User's Guide for the Algorithm Testing System/Version 1.1

Cathleen Diaz

U.S. DEPARTMENT OF COMMERCE
Technology Administration
National Institute of Standards
and Technology
Factory Automation Systems Division
Gaithersburg, MD 20899

NIST

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1. INTRODUCTION

The NIST Algorithm Testing System (ATS) is a software package for evaluating the performance of geometric fitting software. The ATS provides basic capabilities for comparing the results of different fitting routines to a set of reference algorithms. The ATS allows the user to generate test data for various geometries with simulated form errors and simulated measurement errors; run test data through the reference algorithms; import fits computed by other algorithms; and compare the results of algorithms. The system was developed to run on PC compatible computers. This document applies to Version 1.1 of the ATS system and describes how to install and run the ATS on a PC compatible computer.

The ATS is available from NIST on a formatted floppy disk. This distribution disk contains Version 1.1 of the Algorithm Testing System. The disk includes compressed files of the ATS executable, ATS source code, this *User Guide* and several other documents, and data files.

The ATS was developed as part of NIST's contribution to an ongoing effort by industry standards groups to establish a standard for testing software used in inspection systems. The project is sponsored by the Navy Manufacturing Technology Program and by NIST internal funding. In the short term, the project goal is to develop a production version of the Algorithm Testing System. The draft report, *Requirements for a Production Algorithm Testing System*, provides a description of the production version of the ATS. The long-term goal is to develop a standard set of reference algorithms that can be used for testing software. This achievement would allow industry to have a standard method for testing software.

1.1   System Requirements

In order to run the ATS, you must have an IBM PC compatible computer. The minimum configuration necessary is as follows:

    80286 or higher cpu
    DOS Version 3.3 or later
    Hard disk with at least 2 MB free space
    EGA or VGA graphics
    High density 5 1/4" floppy drive
    512 KB free memory (recommend minimum of 640K installed memory)

Optional equipment:
    80 x 87 Math co-processor
    Mouse

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A math co-processor is not required. However, the ATS will use one if it is present. A mouse is not required but is recommended. To install the software as it is distributed, you must have a high density 5 1/4" floppy drive (other formats are available upon request).

1.2   Features

The Algorithm Testing System features the following implementations.

- Least-squares fitting algorithms
- Data generation with simulated form errors, measurement strategy, and measurement error models
- Window-based user interface within the ATS
- Data management capabilities, including data import and export
- Residual analysis of a fit
- Detailed comparison of fit results

1.3   Overview

Section 2 of this document describes the procedure for installing the Algorithm Testing System from the distribution disk onto your system. Section 3 contains a brief overview for starting and operating the system. Section 4 contains a detailed description of the system operation. There are four appendices at the end of the document. Appendix A contains a description of the ATS file formats. Appendix B contains a description of the ATS file names. Appendix C contains details on the parameters of the data generator. Finally, Appendix D describes the parameters reported by the fit result analysis and comparison.

2.   INSTALLATION

The installation diskette contains multiple compressed files and is distributed on an IBM-formatted disk. The distribution diskette includes the NIST Algorithm Testing System; this *User Guide*; the document, *Form Error Models of the NIST Algorithm Testing System*[1]; the draft report, *Least-Squares Fitting Algorithms of the NIST Algorithm Testing System;* and various data files. The documents included are in a WordPerfect 5.1 format.

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[1]Algeo, M. E. A. and Hopp, T. H., *Form Error Models of the NIST Algorithm Testing System*, NISTIR 4740, National Institute of Standards and Technology, Gaithersburg, MD, January 1992.

The ATS is distributed in a compressed format and must be expanded to be used. The **INSTALL** script on the distribution diskette simplifies this process. The **INSTALL** script can be used with one or two arguments, as follows:

Method 1: Using **INSTALL** with one argument

Change to the floppy drive that contains the ATS distribution diskette and enter **INSTALL [target directory]**.

For example, if the distribution diskette is in drive A: and you want the ATS installed in C:\ATS, then enter the following commands:

> **A:<ENTER>**
> **INSTALL C:\ATS<ENTER>**

Method 2: Using **INSTALL** with two arguments

From any drive, specify the absolute path to **INSTALL** and enter **[source drive]:INSTALL [source drive] [target directory]**.

For example, if the distribution diskette is in drive A: and you want the ATS installed in C:\ATS, then enter the following commands:

> **A:INSTALL A: C:\ATS<ENTER>**

3.   OPERATION

This section of the document contains an overview for starting and operating the Algorithm Testing System. For more detailed instructions on using the ATS refer to Section 4.

