IBM® Netezza® Analytics Release 3.3.x.0

Matrix Engine Developer's Guide

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Preface

Audience for This Guide

The nzMatrix Engine is intended for developers and partners interested in working with large matrices on the IBM Netezza appliance. To work with nzMatrix, you should possess a thorough understanding of matrix concepts and linear algebra. You should also be familiar with basic operation and concepts of the IBM Netezza systems and software.

Purpose of This Guide

This guide provides an introduction to Netezza Matrix Engine concepts and usage examples for NZPLSQL stored procedures.

Symbols and Conventions

Note on Terminology: The terms *User-Defined Analytic Process (UDAP)* and *Analytic Executable (AE)* are synonymous.

The following conventions apply:

- ▶ Italics for emphasis on terms and user-defined values, such as user input.
- ▶ Upper case for SQL commands, for example, INSERT or DELETE.
- ▶ Bold for command line input, for example, nzsystem stop.
- ▶ Bold to denote parameter names, argument names, or other named references.
- ➤ Angle brackets (<>) to indicate a placeholder (variable) that should be replaced with actual text, for example, inza-<release_number>.zip.
- A single backslash ("\") at the end of a line of code to denote a line continuation. Omit the backslash when using the code at the command line, in a SQL command, or in a file.
- ▶ When referencing a sequence of menu and submenu selections, the ">" character denotes the different menu options, for example, Menu Name > Submenu Name > Selection.

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CHAPTER 1

Introduction to the Netezza Matrix Engine

The Netezza Matrix Engine (nzMatrix) is a parallelized linear algebra package. It provides a wide range of computations and manipulations that can be run on very large matrices. Using fully distributed and parallelized memory, processing, and database storage, nzMatrix performs computations comparable in size to the available aggregate RAM of the Netezza appliance. It scales to hundreds of gigabytes of RAM, hundreds of processing cores, and hundreds of terabytes of data storage. The Netezza Matrix Engine provides access to highly scalable matrix operations.

With nzMatrix, matrices are transparently stored in IBM Netezza Analytics, allowing matrix data transfer directly to and from the database and the distributed matrix engine.

Netezza Matrix Engine Functions

The Netezza Matrix Engine provides a wide variety of functions:

- Linear algebra functions
 - ▲ Matrix multiplication
 - Linear equation solving
 - ▲ Linear least squares
 - ▲ Matrix inversion
 - ▲ Eigenvalues and eigenvectors
 - ▲ Singular value decomposition
- ▶ Matrix element-wise, pair-wise, and reduction functions
- Inquiry and housekeeping functions
- Random number generators (RNGs)

Applications for nzMatrix

The Netezza Matrix Engine has many areas of application in business and research:

- Principal Component Analysis (PCA)
- Clustering and prediction
- Dimension reduction for data mining
- Customer segmentation, behavioral targeting, customer loyalty
- Social network analysis, such as marketing and counter-terrorism
- Unsupervised learning, latent semantic indexing
- Signal processing, image processing, data compression
- ▶ Recommender systems, such as the Netflix Prize
- Microarray Data Analysis, such as bioinformatics and genomics
- Mathematical finance

Understanding nzMatrix

nzMatrix Layered Architecture

nzMatrix has a layered architecture, consisting of an NZPLSQL layer with its API and a C++ layer, which is not exposed as an API. The C++ layer performs many of its functions by calling the Intel[®] MKL library, including PBLAS and ScaLAPACK routines. PBLAS and ScaLAPACK are proven libraries of highly scalable distributed matrix routines that rely on BLACS and MPI for interprocess communication. For more information on UDAPs, refer to the *User-Defined Analytic Process Developer's Guide*.

Matrix Storage and Access

The Netezza Matrix Engine stores data in the currently connected database using standard Netezza database tables beginning with the prefix NZ_MAT_. As a best practice, you should set privileges to hide these tables from direct access by standard users. The standard Netezza Analytics privilege-granting scripts, create_inza_db.sh and create_inza_db_user.sh are used to modify the permissions. While elevated privileges allow direct access to nzMatrix tables, it is not recommended because direct access could result in code incompatibility with future versions of nzMatrix or data corruption.

The **create_inza_db_user.sh** script grants users the necessary privileges to execute the nzMatrix stored procedures registered in the NZM database. It is recommended that you create additional databases for connection purposes, rather than using the NZM database.

The nzMatrix NZPLSQL stored procedures allow interaction with matrices. nzMatrix provides routines for creating matrices from and saving matrices to user-accessible Netezza database tables in Row/Column/Value format. nzMatrix also provides routines for listing and deleting matrices stored in the database as well as for creating identity matrices, random matrices, and others.

