorization Domains

A unique factorization domain (UFD) is an integral domain with the additional property that each element a falls into exactly one of the following four categories:

1. a is 0.
2. a is a unit, i. e.there exists an element b such that $a \otimes b = 1$.
3. a is prime, i. e.it is neither 0 nor a unit, and for all elements b, c with $b \otimes c = a$, it follows that either b or c is a unit.
4. a is composite, i. e. it has a factorization into two or more primes, with is unique except of order and multiplication by units.

UFDs provide the following methods in addition to the ones for integral domains described in Section 7.1.4:

```
class A
{
public:
   typedef ufd_tag algebra_category;

   bool isUnit(const type&) const;
   bool isPrime(const type&) const;
   bool isIrreducible(const type&) const;
   bool isComposit(const type&) const;

   type unitRecip(const type&) const;
};
```

Together with `is0()`, which was already defined for rings in Section 7.1.2, `isUnit()`, `isPrime()` and `isComposit()` allow to determine to which of the four categories a given element a belongs. For each $a \in A$, exactly one of these four methods returns true. `isIrreducible()` is a synonym for `isPrime()`.

In UFDs, units have always a multiplicative inverse, which can be determined by `unitRecip()`. This method is only defined for arguments that are units in A.

7.1.6 Euclidean Rings

Euclidean rings are UFDs with the additional feature that a division with remainder can be performed, such that the remainder is in some sense smaller than the divisor. To be more specific, there is a function $|\cdot| : A \to \mathbb{N}$, called a norm, with the following properties:[1] $|a| = 0$ if and only if $a = 0$, $|a| = 1$ if and only if a is a unit, and $|a| \leq |a \otimes b| \leq |a|\,|b|$ if $b \neq 0$. In addition to that we have $|a| \leq |b|$ whenever `index(`a`)` $\leq$ `index(`b`)`.

Most noteworthy, for all $a \in A$ and $b \in A \setminus \{0\}$ elements $q, r \in A$ can be found such that $a = (q \otimes b) \oplus r$ and $|r| < |b|$. In other words, the Euclidean algorithm can be performed: the remainder will eventually become zero and the algorithm terminates.

Euclidean rings provide the following methods in addition to the ones for UFDs defined in Section 7.1.5:

```
class A
{
public:
   typedef euclidean_tag algebra_category;

   void div(const type&, const type&, type&, type&) const;
   type quot(const type&, const type&) const;
   type rem(const type&, const type&) const;

   unsigned norm(const type&) const;
   unsigned numOfRemainders(const type&) const;
};
```

`div(`a`,`b`,`q`,`r`)` sets q and r as defined above. If the calculation of only either q or r is required, `quot()` or `rem()` can be used, respectively. `numOfRemainders(`b`)` returns the number of different remainders that can occur when dividing by b, or 0 if this number is infinite. Most algebraic structures will throw `DivisionByZero` if b is 0 while calling any of the these methods. However, some may trap or show some other undefined behavior.

Finally, `norm(`a`)` returns $|a|$.

7.1.7 Fields

A field is an arithmetic structure $(A, \oplus, \otimes)$ such that $(A, \oplus)$ as well as $(A \setminus \{0\}, \otimes)$ are Abelian groups, and the distributive laws hold. Each field is also an Euclidean Ring, with the additional properties that there are no primes and composites, and the remainder of divisions is always 0.

Fields provide the following methods in addition to the ones for Euclidean rings in Section 7.1.6. Keep in mind, that some of the UFD operations (`isPrime()`, `rem()`, ...) become dummies, returning the same value independent of their arguments.

```
class A
{
public:
```

[1] The concept of "norm" used in HINTLIB is not identical to what is used in number theory. For instance, it does not hold in general that $|a \otimes b| = |a|\,|b|$.

```
    typedef field_tag algebra_category;

    unsigned characteristic() const;

    type recip(const type&) const;

    type  div  (const type&, const type&) const;
    type& divBy(      type&, const type&) const;
};
```

`recip(`a`)` returns the multiplicative inverse of a. Most algebraic structures will throw `DivisionByZero` if a is 0. `div(`a`,`b`)` and `divBy(`a`,`b`)` are equivalent to `mul(`a`, recip(`b`))` and a `= div(`a`,`b`)`, respectively.