3.1   Running the ATS

The command to run the ATS is **ats.** For example:

> **C:\ATS\ATS<ENTER>**

starts the ATS executable in the C:\ATS directory. The ATS starts up with a menu bar at the top of the screen displaying five menu items. The menu bar is your primary access to all the menu items and menu commands. Each menu item has a pull-down menu associated with it. The pull-down menus contain commands. In this document, all ATS commands will be

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identified by the menu item name and command name, separated by a vertical bar. For example, the command to exit the ATS is denoted PROGRAM|QUIT.

Here is how you choose menu commands using the keyboard:

1 Press *<F-10>*. This function key makes the menu bar active.
2 Use the *<LEFT/RIGHT>* arrow keys to select the menu item you want and then press *<ENTER>* to obtain the pull-down menu with the commands. The *<DOWN ARROW>* can also be used to pull down command menus.

   As a shortcut for this step, you can just press the highlighted letter of the menu item. For example, from the menu bar, press T to move to and display the TEST menu.

3 Use the *<DOWN/UP>* arrow keys to select the command you want. Then press *<ENTER>*.

   Again, as a shortcut, you can just press the highlighted letter of a command to choose it once the menu is displayed. At this point the ATS either carries out a command, displays a dialogue box, or displays another menu.

4 To cancel an action, press *<ESC>*.
5 To close a menu, press *<ESC>*.

You can also use a mouse to choose menu items and menu commands.

1 Click on the desired menu item to display the menu commands.
2 Click on the desired command.
3 To cancel an action, press *<ESC>*.
4 To close a menu, press *<ESC>*.

Most commands result in a window being displayed by the ATS. The four main window types are test descriptions, data sets, fits, and analysis results. All interaction with the ATS is through these windows. Each window type has its own particular procedures, but several features are common to all main window types.

These common window procedures are as follows:

1 Any selected window can be removed from the display by pressing *<ESC>* and selecting *<OKAY>*.
2 Any window can dragged or moved using the mouse. Select the border of the window with the mouse and move the window while holding down the mouse button.
3 Any window can be selected with the mouse. A window is active when its border is highlighted. Move the mouse to the window until highlighted. Only one window may

be active at any time. Clicking on the border of an active window in the background will bring it to the foreground.

4   The function key <*F-5*> sequences through displayed windows.

3.2   Basic Procedures for Using the ATS

The capabilities of the ATS are: defining a test description for a given geometry, generating a data set for the test, fitting the test data set using the least squares method, and analyzing the fit results. Usually you will use the ATS by going through each of the above steps in sequence.

You define a test description by selecting the TEST|NEW command. A test description window is displayed. This window allows you to select a geometry type. When you select a geometry type, you also must enter numeric parameters defining the ideal (nominal) geometry. These parameters are used to generate data. They are also used as the starting guess for computing reference fits. A test description window also allows you to select and define a form error, a sampling pattern, and a measurement error for the given geometry.

You generate a data set by selecting the DATASET|NEW command. At least one test description window must be opened. The data set is associated with the last test description window you used. A data set window is displayed. This window allows you to select the GENERATE button. This selection will cause the ATS to generate data corresponding to the associated test description. After the data set is generated, the coordinates are displayed in the window.

You calculate a fit by selecting the FITTING|NEW menu command. A fit description window is displayed. This window allows you to select the fitting method to be used (currently only least squares is implemented). You select the COMPUTE FIT button to calculate the fit. You can set iteration limits and a convergence factor to control the fitting algorithm.

You analyze fit results by selecting the ANALYSIS|NEW command.   An analysis window is displayed. This window is divided into three sections. In the upper left is a box listing the names of all fit result windows available for analysis. This list contains the last fit window that you used, together with all other fit windows associated with the same geometry type. You can select any fit for detailed analysis by clicking on it with the mouse or by highlighting it with the arrow keys and pressing <*ENTER*>. If there is more than one fit, a comparison to a reference fit is also done. You can select which fit is used as the reference by pressing R while the fit is highlighted. The bottom half of the window displays the detailed analysis of a single fit. The sum of the squares, standard deviation, maximum, and average of the residuals are displayed. The partial derivatives of the objective function with respect to the fitting parameters are shown. These numbers indicate how close the fit is to a minimum. The upper right section of the analysis window contain the comparative results of a fit to the selected reference fit.

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4.   DETAILED INSTRUCTIONS

This section contains detailed instructions for operating the ATS. Section 4.1 presents an overall description of the menu system. Section 4.2 describes each menu item and the respective menu commands.