When a given database is shared, the matrix namespace is also shared. Therefore, if a matrix is created while connected to a shared database, that matrix is accessible to any user who has the proper privileges to work in the shared database. This is different than tables where, by default, users do not have visibility into other users' tables. Note that you cannot create a new matrix with the same name in the shared database without first deleting the previously created matrix.

nzMatrix General Limitations

nzMatrix uses the 64-bit double precision floating point approximate numeric data type for storage and computation of matrix element values. Row and column indices are stored as 32-bit integer values, allowing up to 2,147,483,647 rows and columns. Row and column indices begin at 1; a zero index value is not permitted.

nzMatrix computations are automatically distributed across the Netezza appliance. Computations that make use of PBLAS and ScaLAPACK are automatically queued FIFO and run one at a time. If a computational step that uses PBLAS or ScaLAPACK is being performed, any other users' attempts to do the same are queued.

To check which tasks are queued, if any, use the following SQL command:

```
CALL NZA..SP MPI STATS();
```

To abort a task, use the following SQL command, replacing the Job Task ID as needed:

```
CALL NZM..KILL ENGINE (< job task ID>);
```

Calculations using PBLAS or ScaLAPACK consume S-Blade RAM for temporarily holding input matrices, intermediate work matrices, and result matrices. Each matrix element consumes 8 bytes. Exceeding available RAM may result in aborted computation and an "Out of memory" user error. Available RAM equals total RAM minus the RAM requirements of the Linux operating system, the Netezza software, and concurrent, unrelated queries.

For example, an IBM Netezza 1000-12 with 12 S-Blades and 16 GB of RAM per S-Blade, performing the matrix multiplication of two 65,000 x 65,000 element matrices, consumes its available RAM and takes approximately 1 hour. Performing the Singular Value Decomposition of a 45,000 x 45,000 element matrix also consumes the available RAM and takes approximately 7 hours. These are maximum limits and assume minimal concurrent queries.

Scalability

Memory requirements and computation time grow rapidly as matrix dimensions increase. The amount of memory required to hold a matrix with n rows and n columns is proportional to n squared, and the number of operations required to multiply, invert, or decompose such matrices is proportional to approximately n cubed.

Random Number Generators

Netezza Analytics provides a set of wrappers for the Intel® Math Kernel Library random number generators (RNGs). The SQL API provides a set of stored procedures that generate matrices filled with

pseudorandom values drawn from given probability distribution. See the *Netezza Matrix Engine Reference Guide* for a description of each stored procedure. See <u>Intel® Math Kernel Library Vector</u> <u>Statistical Library Notes</u> for more information on the RNGs.

Bulk Algorithms

From Version 3, IBM Netezza Analytics provides bulk algorithms that you can use to work on many smaller matrices in parallel.

The bulk algorithms are:

- ▶ Bulk matrix operations
- ▶ Bulk linear regression
- ▶ Bulk principal components analysis (PCA)

For detailed information about bulk algorithms, see the *IBM Netezza In-Database Analytics Developer's Guide*.

CHAPTER 2

Using nzMatrix: An Example

Enabling a Database for nzMatrix Use

To enable nzMatrix functionality, follow the instructions below:

1. Create a new Netezza Analytics-enabled database:

```
$ cd /nz/export/ae/utilities/bin
$ ./create_inza_db.sh MYDB
```

2. Connect to the database:

```
$ nzsql MYDB
```

3. Initialize the nzMatrix engine for the particular database:

```
CALL NZM..INITIALIZE();
```

Refer to the *IBM Netezza Analytics Administrator's Guide* for additional examples and detailed information on creating Netezza Analytics-enabled databases and setting database permissions.

nzMatrix Using the SQL Interface

This example demonstrates using nzMatrix by calling NZPLSQL stored procedures. It illustrates a wide variety of nzMatrix capabilities, ranging from simple matrix addition to complex linear algebra operations such as Singular Value Decomposition (SVD). The example is not intended to solve a specific issue, but rather to illustrate syntax and usage. Refer to the *Matrix Engine Reference Guide* for additional examples and detailed information on each stored procedure.

Note: nzMatrix does not overwrite existing matrices. Therefore, you may need to delete any preexisting matrices before running this example and again after the example is complete. The DELETE_ALL_MATRICES() procedure deletes all matrices in the current database and should be used only if you are certain that the database does not contain matrices needed by other users. If the

database does contain matrices belonging to another user, use the Delete_MATRIX() procedure to delete matrices by name.

