Recursive function templates as a solution of linear algebra expressions in C++

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Abstract

The article deals with a kind of recursive function templates in C++, where the recursion is realized corresponding template parameters to achieve better computational performance. Some specialization of these template functions ends the recursion and can be implemented using optimized hardware dependent or independent routines. The method is applied in addition to the known expression templates technique to solve linear algebra expressions with the help of the BLAS library. The whole implementation produces a new library, which keeps object-oriented benefits and has a higher computational speed represented in the tests.

Introduction

The C++ programming language has a powerful template facility that enables the development of flexible software without incurring a large abstraction penalty [1],[2]. The main goal is the resolving of all templates of a program during the compilation time. In this way C++ language can be meant as a two-level language [5]. A function template takes both template parameters (solved in the compilation time) and function arguments (work dynamically in the program code).

A naive implementation of linear algebra operations in C++ using the known object-oriented features, such as providing of classes and operator overloading, yields an inefficient code. The main reason for that is generation of temporary objects by each overloaded operator [1]. This problem is usually solved by expression templates technique [4],[6], which is implemented in the known optimized C++ libraries for linear algebra, e.g. valarray standard library (Linux RedHat 7.2), Blitz++ etc. Their tests and descriptions [8] prove that computational performance of such libraries can be equal to ones written in FORTRAN without any object-oriented limitations.

But there are some processor and cash oriented implementations, which have better performance. The best example of such linear algebra library is Basic Linear Algebra Subprograms [7]. They exist for most of the hardware platforms with the same interface, although specifically implemented (in FORTRAN or Assembler) for some types of commonly used processors.

\begin{align*}
  z &= c \times x + y \\
  z &= t_1 + y \\
  z &= t_2 
\end{align*}
Therefore the combination of an expression templates abstraction with the incorpo-
ration of BLAS in a specialization can produce a better performance than the best pure
C++ libraries.

Expression templates

We consider a simple example of a vector expression (2) to see, how the expression tem-
plates are used to collect the arguments and the operators of the vector expression.

\[ X = A + B + C. \] (2)

As assumed in C++, the right hand side of the equation (2) is resolved from left to
right before the assign operator is applied. So, we have the series of operators:

1. \( X = A + B + C \). The first operator '+' is applied.
2. \( X = BinClos < A, B, + > + C \). The second operator '+' is applied.
3. \( X = BinClos < BinClos < A, B, + >, C, + > \). The assign operator '=' is applied.

We have just introduced a new symbolic notation \( BinClos \) for a binary operation. It looks
intentionally like a template class, where \( A \), \( B \) and '+' must be data types as template
parameters. The basic trick of the approach is to substitute a template class as a template
parameter into itself and to build parse trees using operator overloading [4].

The C++ class for description of binary expression closure is defined using three
template parameters: the right and the left hand side and the operation. But it has also
to save references (not the values) to the arguments of the binary expression:

```c++
template<class Left, class Right, class Oper>
struct BinClos {
    const Left& arg1;
    const Right& arg2;
    BinClos(const Left& a, const Right& b):arg1(a),arg2(b) {} //constructor
};
```

Now we have to declare the class for a vector, which can be implemented later. Further,
the addition operator should be described as a data type. The simple structure includes
only the function `apply` to realize the addition:

```c++
class Vector; // some vector class
struct add { // encapsulates the '+' operation
    static double apply(double a, double b) {
        return a+b;
    }
};
```

For the whole minimal implementation we need a C++ operator, that yields the structure
`BinClos`. There are some possibilities to define this operator. The following example
represents an addition of any object of type `Left` with a vector:

```c++
template<class Left>
BinClos<Left,Vector,add> operator + (Left& a, Vector& b) {
    return BinClos<Left,Vector,add>(a,b);
}
```
So, the right hand side of the equation (2) is gathered in the compile time to the single template structure:

\[
\text{BinClos<BinClos<Vector,Vector,add>,Vector,add>}
\]  

(3)

The next step in the solution of (2) is to assign the last complicated template structure (3) to the resulting vector \(X\). We consider, at first, the usual approach that exists in the optimized C++ libraries, such as valarray and Blitz++ [4]. It uses the operator overloading to assign the whole expression in only one loop per component (4).

\[
X_i = A_i + B_i + C_i.
\]  

(4)

The structure BinClos is supplemented with an operator[], that adds \(i\)-th components of two data members arg1 and arg2 of the structure. If the arg1 (or arg2) is a simple vector, than the operator[] is called in the class Vector, else the same operator is called recursively in the structure BinClos. That process is started by operator=, which is represented by the single loop and calls operator[] due to the expr[i]:

```
template<class Left, class Right, class Oper>
struct BinClos {
    const Left& arg1;
    const Right& arg2;
    BinClos(const Left& a, const Right& b):arg1(a),arg2(b) {}  
    double operator[](int i) {
        return Oper::apply(arg1[i],arg2[i]);
    }
};

class Vector {
    double* data;
    int size;
public:
    ... //definition of constructors
    template<class Left, class Right, class Oper>
    void operator=(const BinClos<Left,Right,Oper>& expr) {
        for (int i=0; i<size; ++i) data[i]=expr[i];
    }
    double operator[](int i) { return data[i]; }
};
```

As it can be seen, the solution is distributed to some overloaded operators. Therefore, there is no possibility to substitute an external optimized subprogram. The next approach provides another template technique to realize the last step of the solution.

