

Elements of Design for Containers and Solutions in the LinBox library

Extended abstract

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Abstract. We develop in this paper design techniques used in the C++ exact linear algebra library LinBox, intended to make the library safer and easier to use, while keeping it generic and efficient. First, we review the new simplified structure for containers, based on our *founding scope allocation* model. We explain design choices and their impact on coding: unification of our matrix classes, clearer model for matrices and submatrices, *etc.* Then we present a variation of the *strategy* design pattern that is comprised of a controller–plugin system: the controller (solution) chooses among plug-ins (algorithms) that always call back the controller. We give examples using the solution `mul`. Finally we present a benchmark architecture that serves two purposes: Providing the user with easier ways to produce graphs using C++; Creating a framework for automatically tuning the library and provide regression testing schemes.

Keywords: LinBox; design pattern; algorithms and containers; benchmarking; matrix multiplication algorithms; exact linear algebra.

1 Introduction

This article follows several papers and memoirs on the LinBox⁶ (*cf.* [2, 7, 8, 12, 18]) and builds upon them. LinBox is a C++ template library for fast and exact

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⁶ See <http://www.linalg.org>.

linear algebra. It is designed with generality and efficiency in mind. The LinBox library is under constant evolution, driven by new problems and algorithms, by new computing paradigms, new compilers and architectures. This poses many challenges. To address these changes, we are incrementally updating the *design* of the library towards a 2.0 release.

Let us start from a basic consideration: we show in the Table 1 the increase in the “lines of code” size ⁷ of LinBox and its co-evolved dependencies Givaro and FFLAS-FFPACK. This increase affects the library in several ways. First, it demands

LinBox	1.0.0 ^{†‡}	1.1.0 ^{†‡}	1.1.6 [‡]	1.1.7 [‡]	1.2.0	1.2.2	1.3.0	1.4.0
loc (×1000)	77.3	85.8	93.5	103	108	109	112	135
FFLAS-FFPACK	n/a	n/a	n/a	1.3.3	1.4.0	1.4.3	1.5.0	1.8.0
loc	—	—	—	11.6	23.9	25.2	25.5	32.1
Givaro	n/a	n/a	3.2.16	3.3.3	3.4.3	3.5.0	3.6.0	3.8.0
loc	—	—	30.8	33.6	39.4	41.1	41.4	42.8
total	77.3	85.8	124	137	171	175	179	210

Table 1: Evolution of the number of lines of code (loc, in thousands) in LinBox, FFLAS-FFPACK and Givaro ([†]contains Givaro, [‡]contains FFLAS-FFPACK).

a stricter development model, and we are going to list some techniques we used. For instance, we have transformed FFLAS-FFPACK⁸ (*cf.* [9]) into a new stand-alone header library, resulting in more visibility for the FFLAS-FFPACK project and also in better structure and maintainability of the library. A larger template library is harder to manage. There is more difficulty to trace, debug and write new code. Techniques employed for easier development include reducing compile times, enforcing stricter warnings and checks, supporting more compilers and architectures, simplifying and automating version number changes, automating memory leak checks, setting up build-bots to check the code frequently,...

This size increase also requires more efforts to make the library user friendly. For instance, we have: Developed an `auto-install.sh` script that installs automatically the latest stable or development versions of the trio, resolving the version dependencies; Facilitated the discovery of the BLAS/LAPACK libraries; Simplified and sped up the checking process while covering more of the library; Updated the documentation and distinguished user and developer oriented docs; Added comprehensive benchmarking tools,...

Developing generic and high-performance libraries is difficult. We can find a large literature on coding standards and software design references in (*cf.* [1, 10, 14, 16, 17]), and many internet sources and experience acquired by/from free software projects. Another motivation for developing a high-performance mathematical library is to make it available and easy for researchers and engineers that will use it for producing quality reliable results and quality research papers.

⁷ Using `sloccount`, available at <http://sourceforge.net/projects/sloccount/>.

⁸ See <http://www.linalg.org/projects/fflas-ffpack/>.

We describe advances in the design of LinBox in the next three sections. We will first describe the new *container* framework in Section 2, then the improved *matrix multiplication* algorithms in Section 3 made by contributing special purpose matrix multiplication plug-ins, and, finally, we present the new *benchmark/optimisation* architecture (Section 4).