`div()` is equivalent to `quot()`. The reason for introducing an additional name is to allow stricter type checking in templates. While `quot()` is available also for Euclidean rings, `div()` is guaranteed to return a result that is unbiased by any remainder.

For finite fields, `characteristic()` returns the characteristic of the field, i. e. the smallest number n such that $\sum_{i=1}^{n} x$ is equal to 0 for all x. The characteristic is always a divisor of the field size. If the field is infinite, 0 is returned.

7.1.8 Fields with Cyclic Additive Groups

In general, the additive group of a field is not cyclic. However, for finite fields of size p, with p prime, this is the case. This special situation is declared by setting `algebra_category` to `cyclic_tag`, a subclass of `field_tag`.

```
class A
{
public:
    typedef cyclic_tag algebra_category;
};
```

There are no additional methods for fields with cyclic additive groups.

7.1.9 Polynomial Rings

Polynomials p are terms of the form

$$a_n x^n + a_{n-1} x^{n-1} + \cdots + a_1 x + a_0$$

with a_i denoting coefficients from some ring, and x a formal parameter that is not further defined. a_n is different from 0 and is called the leading coefficient of p. Addition and multiplication can be defined as

$$(a_n x^n + \cdots + a_1 x + a_0) \oplus (b_m x^m + \cdots + b_1 x + b_0) := \sum_{i=0}^{\infty} (a_i + b_i) x^i$$

and

$$(a_n x^n + \cdots + a_1 x + a_0) \otimes (b_m x^m + \cdots + b_1 x + b_0) := \sum_{i=0}^{\infty} x^i \sum_{j=0}^{i} a_j b_{i-j}$$

with a_i and b_j assumed to be 0 for $i > n$ and $j > m$, respectively.

Polynomial rings are always rings, sometimes even domains, UFDs or Euclidean rings, and inherit all properties described in Sections 7.1.3, 7.1.4, 7.1.5, and 7.1.6, respectively. In addition to that, they provides the following methods:

```
class A
{
public:
   typedef polynomial_tag polynomial_category;
   typedef _ coeff_algebra;
   typedef coeff_algebra::type coeff_type;
   typedef _                   coeff_reference;

   coeff_algebra getCoeffAlgebra() const;

   bool isMonic(const type&) const;

   coeff_type evaluate (const type&, const coeff_type&) const;
};
```

`coeff_algebra` is the type of the ring used for the coefficientes of the polynomials; `coeff_algebra::algebra_category` it is always as subclass of `ring_tag`. `getCoeffAlgebra()` returns an instance of the `coeff_algebra` in use.

`coeff_type` is the type of a single coefficient. `coeff_reference` is the type used to reference a single coefficient inside the polynomial, used for instance by `type::operator[]()`. If some kind of packed data layout is used for the polynomial, this type will not be `coeff_type&`!

`isMonic()` returns true, if the leading coefficient is 1 or if the polynomial is 0. `evaluate(`p`,`a`)` returns $p(a)$, ie the ring element a is substituted for the formal parameter x in the polynomial, and the whole expression is evaluated using normal ring arithmetic.