**Recursive function templates**

The basic idea of the following approach is to divide the right hand side of (2) into simple units, which are bounded by addition or subtraction and than to apply the operations consequently to the vector \(X\) (fig. 1). We have always two types of arguments and a type of operation at the top level of recursive built structure (3). These two types can be applied to the \(X\) with the type of the operation. If an argument is complicated, than the process continues in the same way recursively, else we get a simple addition or subtraction of a vector \(X\) with another vector. The last can be done in a single function without any overloading of operators. In the next step we have to construct the recursion using such
\[ X = A + B + C \quad \text{or} \quad X = A + B + C \]

Figure 1: Basic idea of the recursive solution

functions. The optimal decision in terms of maintaining the efficiency is to apply recursion with respect to the template parameters of the functions. In order to minimize the number of the function parameters the functions are implemented as member functions of the structure BinClos.

We need first to implement a C++ trait \([4]\) to represent the rule of addition. In the terms of the set theory, we have a mapping:

\[
\{+,+\} \rightarrow \{+\}, \quad \{+,-\} \rightarrow \{-\}, \quad \{-,+\} \rightarrow \{-\}, \quad \{-,-\} \rightarrow \{+\}. \tag{5}
\]

Both addition and subtraction operations are now implemented as two empty structures and are used as template parameters for the recursive functions. They have only a meaning of different data types.

```cpp
struct add {};
struct sub {};
```

The trait `add_rule` receives two such empty structures as template parameters and produces the result of the data type `oper`. Two members of the mapping (5) are described by the next template instantiation:

```cpp
template<class Op1, class Op2>
struct add_rule {
    typedef Op2 oper;
};
```

and the other two are specialized:

```cpp
template<>
struct add_rule<sub,add> {
    typedef sub oper;
};
template<>
struct add_rule<sub,sub> {
    typedef add oper;
};
```

We have now all tools to implement recursive function templates. These are functions `Assign` and `Operation` (either addition or subtraction). The first function `Assign` assigns the first argument `arg1` due to the recursive call of itself (see below). If the argument is simple, e.g. vector, than the same function has to be implemented in the corresponding class (e.g. class `Vector`). The function `Assign` has one template parameter, which defines the return type. Thus, it is generalized for any operation.

The second argument `arg2` of the binary closure have to be added or subtracted from `x`. For this purpose, the function `Operation` is called. It receives also the second template parameter `LeftOp` to recognize the operation. The second function `Operation` is recursive too and used especially for C++ like expressions, e.g. \( X + = A - B \). In this case the first argument `A` is added (first line of `Operation` implementation) and the second is subtracted. The last subtraction is obtained by compiler from two symbols \{+,-\} as data types with the help of the addition rule trait.
The function recursion must be finished. It means that two described template functions must be specialized as the member functions in each of the class (e.g. class Vector) that occurs in expressions resolved by this method.

```cpp
template<class Left, class Right, class Oper>
struct BinClos {
    const Left& arg1;
    const Right& arg2;
    BinClos(const Left& a, const Right& b):arg1(a),arg2(b) {}

template<class Ret>
void Assign(Ret x) {
    arg1.Assign<Ret>(x);
    arg2.Operation<Oper,Ret>(x);
}
template<class LeftOp, class Ret>
void Operation(Ret x) {
    arg1.Operation<LeftOp,Ret>(x);
    arg2.Operation<typename add_rule<LeftOp,Oper>::oper,Ret>(x);
}
};
```

The specialization in the class Vector is very simple using the BLAS library. The recursion process is initiated also in the class Vector from an overloaded operator, e.g. `operator=`, by corresponding call of the template function (e.g. `Assign`):

```cpp
class Vector {
    double* data;
    int size;
public:
    // definition of constructors
    template<class Left, class Right, class Oper>
    void operator=(const BinClos<Left,Right,Oper>& expr) {
        expr.Assign(data);
    }
    template<class LeftOp, class Ret>
    void Operation(Ret x) {
        cblas_daxpy(size,1.,data,1,x,1); // sample specialization using CBLAS
    }
};
```

The provided template functions can be specialized in the structure BinClos for some often used short algebraic expressions. It also leads to the increase in computational efficiency. For instance:

```cpp
template<> template<> inline void BinClos<Vector,Vector,add>::Assign<double*>(double*x) { // X=A+B
    ...
}
template<> template<> inline void BinClos<Vector,double,mul>::Operation<add,double*>(double*x) { // X+=c*A
    ...
}
```
Moreover, multiplication operations, such as vector-constant and vector-matrix multiplications, must necessarily be specialized, because they cannot be partially applied to the vector $X$.