2 Containers architecture

LinBox is mainly conceived around the RAII (Resource Acquisition Is Initialisation, see [16]) concept with re-entrant function. We also follow the founding scope allocation model (or *mother model*) from [8] which ensures that the memory used by objects is allocated in the constructor and freed only at its destruction. The gestion of the memory allocated by an object is then exclusively reserved to it.

LinBox essentially uses matrix and vectors over fields and rings as data objects (containers). The fragmentation of the containers into various matrix and blackbox types needed to be addressed and simplified. The many different matrix and vector types with different interfaces needed to be reduced into only two (possibly essentially one in the future) containers: **Matrix** and **Vector**.

2.1 General Interface for Matrices

First, in order to allow operations on its elements, a container is parametrized by a field object (Listing 1.1), not the field's element type. This simpler and more general. The storage type is given by a second template parameter that can use defaults, *e.g.* dense BLAS matrices (stride and leading dimension or increment).

```
template< class _Field, class _Storage = denseDefault >
class Vector ;
```

Listing 1.1: Matrix or Vector classes in LinBox.

In the mother model, we must distinguish containers that own (are responsible for allocated memory) and containers that share some memory. The **SubMatrix** and **SubVector** types share the memory while **Matrix** and **Vector** own it. The common interface shared by all container matrices is the **BlackBox** interface described in the following paragraphs, that accomodates both owner and sharer container types.

Input/Output. Our matrix all read and write from MatrixMarket format⁹) which is well established in the numerical linear algebra community. This allows for easy exchange and interoperability, but LinBox containers can also add some comments to the file, for instance the field characteristics (modulo, irreducible polynomial, **init** function, rank,...) We can adapt the header to suit our needs, and even create new formats that save space (CSR fashion saving roughly a third space over COO), or dedicated to structured matrices.

⁹ See <http://math.nist.gov/MatrixMarket/>.

Accessing Elements. The function `setEntry` can be used to populate the matrix (from some `init()` until a `finish()` is emitted). The function `setEntry` can be (very) costly (for some sparse formats for instance) Other functions such as `refEntry` (that retrieves a writable reference to an entry) may be difficult to implement or inefficient (compressed fields, sparse matrices); `getEntry` may be specialized, in all cases, there is a solution for this operation falling back to the `apply` method. Accessing (read or write) elements, rows or columns through iterators, although handy, is not required because it can be tricky to implement (compressed fields, hybrid or recursive formats). Traits on matrices where efficient iterators are available allow for their selections in some algorithms.

Apply method. This is essential in the `BlackBox` interface (Sections 2.2 and 3).

Rebind/Conversions. Rebind from one field to the other (if possible, using some default homeomorphism). Conversion mechanisms between formats are added to the interface when convenient, for instance all sparse matrix formats can convert to/from CSR format. This ‘star’ mechanism can simplify the code (to the expense of memory usage) and may speed it up when the mother format (CSR for instance) is well tuned for some task. Such tasks could be read/write from a file for instance, or update the matrix.

This is a common minimal interface to all our matrices that can be used by all of our algorithms. Additional elements to a container can be added, and flagged with a trait. This model also ensures basic “linear application” use of a matrix (blackbox) which is the least one can request from a matrix. For instance, this interface is shared by: Our *dense* containers (BLAS type or vector of rows); Our *permutations* containers (compressed LAPACK or cycle representation); Our *sparse* formats (based on common formats such as COO, CSR,... or based on STL containers such as `map`, `deque`, `pair`,...); Our *structured* containers (Diagonal, Hankel, Butterfly,...); Our *compound* containers (Sum, Compose, Submatrix,...).

2.2 The apply method

The `apply` method (left or right) is arguably the most important feature in the matrix interface and the `LinBox` library. It performs what a linear application is defined for: apply to a vector (and by extension a block of vectors, *i.e.* a matrix).

We propose the new interface (Listing 1.2), where `_In` and `_Out` are vector or matrices, and `Side` is either `Tag::Right` or `Tag::Left`, whether the operation $y \leftarrow A^\top x$ or $y \leftarrow Ax$ is performed. We also generalize to the operation $y \leftarrow \alpha Ax + \beta y$ as it is often handy and efficient to allow for accumulation.

```
// y = A.x
template< class _In, class _Out >
_Out& apply(_Out &y, const _In& x, enum Side) ;
```

Listing 1.2: Apply methods.

This method is important for two reasons: first it is the building block of the `BlackBox` algorithms (for instance `Wiedemann` and `block-Wiedemann`); second

the matrix multiplication is a basic operation in linear algebra that needs to be extremely efficient (this is the matter of Section 3). The implementation of the apply method can be left to the `mul` solution (see Section 3), with possibly a helper/method argument if the apply parameters are specialized enough.

