Notes on the bigalgebra Package

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1 Introduction

The bigalgebra package provides linear algebra operations for "Big Matrices" defined in the bigmemory package. The package includes matrix and vector arithmetic operations and several matrix factorizations. Standard infix arithmetic operators are overloaded to use bigalgebra functions, keeping syntax familiar and simple.

The bigalgebra package may be optionally compiled with high-performance, multithreaded numeric libraries, which may also provide large-index support. Large indices support linear algebra computation on matrices and vectors with up to 2^{51} total entries (the usual R limit constrains objects to less than 2^{31} total entries). The package also supports computations on arrays that are larger than available RAM using bigmemory's file-backed big matrix objects. The bigalgebra package presently supports double-precision computation.

2 Installation

The default installation uses available system and R BLAS and LAPACK libraries. The bigalgebra package may be optionally compiled with alternate libraries that offer performance and threading optimizations as well as large index support.

Installation assumes the standard R toolchain and GNU compiler suite, and requires setting one or more configuration options:

- --with-incDir Extra required include directories and compiler options.
- --with-blasHeader Alternate BLAS header file.
- --with-blas The BLAS library linker instructions.
- --with-lapcakHeader Alternate LAPACK header file.

- --with-lapack The LAPACK library linker instructions.
- --with-int64 The integer index type (usually long or long long).

2.1 Installation with Reference BLAS (with large index support)

The bigalgebra package includes reference BLAS and LAPACK libraries from Netlib with large index support. The libraries are not tuned for performance—use high-performance libraries instead when possible.

The following example illustrates installation with the reference large-index BLAS and LAPACK libraries:

R CMD INSTALL --configure-args='--with-blas=refblas64' bigalgebra

2.2 Installation with Intel MKL

The Intel® Math Kernel Library (MKL), available from http://software.intel.com/en-us/intel-mkl/, is a set of highly optimized and extensively threaded numeric routines for x86, x86-64, and Intel architecture (Itanium) processors. The library is available in standard and large-index versions.

We assume below that the MKL is installed in the <code>/opt/intel/mkl/10.2.5.035/</code> directory—substitute your installation path as required. We illustrate the command-line installation procedure below. Installation from the R console with the <code>install.packages</code> command follows similarly. We outline dynamic linkage against MKL which requires that the MKL libraries lie in the system library path.

2.2.1 Example: MKL Large-index support on x86-64 systems using GNU Open MP

```
R CMD INSTALL --configure-args='
--with-incDir="-DMKL_ILP64 -I/opt/intel/mkl/10.2.5.035/include/"
--with-blasHeader="refblas64longlong.h"
--with-blas="-L/opt/intel/mkl/10.2.5.035/lib/em64t/
-lmkl_gf_ilp64 -lmkl_gnu_thread -lgomp -lmkl_core"
--with-lapack="-L/opt/intel/mkl/10.2.5.035/lib/em64t/
-lmkl_gf_ilp64 -lmkl_gnu_thread -lgomp -lmkl_core"
--with-lapackHeader="mkl.h"
--with-int64="long long"' bigalgebra
```

Note that we use the "refblas64longlong.h" BLAS header file supplied with the bigalgebra package. Additional MKL compilation examples can be found in the Intel MKL documentation.

2.3 Installation with AMD ACML

The AMD® Core Math Library (ACML) is available from http://developer.amd.com/cpu/libraries/acml/page The ACML provides a highly-threaded set of numeric libraries optimized for performance on x86 and x86-64 processor architectures. The library is available in standard and large-index versions.

We assume that the ACML is installed in the /opt/acml4.4.0/ directory.

2.3.1 Example: ACML Large-index support on x86-64 systems

```
R CMD INSTALL --configure-args='
--with-incDir="-I/opt/acml4.4.0/gfortran64_int64/include/"
--with-blasHeader="acml.h"
--with-blas="-L/opt/acml4.4.0/gfortran64_int64/lib -lacml -lacml_mv"
--with-lapack="-lacml -lacml_mv"
--with-lapackHeader="acml.h"
--with-int64=long' bigalgebra
```

2.4 Installation with GOTO BLAS

3 Examples

```
> library('bigalgebra')
XXX
```