In addition to the members of the polynomial ring itself, the type used to store the polynomials, `type`, is a class that is guaranteed to have the following members:

```
class Poly
{
public:
   typedef _ coeff_type;
   typedef _ coeff_reference;

   Poly ();
   Poly (const Poly& p);
   template<typename I> Poly (I i, I i);

   Poly& operator= (const Poly& p);
   int degree() const;

   coeff_type      operator[] (unsigned i) const;
   coeff_reference operator[] (unsigned i);

   coeff_type      lc() const;
   coeff_reference lc();

   bool operator== (const Poly& p) const;
   bool operator!= (const Poly& p) const;
};
```

7.1.10 Vector Spaces

A Vector Space V with dimension d over a ring or field A (denoted as $V = A^d$) is the set of all d-tuples $\boldsymbol{x} = (x_1, \ldots, x_d)$ with $x_i \in A$. x_i is called the i-th coordinate of $\boldsymbol{x}$. There is an addition

$\oplus : V \times V \to V$, which is performed coordinate wise, making $(V, \oplus)$ an additive group with the neutral element $(0, \ldots, 0)$. In addition to that, there is a multiplication $\otimes : A \times V \to V$, which is defined as $\lambda \otimes (x_1, \ldots, x_d) := (\lambda x_1, \ldots, \lambda x_d)$.

In addition to the operations for groups presented in Section 7.1.2, vector spaces provide the following methods and types:

```
class VectorSpace
{
   typedef vectorspace_tag algebra_category;

   typedef _ scalar_algebra;
   typedef scalar_algebra::type scalar_type;
   typedef _ scalar_reference;

   scalar_algebra getScalarAlgebra() const;

   unsigned dimension() const;

   scalar_type coord (const type&, unsigned) const;
   scalar_reference coord  (type&, unsigned) const;

   template<typename I> void toCoord (const type&, I) const;
   template<typename I> void fromCoord (type&, I) const;

   type  mul (const type&, scalar_type) const;
   type& scale (    type&, scalar_type) const;
};
```

`scalar_algebra` defines the type of the algebraic structure A the vector space V is based on. `scalar_algebra::algebra_category` is always a subclass of `ring_tag`. `getScalarAlgebra()` returns an instance of the `scalar_algebra` in use

Coordinates and scalars are of the type `scalar_algebra::type`, which is also directly available as `scalar_type`. It is convenient to use a certain coordinate of a vector as an lvalue. Depending on the implementation of `type`, `scalar_type&` is not always appropriate to accomplish this. Therefore, `scalar_reference` is provided, which allows direct write access to coordinates.

`dimension()` returns the dimension of the vector space.

`mul()` and `scale()` provide multiplication with scalars in the obvious way, with `scale(`a`,`λ`)` identical to a `= mul(`a`,`λ`)`.

`coord()` is used to access a given coordinate. Two versions are available: the first one used for `const type&` arguments, returning `scalar_type` directly. The second one, requiring a non-const `type&` argument, returning a `scalar_reference`, which can be written to.

If access to more or all coordinates is required at the same time, `toCoord()` and `fromCoord()` can be used. They copy the coordinates to and from a output / input iterator, respectively.

7.2 Implemented Algebraic Structures

This section describes all algebraic structures which are readily available in HINTLIB.

Actually, it describes only some of the implemented algebraic structures, and text ist very incomplete. :-(

R::algebra_category	algebra_category of the polynomial ring
ring_tag	ring_tag
domain_tag	domain_tag
ufd_tag	domain_tag (see text)
field_tag	euclidean_tag

Table 7.3: algebra_category of polynomial rings

7.2.1 Basic Structures

The field of real numbers, $\mathbb{R}$, is constructed using `RealField()`. Internally, all operations are based on the type `real`.

The Euclidean ring of the integers, $\mathbb{Z}$, is constructed using `IntegerRing<T = int>()`. All operations are performed using standard integer arithmetic based on `T`, ie care has to be taken to avoid overflow or division by zero. `element()` enumerates the integers in the order $0, 1, -1, 2, -2, 3, -3, \ldots$, `norm(`$a$`)` returns $|a|$.