3 Improving LinBox matrix multiplication

3.1 Plug-in structure

We propose the following *design pattern* (the closest design pattern to our knowledge is the *strategy* one, see also [6, Fig 2.]). The main advantage of this design pattern is that the modules always call back the controller so that the best choice is always chosen. Besides modules can be easily added as *plug-ins*. An analogy can be drawn with dynamic systems—once the controller sends a correction to the system, it receives back a new measure that allows for a new correction.

For instance, we can write (Figure 2) the standard cascade algorithms (see [9]) in that model. Cascade algorithms are used to combine several algorithms that are switched using thresholds, ensuring better efficiency than any of the algorithms within used separately. This method allows for the reuse of modules and ensures efficiency. It is then possible to adapt to the architecture, the available modules, the resources. The only limitation is that the choice of the module should be done fast.

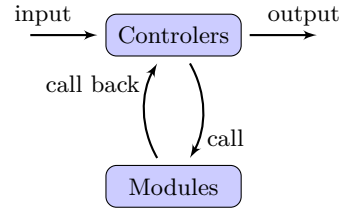


Fig. 1: Controller/Module design pattern

Algorithm 1: Algo: controller	Algorithm 2: Algo: recursive module
Input: A and B , denses, with resp. dimensions $n \times k$ and $k \times n$.	Input: A, B, C as in controller.
Input: H Helper	Input: H , RecursiveCase Helper
Output: $C = A \times B$	Output: $C = A \times B$
if $\min(m, k, n) < H.\text{threshold}()$	Cut A, B, C in S_i, T_i
then	...
Algo($C, A, B, \text{BaseCase}()$) ;	$P_i = \text{Algo}(S_i, T_i, H)$
else	...
Algo($C, A, B, \text{RecursiveCase}()$)	
end	

Fig. 2: Conception of a recursive controlled algorithm

On top of this design, we have Methods/Helpers that allow (preferred) selection of algorithms and cut short in the strategy selection of Section 3.1.

This infrastructure also invites to modularise the code. For instance, `FFLAS-FFPACK` has seen major modularization (addition, scaling, reduction,...). Not only

it allows to write code with hardly more line than it takes for pseudo-code listings in [5] (compared to $\approx 2.5\times$ on some routines before) but also it automatically brings performance, because we can the separately improve on these modules and can switch easier between them. Also, this reduces the lines of code, hence the probability for bugs, and eases the tracing/traking of bugs, allows for more unit tests. Modularising the code comes at almost no cost because we may add $O(1)$ operations that 1) don't cost much compared to $O(n^2)$ or more complexity of the modules; 2) allow early decisions and terminations (*e.g.* by testing against 0, ± 1 , checking leading dimensions and increments); 3) allow better code (AVX, SSE, copy–cache friendly operation–copy back, representation switching,...)

3.2 New algorithms/infrastructure

We introduce now several new algorithms that improve on matrix multiplication in various ways: reducing memory consumption, introducing new efficient algorithms, using graphics capabilities, generalizing the BLAS to integer routines.

New algorithms: low memory The routine `fgemm` in `FFLAS` uses the classic schedules for the multiplication and the product with accumulation (*cf.* [5]), but we also implement the lower memory routines therein. The difficulty consists in using the part of the memory contained in a sub-matrix of the original matrix. It is two-fold. – First we have to use some part of a memory that has already been allocated to the input matrices, therefore we cannot free and reallocate part of it. – Second, several of these algorithms are meant for square matrices.

New algorithms: Bini. In [3], we use Bini's approximate matrix multiplication formula to derive a new algorithms that is more efficient that the Strassen–Winograd implementation in `fgemm` by $\approx 5 - 10\%$ on sizes 1 500–3 000. This is a cascade of Bini's algorithm and Strassen–Winograd algorithm and/or the naïve algorithm (using BLAS). The idea is to analyse precisely the error term in the approximate formula and make it vanish.

Integer BLAS. In order to provide fast matrix multiplication with multiprecision integers, we rely on multi-modular approach through the chinese remainder theorem. Our approach is to reduce as much as possible to `fgemm`. Despite, the existence of fast multimodular reduction (*resp.* reconstruction) algorithm [11], the naive quadratic approach can be reduced to `fgemm` which makes it more efficient into practice. Note that providing optimized fast multimodular reduction remains challenging. This code is directly integrated into `FFLAS`.