4.1   The Menu System

The ATS starts up with a menu bar across the top of the screen. The menu items are listed across this menu bar. The commands of each menu item are organized into pull-down menus. Each pull-down menu contains a series of commands. The menu items are PROGRAM, TEST, DATASET, FITTING, and ANALYSIS. Whenever the menu bar is active, one of the menu items is highlighted to indicate which item of the menu bar is currently active. Figure 1 is a diagram of how the menu system would appear if all of the menus were pulled down at the same time. (The ATS allows only one menu at a time to be pulled down.)

ATS	Program	Test	Dataset	Fitting	Analysis
	About	New	New	New	New
	Directory	Open	Open	Open	
	Quit	Save	Save	Save	
		Delete	Delete	Delete	
			Import	Import	
			Export		
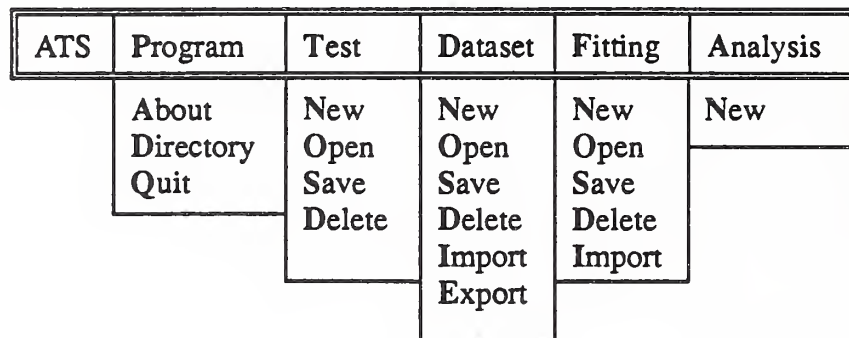
Figure 1: Menu bar from Algorithm Testing System with all menus pulled down

4.1.1   The Menu Bar, the Mouse, and the Keyboard

The ATS allows you to access the system via the menu bar. The menu bar can be accessed with function keys from the keyboard, with a mouse, and with keystrokes from the keyboard.

Here is how to access the menu bar with function keys:

1   If no menu item is highlighted, press the **<F-10>** function key. This action activates the menu bar. (The menu bar must be active to select an item.)
2   Use the **<LEFT/RIGHT>** arrow keys to move along the menu bar and select an item.

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3 Use the *<ENTER>* or *<DOWN>* arrow key once an item is selected to pull down the corresponding menu.

4 Use the *<UP/DOWN>* arrow keys to move through and select a command from the menu.

5 Use the *<ENTER>* key to execute the selected command.

Here is how to access the menu bar with the mouse:

1 Click on the desired menu item to display the menu. This will automatically activate the menu bar.

2 Click on the desired command to be executed.

Here is how to access the menu bar with keystrokes from the keyboard:

1 If necessary, press the *<F-10>* function key to activate the menu bar.

2 Press the highlighted letter from the desired menu item. This action activates its corresponding command menu.

3 Press the highlighted letter from the desired menu command. This action executes the corresponding command.

The following table lists the function keys available to you.

Keys	Function
<F-5>	Sequences through window displays.
<F-10>	Activates menu bar.
<ESC>	Close active window or menu display.

Table 1: General function keys

The following tables list the menu items shortcut keys and the menu commands shortcut keys.

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Keys	Menu item	Function
P	Program menu	Takes you to the Program menu
T	Test menu	Takes you to the Test menu
D	Dataset menu	Takes you to the Dataset menu
F	Fitting menu	Takes you to the Fitting menu
A	Analysis menu	Takes you to the Analysis menu

Table 2: Menu items shortcut keys

Keys	Menu command	Function*	Menus
N	New	Create a new object	Test, Dataset, Fitting, Analysis
O	Open	Open a saved object	Test, Dataset, Fitting
S	Save	Save an object	Test, Dataset, Fitting
D	Delete	Delete a saved object	Test, Dataset, Fitting
I	Import	Import an object	Fitting, Dataset
E	Export	Export an object	Dataset
A	About	Show program information	Program
D	Directory	Change directory	Program
Q	Quit	Exit the program	Program
		*An object is a test description, dataset, fit, or analysis.	

Table 3: Menu commands hot keys

4.2   Menu Items and Commands

The menus shown in Figure 1 are described in detail in sections 4.2.1 through 4.2.5.

4.2.1 The PROGRAM Menu

The PROGRAM menu contains the PROGRAM|ABOUT command, the PROGRAM|DIRECTORY command, and the PROGRAM|QUIT command. The PROGRAM|ABOUT command displays some general information about the Algorithm Testing System. It is an information screen that tells where, when and by whom the system was developed. The PROGRAM|DIRECTORY command allows you to change directories. For example, the ATS could be running in one directory and the files containing data sets could be in another directory. The PROGRAM|QUIT command allows you to exit the ATS.