7.2.2 Modular Arithmetic

Given an Euclidean ring R and an element $p \in R$, a new ring R/pR can be constructed, containing the elements of R modulo p. If p is irreducible in R, it can be shown that the resulting ring is actually a field. The compiler cannot determine if p is irreducible, thus, the user has to specify if a field is expected by using the proper class.

`ModularArith<R>(const R& `R`, const type& `p`)` constructs the ring R/pR. Given that p is irreducible in R, `ModularArithField<R>(const R& `R`, const type& `p`)` produces the same structure including the additional operations for fields. `R::algebra_category` must be a subclass of `euclidean_ring` in both cases.

$\mathbb{Z}/p\mathbb{Z}$ could be implemented using `ModularArith<IntegerRing<T>>`, however, this turns out to be inefficient. Specializations `ModularArith<T>` and `ModularArithField<T>` have been provided for `T` equal to `unsigned char` and `unsigned short`. These classes use `T` as `type`, and perform all internal calculations based on `unsigned`.

7.2.3 Polynomials

Polynomial rings over an arbitrary ring R can be constructed using `PolynomialRing<R>(const R& `R`)`.

The `algebra_category` of the resulting polynomial ring is determined by `R::algebra_category` according to Table 7.3. If R is an UFD, we would expect the resulting polynomial ring to be an UFD, too. However, implementing the required member functions based only on the UFD-properties of R turns out to be rather hard, so it is not done yet.

For polynomials over $\mathbb{F}_2$ an optimized implementation storing the coefficients in bits of a computer word is available as `Polynomial2Ring<T>`, with `T` being either `u32` or `u64`.

7.2.4 Finite Fields

A large number of classes realizing finite fields in HIntLib are available

Special Cases

An optimized version for the field with two elements, $\mathbb{F}_2$, can be constructed using `GF2()`.

Direct Calculation of General Finite Fields

A finite filed with $b = p^q$ elements, with p prime, has always the structure of the ring of polynomials over the field $\mathbb{Z}_p$, modulo an irreducible polynomial in this ring with degree q. Therefore it could be realized using `ModularArithField<PolynomialRing<ModularArithField<B> > >`. However, this is tedious because the user has to calculate an irreducible polynomial of the appropriate degree by hand. The class `GaloisField<>` takes care of the required setup.

```
template <typename T>
class GaloisField
   : public ModularArithField<PolynomialRing
                 <ModularArithField<B> > >
{
public:
   GaloisField (unsigned base, unsigned exponent);
   GaloisField (unsigned size);
};
```

In addition to all the members inherited from `ModularArithField<PolynomialRing<ModularArithField<B>>>`, the constructors take care of setting up everything properly, given either the size $b = p^q$ of the field or the values p and q separately.

Field Arithmetic Using Table Lookups

`LookupGaloisField<>`, `LookupGaloisFieldPow2<>`, and `LookupGaloisFieldPrime<>`.

Appendix A

Installation

HINTLIB is installed using the common GNU installation procedure, which is

```
./configure
make
make install
```

maybe with an additional

```
make check
```

`./configure` determines all properties of the host system that affect building HINTLIB. It also allows the user to specify additional configuration options or to override settings that otherwise would be determined automatically by `configure`.

`make` compiles and links the library.

`make install` installs HINTLIB on the system. Usually this is done in /usr/local/, therefore you need root permissions while executing `make install`. If you do not have root permissions or want to install HINTLIB somewhere else for some other reason, see Section A.1.2.

Finally, `make check` runs the test suite. This can be done before or after installing the library with `make install`.

More general information about the GNU build process can be found in the file `INSTALL` in the HINTLIB source directory.

A.1 Configuring HINTLIB

The process of configuring HINTLIB is started by calling `./configure` in the top-level HINTLIB source directory (which is the directory that also contains this manual).

All the options discussed here are to be added to the `configure` command line.

A.1.1 Selecting the Compiler and Compiler Options

`configure` tries determine the proper way of calling your C++ compiler. If it does not get it right or if you want to select between different compilers installed on your system, you can specify the correct compiler using "`CXX=`*`your_compiler`*".