In a whole library for linear algebra we need to implement besides the binary expression closure in the same way a unary expression closure and a unary and a binary function closure. It is also important to consider that the described method of recursive functions does not work if any unspecialized expression in some mathematical function is substituted, for instance:

$$X = \sin(A + B + C), \quad \text{where } X, A, B, C \text{ are vectors.} \quad (6)$$

The acceptable solution allows the library to yield a temporary vector $T$. This vector receives the expression value in the mathematical function ($T = A + B + C$) and than is plugged into the function ($X = \sin(T)$). The copying of a complicated argument result to the temporary vector does not reduce the computational performance significantly. This can be evidently proved by the following performance tests.

### Performance tests

Three performance tests were developed to verify the functionality of the library and to find its weak points.

- **Test 1:** Short expressions. A vector-matrix product and a vector-constant product are repeated 1000 times. That combination is often used in many mathematical and engineering computations.
  $$x = Ay, \quad y = y + cx, \quad c = \text{const}$$

- **Test 2:** Long expressions. The sum of 7 vector-constant products are calculated 100000 times. The test can show how slower is the evaluation using some loops (with the help of BLAS) and a single loop (due to overloaded `operator[]`).
  $$y = y + c1u1 + ... + c7u7, \quad y = c8y, \quad c_i = \text{const}$$

- **Test 3:** Long function expressions. The sum of 3 mathematical functions are calculated 50000 times. It has the same aim as the second test. The temporary vectors in the computation of mathematical functions and their penalty are tested.
  $$y = y + \log(u_1) - \cos(c2u2 + u3) + \sin(c4u4 + c5u5 - u6), \quad y = c6y, \quad c_i = \text{const}$$

The tests were performed on two completely different hardware platforms, that have their own specific optimized BLAS version:

- **Intel Pentium III 800MHz with Linux RedHat 7.3.**
  Compiler: GNU C++, gcc 2.96 version. BLAS: Intel Math Kernel Library.
  The first three bars of the test diagram (fig. 2) show the CPU time of the pure C++ implementation. It proves that the new implementation (third bar) has a performance similar to optimized libraries `valarray` and Blitz++. The implementation using BLAS is quicker in the most cases (test 1 and test 3), especially using hardware specific BLAS version Intel MKL. The last two bars in the tests 1 and 2 estimate the abstraction penalty, that is acceptable.

- **IBM M80 enterprise server having 8 Power3 500MHz processors and IBM AIX operating system.** (Each test uses one processor).
  Compiler: GNU C++, gcc 2.95 version. BLAS: IBM ESSL library.
  The both tests (fig. 3) do not show any abstraction penalty of the new library. The optimized BLAS (ESSL) library requires 2-3 times less computational time compared to the pure C++ implementation to the same task.
Test 1: matrix-vector and vector-constant products

Test 2: long vector-constant expressions

Test 3: long function expressions

Figure 2: Performance tests on the Intel PIII-800 platform

Figure 3: Performance tests on the IBM M80 with Power3 500MHz processors
The same compiler with following optimization options was used on the both hardware platforms:

-07 -ffast-math -funroll-loops -fomit-frame-pointer -fexpensive-optimizations

Conclusions

The new library for the linear algebra was developed, which uses the expression templates technique and the optimized BLAS to achieve higher computational performance than the known C++ libraries. According to the BLAS specification the library provides vectors and matrices of only single and double precision types. Any other types are not allowed, although, the algebraic expressions resolved by the library are not limited and implemented traditionally for both general and sparse vectors and matrices.

The main trick of the implementation is the recursion of function templates realized by factitious empty classes add and sub. They have the aim to separate definition of structure BinClos and member function templates for addition and subtraction operations in the compilation time. Some old compilers do not allow to write function template if one of the template parameters is not a data type of an argument. For some C++ developer it can seem to be a mistake. But it works efficiently in the described implementation, since the template parameters are resolved in the compilation time without loss of the code performance. This code can be produced by some commonly used compilers:

- GNU C++, gcc 2.95x, gcc 2.96x, gcc 3.x versions
- Intel C++ compiler, version 5.0
- KAI C++ compiler

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