4.2.2 The TEST Menu

The TEST menu contains the commands for creating, opening, saving, and deleting test descriptions. The four available commands are TEST|NEW, TEST|OPEN, TEST|SAVE, and TEST|DELETE. These commands are described in detail in sections 4.2.2.1 through 4.2.2.4.

4.2.2.1   The TEST|NEW Command

The TEST|NEW command allows you to create a new test description. The information that is required to create a test description is displayed in a window. The window requests that a geometry be defined, form errors identified, sampling pattern chosen, and measurement error be identified. You cannot define a form error or a sampling pattern until you have defined a geometry. The information needed to create a test description is described in detail below. See Appendix C for more detailed information.

GEOMETRY   The GEOMETRY field allows you to choose the geometry for the test description. Select GEOMETRY to obtain the following options: LINE, CIRCLE, PLANE, SPHERE, CYLINDER, and CONE. When the geometry is chosen another window is displayed. The new window allows you to enter a location, a direction, a size, an angle and an extent for the geometry (only those that are relevant to the geometry are displayed). The geometry types are described in detail in Appendix C of this document.

FORM ERROR   The FORM ERROR field allows you to choose the type of form error to be simulated in the sampling of points. Select FORM ERROR to obtain the options for the types of form errors available. The form errors vary depending on the

type of geometry selected. The form errors are described in detail in Appendix C of this document.

SAMPLING

The SAMPLING command allows you to indicate the sampling pattern to be used in generating data sets. Select the SAMPLING command to obtain the following options for sampling patterns: RANDOM, EQUISPACED WITH ENDS, EQUISPACED NO ENDS, and STRATIFIED. The <ENTER> key here selects the next information field to be entered (a command is not executed). The sampling patterns are described in detail in Appendix C of this document.

MEASUREMENT ERROR

The MEASUREMENT ERROR field allows you to indicate the type of measurement error that should be simulated to generate the data points. Select the MEASUREMENT ERROR command to obtain the following options: NONE, UNIFORM, and NORMAL. The measurement errors are described in detail in Appendix C of this document.

4.2.2.2   The TEST|OPEN Command

The TEST|OPEN command opens a previously saved test description (see TEST|SAVE below). Once the TEST|OPEN command is selected, a new window is displayed. The window shows a list of names of saved test descriptions. You select a name and a test description window is displayed on the screen. The test description window will contain all the information that was stored. Press <ESC> to cancel the operation.

4.2.2.3   The TEST|SAVE Command

The SAVE command saves the current test description. The description is saved in a file in the current directory. (ATS system file names are discussed in Appendix B of this document.) Once a test description is created you can save it by selecting the TEST|SAVE command from the TEST menu on the main menu bar. You will be prompted for a test description name. This name should be no longer than eight characters and should not be given an extension.

4.2.2.4   The TEST|DELETE Command

The TEST|DELETE command deletes a test description that has been previously saved. Select the TEST|DELETE command and then select the test description to be deleted from the displayed list.

You must then confirm or cancel the request by selecting OKAY or CANCEL. Deleting a test description will invalidate any saved dataset that was created from the test. It is valid to delete an already open test description. However, the test description will be lost if the window is closed without saving it again.

4.2.3   The DATASET Menu

The DATASET menu contains the commands for creating, saving, and deleting data sets. The data can be generated by the data generator or imported from an external file. Data sets can also be exported to a data file (for use by other programs). A data set is always associated with and dependent upon the test description. The six available commands in this menu are: DATASET|NEW, DATASET|OPEN, DATASET|SAVE, DATASET|DELETE, DATASET|IMPORT, and DATASET|EXPORT. These commands are described in detail in sections 4.2.3.1 through 4.2.3.6.

4.2.3.1   The DATASET|NEW Command

The DATASET|NEW command allows you to generate a new data set. The data set is automatically associated with the last active test description. A data set cannot be generated without an active test description. A window is displayed when the NEW command is selected. This window allows you to select the GENERATE button. This button invokes the data generator, which generates data points based on the associated test description. After the points are generated they are displayed in the window as x, y, and z coordinate values. You can use the arrow keys or page up and down to scroll through the points. (You must be at the GENERATE button to be able to leave the window using the keyboard). If you make changes to the test description after a data set has been generated, selecting GENERATE again will cause the data set to be replaced with new data corresponding to the test description values.