Compiler options (for instance options for optimization or target specific options) can be added using "`CXXFLAGS=`*`your_options`*".

A.1.2 Installation Directory

By default HINTLIB is installed in /usr/local/. To be precise, the header files are stored in /usr/local/include/HIntLib/, the library in /usr/local/lib/, and the precalculated Niederreiter/Xing generator matrices in /usr/local/share/HIntLib/.

If you have root access to the system and can run `make install` as root, this default is probably the best solution.

If you want to install HINTLIB somewhere else (for instance in your home directory, because you do not have write access to /usr/local), you can use the "`--prefix=...`" on the `configure` command line. `./configure --help` gives you more information on selecting the installation directory.

A.1.3 The MPI Header File

By default HINTLIB is built as a sequential as well as a parallel library using MPI (see [11]).

If MPI is not installed on your system or if you do not want to build the parallel library, you can disable the MPI version of HINTLIB using "`--disable-MPI`".

If the MPI header file `mpi.h` is not in your default search path for header files, you can use "`MPI_HEADER_PATH=`*`directory_with_mpi.h`*". The path you specify will only be added to the header search path for building the parallel part of the library.

A.1.4 Building Static Libraries

If this is supported by the the host system, HINTLIB is built as a shared library by default.

If you want to build a static library in addition to the shared library, add "`--enable-static`" to the `configure` command line.

If you want to build only a static library, add "`--enable-static --disable-shared`" to the `configure` command line.

A.1.5 Building HINTLIB Outside the Source Directory

HINTLIB can be built outside the source directory (given that the make program supports the VPATH variable). This is useful if you want to build HINTLIB multiple times, for instance to accomodate different platforms or different configuration settings.

Change to an empty directory which you want to used for the next build and call `configure` using *`path_to_HIntLib_source_dir`*`/configure`.

A.1.6 Cross Compilation

It is not possible to cross compile HINTLIB, because a number of source files are created during the build-process by C++ programs.

A.1.7 The Size of the Index Data Type

The datatype `HIntLib::Index` is an unsigned integer variable with either 32 or 64 bits precision (see Section 2.3).

By default, `Index` has 64 bits if and only if `unsigned long int` has at least 64 bits.

You can force it to be 32 bits (to be precise: to be a typedef for `u32`) by adding "`--with-index=32`" to the `configure` command line, or to 64 bits (`u64`) by adding "`--with-index=64`".

A.1.8 The Datatype for Real Numbers

By default, the datatype `HIntLib::real` is a typedef for `double` (see Section 2.4). It can be set to `float` or `long double` by adding "`--with-real=float`" or "`--with-real=long`" to the `configure` command line, respectively.

Using `long double` is useful if you need the extra precision. Using `float` could be faster on some systems, however I do not know about any modern system where this is actually the case.

A.2 Comments for some Architectures

This section contains some information that may be useful for building and installing HINTLIB on certain architectures.

A.2.1 Linux with GNU C++ Compiler

This should run out-of-the-box, for 2.95.x as well as for 3.x versions of the compiler.

- If you want to, you can disable debugging information using "`CXXFLAGS=-O2`", which replaces the "`CXXFLAGS=-g -O2`" default chosen by `configure` for the GNU C++ compiler.

A.2.2 Linux with the Intel C++ Compiler

- Select the Intel C++ compiler by using "`CXX=icpc`".

A.2.3 Sun Solaris with GNU C++ Compiler

- Select the GNU C++ compiler by using "`CXX=g++`".
- If you want to, you can disable debugging information using "`CXXFLAGS=-O2`", which replaces the "`CXXFLAGS=-g -O2`" default chosen by `configure` for the GNU C++ compiler.
- If you have a 64-bit processor (Ultra SPARC), add "`--with-index=64`".
- If you want to build a 64-bit ABI version of HINTLIB, you have to use "`CXXFLAGS=-O2 -m64`". However, the only reason for doing so is to link HINTLIB to an executable that has to use the 64-bit ABI for some other reason. There is no advantage for HINTLIB using the 64-bit ABI.