nzMatrix Run from Netezza SQL

This example can be run from the nzsql command line or from any other SQL-based application.

```
-- Note: All procedures return a value of true, except where noted.
-- Initialize nzMatrix
CALL NZM..INITIALIZE();
-- Uncomment the next line to delete all matrices in the current database
-- CALL NZM..DELETE ALL MATRICES();
-- Generate matrices
CALL NZM..UNIFORM('A', 5, 5); -- Uniformly distributed random numbers
CALL NZM..NORMAL('B', 5, 5); -- Normally distributed random numbers
CALL NZM..CREATE RANDOM MATRIX('A53', 5, 3); -- Same as UNIFORM
CALL NZM..CREATE IDENTITY MATRIX('A IDENT', 5); -- Identity matrix
CALL NZM..CREATE ONES MATRIX('A ONES', 5, 5); -- Matrix of ones
-- Set and Get the value of a matrix element
CALL NZM..SET_VALUE('A', 3, 2, 0.12345);
CALL NZM..GET VALUE('A', 3, 2); -- Returns 0.12345
-- Bulk export of matrix data to a Netezza table
DROP TABLE MYTABLE; -- In case MYTABLE already exists
CALL NZM..CREATE TABLE FROM MATRIX('A53', 'MYTABLE');
SELECT * FROM MYTABLE ORDER BY ROW, COL; -- Confirm contents of MYTABLE
-- Create a matrix from a table - bulk import of data
CALL NZM..CREATE MATRIX FROM TABLE ('MYTABLE', 'B53', 5, 3);
-- Confirm that B53 has been correctly created
CALL NZM.. TEST DENSE VALID('B53'); -- Returns true
CALL NZM..LIST MATRICES(); -- Returns current list of matrices
CALL NZM..GET NUM ROWS('B53'); -- Returns 5
CALL NZM..GET NUM COLS('B53'); -- Returns 3
-- Element-by-element add, subtract, multiply, divide
CALL NZM..ADD('A', 'B', 'A_PLUS_B');
CALL NZM..SUBTRACT ('A', 'B', 'A MINUS B');
CALL NZM..MULTIPLY ELEMENTS('A', 'B', 'A TIMES ELEM B');
CALL NZM..DIVIDE ELEMENTS ('A', 'B', 'A DIV ELEM B');
-- Element-by-element comparisons
CALL NZM..EQ('A', 'B', 'A EQ B'); -- Equal
CALL NZM..NE('A', 'B', 'A NE B'); -- Not equal
CALL NZM..GT('A', 'B', 'A GT B'); -- Greater than
CALL NZM..GE('A', 'B', 'A GE B'); -- Greater than or equal
CALL NZM..LT('A', 'B', 'A_LT_B'); -- Less than
CALL NZM..LE('A', 'B', 'A_LE_B'); -- Less than or equal
CALL NZM..MAX('A', 'B', 'MAX_A_B'); -- Pair-wise maximum
CALL NZM..MIN('A', 'B', 'MIN A B'); -- Pair-wise minimum
-- Functions of matrix elements
```

```
CALL NZM..ABS ELEMENTS('A','A ABS'); -- Absolute value
CALL NZM..CEIL_ELEMENTS('A','A_CEIL'); -- Ceiling
CALL NZM..FLOOR ELEMENTS('A', 'A FLOOR'); -- Floor
CALL NZM..EXP ELEMENTS ('A', 'A EXP'); -- Exponential
CALL NZM..LN ELEMENTS('A', 'A LN'); -- Natural logarithm
CALL NZM..LOG ELEMENTS ('A', 'A LOG'); -- Base 10 logarithm
CALL NZM..INT ELEMENTS('A','A INT'); -- Truncate toward zero
-- Round to the specified number of decimal digits
CALL NZM..ROUND ELEMENTS('A', 'A ROUND', 2);
-- Show the contents of a matrix
CALL NZM..PRINT('A ROUND', FALSE); -- Returns the contents of A ROUND
-- Modulo (remainder) function
CALL NZM..MOD ELEMENTS('A', 'A MOD', 3);
-- Reductions
CALL NZM..RED_MAX('A'); -- Returns the maximum value in A
CALL NZM..RED MIN('A'); -- Returns the minimum value in A
CALL NZM..RED MAX ABS('A'); -- Returns the maximum absolute value in A
CALL NZM..RED MIN ABS('A'); -- Returns the minimum absolute value in A
CALL NZM..RED_SUM('A'); -- Returns the sum of the values in A
CALL NZM..RED SSQ('A'); -- Returns the sum of the squares of the values
CALL NZM..RED TRACE('A'); -- Returns the trace of A (the sum of the
diagonal
                             elements)
CALL NZM..ANY NONZERO('A'); -- Returns one if any of A's values are
nonzero.
                            Otherwise, returns zero.
CALL NZM..ALL NONZERO('A'); -- Returns one if all of A's values are
nonzero.
                               Otherwise, returns zero.
-- Copy a submatrix
CALL NZM..COPY SUBMATRIX('A', 'A SUB', 2, 3, 1, 4);
CALL NZM..GET NUM ROWS('A SUB'); -- Returns 2
CALL NZM..GET NUM COLS('A SUB'); -- Returns 4
-- Transpose (interchange rows and columns)
CALL NZM..TRANSPOSE('A', 'A TRANS');
-- Concatenate vertically (number of columns stays the same)