Polynomial Matrix Multiplication over small prime fields. The situation is similar to integer matrices since one can use evaluation/interpolation techniques through DFT transforms. However, the optimized Fast Fourier Transform of [15] makes fast evaluation (*resp.* interpolation) competitive into practice. We thus rely on this scheme together with `fgemm` for pointwise matrix multiplications. One can find some benchmark of our code in [13].

OpenCL [△](#)dave

Sparse Matrix-Vector Multiplication Sparse matrices are usually problematic because the notion of *sparsity* is too general *vs.* the specificity of real world sparse matrices: the algorithms have to adapt to the shape of the sparse matrices — which is not really the case for the dense case. Getting the best performance for an sparse matrix as an **BlackBox** is a challenging task. There is a huge literature on SpMV(Sparse Matrix Vector multiplication) and on sparse matrix formats, some of which are becoming standard (COO, CSR, BCSR, SKY,...). In [4] we developped some techniques to improve the SpMVoperation in **LinBox**. Just like the BLAS numerical routines, we would also like to take advantage of existing high performance numerical libraries (come back to this later).

The addition of standard matrix format is driven by the availability of numerical routines and the expectation of better performance in the SpMVoperation. The issue in the SpMVoperation is taking advantage of existing numerical routines. There is a Sparse BLAS specification, but it is not widely implemented (Intel's MKL does, there is a cuSPARSE library in the Nvidia Cuda toolkit). Contrary to dense BLAS representation, there is no way of viewing a sparse submatrix in most of the standard formats, so we cannot apply the same techniques as those in FFLAS for Z/pZ . However, we develop hybrid structures that represent a matrix A as a sum $A_1 + A_2 + \dots + A_k$. For instance, the number of non zeros in each row of each A_i will not overflow a dot product and numerical sparse BLAS can be used. Besides, the format of each submatrix is independant and we can create some ELL+CSR format for instance. Besides, sparse matrices from many domains have only ± 1 as non zero entries and we take advantage of that (no multiplication, accumulation further delayed, no need to store the data).

Contrary to the BLAS case, the apply using the transpose of A can be very inefficient compared to the apply on A . In this case, we create a helper function that (if memory allows) just stores A^T in an optimised hybrid format too. Setting up the hybrid representation of A usually costs the order of 5to 10 non optimised SpMVoperations: the conversion is performed only for larger matrices that will be used repeatedly for the SpMVoperation and remains constant.

Using conversions

- double- ζ float
- using flint for integer matmul is faster, even with conversion. Need better CRA implementation (but with the plugins, we can do without our faulty code and just use flint).
- implementation of Toom-Cook for GF(q)
- when does spmv choose to optimise ?
- transition to benchmarking

[△](#)dave some words on the Domain architecture that you support and why it is best than functions (for instance for mul or apply) ?

4 Benchmarking for automatized tuning and regression testing

Benchmarking was introduced in LinBox for several reasons. First, It would give the user a user-friendly way for producing quality graph with no necessary knowledge of a graphing library like `gnuplot`¹⁰ or provide the LinBox website with automatically updated tables and graphs. Second, it would be used for regression testing. Finally, it would be used for selecting default method, threshold. A lot of libraries do some automatic tuning at installation (fftw, ATLAS, NTL,...).

What do we do differently ? Selection between "larger" algorithms, takes more time. Interpolation.

4.1 Performance evaluation

Our plotting mechanism is based on two structures: `PlotStyle` and `PlotData`. The `PlotGraph` structure uses the style and data to manage the output. We allow plotting in standard image formats, html and \LaTeX tables, but also in raw csv or xml. The last raw formats allow for file exchange, data comparisons and extrapolation. \triangle Dave benchmark formats discussion ?

4.2 Automatized regression testing

Saving graphs in raw format can enable automatic regression testing on the buildbots. For some determined matrices (of different shape and size) over a few fields, we can accumulate over time the timings for some of our solutions (rank, det, mul,...). At each new release, when we update the documentation, we can check any regression on these base cases and automatically update the regression plots. \triangle We need to implement this framework (not difficult; anybody?).

4.3 Automatized tuning and method selection

CPU throttling for ATLAS, FFLAS-FFPACK not reliable. XXX Default are provided, method can be selected via a benchmark (cf `wino_threshold`)
XXX howto feature matrix

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¹⁰ <http://www.gnuplot.info/>

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