A.2.4 SGI IRIX with Native C++ Compiler

The exception handling code in the C++ library that comes with version 7.4 of the MIPS Pro C++ compiler seems to be broken. You will see frequent crashes with the following error message:

```
Assertion failed in file "../../libC/lang_support/throw.cxx",
line 1618
```

Version 7.3.x of the compiler does not have this problem.

- Add "`CXX=CC`" and "`CXXFLAGS=-O2`" to the `configure` command line.
- If you have a 64-bit processor, add "`--with-index=64`".

- If you want to build a 64-bit ABI version of HINTLIB, you have to use "`CXXFLAGS=-O2 -64`". However, the only reason for doing so is to link HINTLIB to an executable that has to use the 64-bit ABI for some other reason. There is no advantage for HINTLIB using the 64-bit ABI.

A.2.5 MS Windows + Cygwin with GNU C++

At least with Cygwin versions up to 1.3.10, it is impossible to propagate C++ exceptions from a DLL to the calling program. If an exception is thrown and not caught inside the DLL, the program aborts immediately, without giving the calling program the chance to catch the exception.

With Cygwin, HINTLIB can be built as a shared library (i. e. a Windows DLL). However, applications will abort if an exception is thrown by the library.

- If you want to be able to catch exceptions thrown by HINTLIB, a static library must be built, using "`--enable-static --disable-shared`". If you decide to build HINTLIB as a DLL, a number of programs in the test suite will fail, too, because they also use exceptions.
- If you want to, you can disable debugging information using "`CXXFLAGS=-O2`", which replaces the "`CXXFLAGS=-g -O2`" default chosen by `configure` for the GNU C++ compiler.

Appendix B

The GNU General Public License

Version 2, June 1991

59 Temple Place - Suite 330, Boston, MA 02111-1307, USA

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END OF TERMS AND CONDITIONS

Appendix: How to Apply These Terms to Your New Programs

If you develop a new program, and you want it to be of the greatest possible use to the public, the best way to achieve this is to make it free software which everyone can redistribute and change under these terms.

To do so, attach the following notices to the program. It is safest to attach them to the start of each source file to most effectively convey the exclusion of warranty; and each file should have at least the "copyright" line and a pointer to where the full notice is found.

> one line to give the program's name and a brief idea of what it does.
> Copyright (C) yyyy name of author
>
> This program is free software; you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation; either version 2 of the License, or (at your option) any later version.
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Also add information on how to contact you by electronic and paper mail.
If the program is interactive, make it output a short notice like this when it starts in an interactive mode:

> Gnomovision version 69, Copyright (C) yyyy name of author
> Gnomovision comes with ABSOLUTELY NO WARRANTY; for details type 'show w'.
> This is free software, and you are welcome to redistribute it under certain conditions; type 'show c' for details.

The hypothetical commands `show w` and `show c` should show the appropriate parts of the General Public License. Of course, the commands you use may be called something other than `show w` and `show c`; they could even be mouse-clicks or menu items—whatever suits your program.

You should also get your employer (if you work as a programmer) or your school, if any, to sign a "copyright disclaimer" for the program, if necessary. Here is a sample; alter the names:

> Yoyodyne, Inc., hereby disclaims all copyright interest in the program
> 'Gnomovision' (which makes passes at compilers) written by James Hacker.
> signature of Ty Coon, 1 April 1989
> Ty Coon, President of Vice

This General Public License does not permit incorporating your program into proprietary programs. If your program is a subroutine library, you may consider it more useful to permit linking proprietary applications with the library. If this is what you want to do, use the GNU Library General Public License instead of this License.

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