CALL NZM..CONCAT('A', 'B', 'A B CONCAT V', 'V');
CALL NZM..GET NUM ROWS('A B CONCAT V'); -- Returns 10
CALL NZM..GET NUM COLS('A B CONCAT V'); -- Returns 5
-- Concatenate horizontally (number of rows stays the same)
CALL NZM..CONCAT('A', 'B', 'A_B_CONCAT_H', 'H');
CALL NZM..GET NUM ROWS('A B CONCAT H'); -- Returns 5
CALL NZM..GET NUM COLS('A B CONCAT H'); -- Returns 10
-- Kronecker product
CALL NZM..KRONECKER('A', 'B', 'A B KRON');
CALL NZM..GET NUM ROWS ('A B KRON'); -- Returns 25
```

```
CALL NZM..GET NUM COLS('A B KRON'); -- Returns 25
-- Housekeeping
CALL NZM..MATRIX EXISTS ('A');
CALL NZM..DELETE MATRIX('A');
CALL NZM..MATRIX EXISTS('A'); -- Returns false
-- Linear algebra
CALL NZM..CREATE RANDOM MATRIX('A', 1000, 1000);
-- Matrix inversion
CALL NZM..INVERSE('A', 'A_INV');
-- Matrix multiplication
CALL NZM..GEMM('A', 'A_INV', 'A_A_INV');
-- Verify that A INV is the inverse of A, within floating point precision
CALL NZM..CREATE IDENTITY MATRIX('I', 1000);
CALL NZM..SUBTRACT('A_A_INV', 'I', 'A_A_INV_MINUS_I');
CALL NZM..RED MAX ABS('A A INV MINUS I'); -- Returns a value close to
-- Linear Equation Solving
-- Solve A X = RHS for X
CALL NZM...NORMAL('RHS', 1000, 10);
CALL NZM..SOLVE('A', 'RHS', 'X');
-- Verify that A X = RHS, within floating point precision
CALL NZM..GEMM('A', 'X', 'A X');
CALL NZM..SUBTRACT ('A X', 'RHS', 'A X MINUS RHS');
CALL NZM..RED MAX ABS('A X MINUS RHS'); -- Returns a value close to zero
-- Linear Least Squares
-- For over/underdetermined systems A X LLS = RHS,
-- find linear least squares solution X LLS
CALL NZM..SOLVE LINEAR LEAST SQUARES('A', 'RHS', 'X LLS');
-- Singular Value Decomposition
CALL NZM..SVD('A', 'U', 'S', 'VT');
-- Create a diagonal matrix from the one-column matrix S
CALL NZM..VEC TO DIAG('S', 'SIGMA');
-- Verify that A = U SIGMA VT, within floating point precision
CALL NZM..GEMM('U', 'SIGMA', 'U SIGMA');
CALL NZM..GEMM('U_SIGMA', 'VT', 'U_SIGMA_VT');
CALL NZM..SUBTRACT('A', 'U SIGMA VT', 'A MINUS U SIGMA VT');
CALL NZM..RED MAX ABS('A MINUS U SIGMA VT'); -- Returns a value close to
zero
-- Eigenvalues and eigenvectors of a symmetric matrix
-- Create a symmetric matrix
CALL NZM..TRANSPOSE('A', 'A TRANSP');
CALL NZM..ADD('A', 'A TRANSP', 'A SYMM');
```

```
-- Compute Eigenvalues W and Eigenvectors Z
CALL NZM..EIGEN('A_SYMM', 'W', 'Z');
```

Note: In actual operation, the CALL NZM.._TEST_DENSE_VALID(); command used in the example outputs notice messages that provide some informational text on the tests it is performing. The call ultimately returns TRUE or FALSE, depending on whether the matrix passes all of the validity tests. The notice text was omitted from the example for clarity.

APPENDIX A

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Product may be powered by redundant power sources. Disconnect ALL power sources before servicing. High leakage current. Earth connection essential before connecting supply. Courant de fuite élevé. Raccordement à la terre indispensable avant le raccordement au réseau.

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This equipment has been tested and found to comply with the limits for a Class A digital device, pursuant to part 15 of the FCC rules. These limits are designed to provide reasonable protection against harmful interference when the equipment is operated in a commercial environment. This equipment generates, uses, and can radiate radio-frequency energy and, if not installed and used in accordance with the instruction manual, may cause harmful interference to radio communications. Operation of this equipment in a residential area is likely to cause harmful interference, in which case users will be required to correct the interference at their own expense.

This Class A digital apparatus meets all requirements of the Canadian Interference-Causing Equipment Regulations.

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