4.2.3.2   The DATASET|OPEN Command

The DATASET|OPEN command allows you to open a previously saved data set. This command also opens a window for the test description associated with the data set. Select the OPEN command to obtain a list of available data sets. Once a data set is selected, two windows are displayed. One window contains the test description for the data set. The other window contains the data set itself. (If the test description is already displayed in a window, only one new window is opened.)

4.2.3.3 The DATASET|SAVE Command

The DATASET|SAVE command saves the current data set. Once the DATASET|SAVE command is selected, a form is displayed for you to enter the name of the data set to be saved. You have the option to confirm the save by selecting OKAY or to cancel by selecting CANCEL. If OKAY is selected the data set will be saved. The data set name must not exceed eight characters in length and should not be given an extension. (A detailed description of the ATS system filenames is discussed in Appendix B of this document.)

4.2.3.4 The DATASET|DELETE Command

The DATASET|DELETE command deletes a previously saved data set. Once the DELETE command is selected, a window is displayed with a list of saved data sets. This window allows you to select the data set to be deleted. You can confirm by selecting OKAY or cancel by selecting CANCEL. The DATASET|DELETE command only deletes the dataset, not the associated test description. It is valid to delete an already open data set. However, the data set will be lost if the window is closed without saving it again.

4.2.3.5 The DATASET|IMPORT Command

The DATASET|IMPORT command imports an external file containing x-y-z coordinate data. This command displays a data set (data sets generated outside of the ATS) in a data set description window. In the ATS three types of file formats can be imported. The **PTB A Series, PTB B Series**, and the **Generic** format. (The files with **PTB** data sets are data points that were generated during previous tests done in Germany by the Physikalisch Technische Bundesanstalt.) Refer to Appendix A for more details on the ATS file formats.

The ATS allows you to import these files and run the reference algorithm on the data sets. The ATS allows you to run the reference algorithm with data sets from different sources that represent the same geometry. Once the DATASET|IMPORT command is selected, the ATS displays a window that lists the data set formats available, **Generic, PTB A Series**, and **PTB B Series**. After selecting a format you enter the name of the file to be imported. If you use wildcard characters ('*' or '?') in the file name a file selection window is displayed. You can then select the specific file to be imported. Like the DATASET|NEW command, the DATASET|IMPORT command will only work if you have already opened a test description window.

4.2.3.6 The DATASET|EXPORT Command

The DATASET|EXPORT command exports a data set to a file. The window displayed when DATASET|EXPORT is selected allows you to give the file a name. You can enter a fully qualified

file name, with a path and extension if desired. Confirm the selection with the OKAY button or cancel with the CANCEL button. The DATASET|EXPORT command does not create a test description file and does not add an extension to the file name. The DATASET|EXPORT command saves the file in the **Generic** format.

4.2.4   The FITTING Menu

The FITTING menu contains the commands for creating, saving, and deleting fits. A fit description is always associated with and is dependent upon a data set. (The data set in turn is associated with a test description.) The five available commands in this menu are: FITTING|NEW, FITTING|OPEN, FITTING|SAVE, FITTING|DELETE, and FITTING|IMPORT. These commands are described in detail in sections 4.2.4.1 through 4.2.4.5.

4.2.4.1   The FITTING|NEW Command

The FITTING|NEW command allows you to calculate a fit using the algorithms that come with the ATS. A fit cannot be calculated without an active data set. The ATS currently implements the least squares method of fitting. Each fit uses the test description and the data set description to obtain the data necessary to calculate the fit. The OBJECTIVE button allows you to select the fitting method to be used (least squares for now). You can also set an iteration limit and a convergence factor for the fit. The convergence factor and the iteration limit are discussed in detail in the draft report, *Least-Squares Fitting Algorithms of the NIST Algorithm Testing System.* A positive convergence factor is an absolute convergence test. A negative convergence factor is a relative convergence test. The COMPUTE FIT button is selected to calculate the fit. The results of the fit are displayed in the fit description window. The fit reports the sum of the squares of errors (sse). The location is reported in x, y, and z coordinates. The direction, size and angle are reported for some of the geometries. While the ATS is computing a fit, it displays a status message. Some fitting problems may take considerable time. If you wish to interrupt a fit, press the <BREAK> key while holding down the <CTRL> key. (On some computer systems, there may be a delay before this keystroke is recognized and the fit is interrupted.)

4.2.4.2   The FITTING|OPEN Command

The FITTING|OPEN command allows you to open a file containing a previously saved fit. This command causes the ATS to also open the test description window and the data set window associated with the fit. Once the FITTING|OPEN command is selected, a window displays a list of previously saved files. You select a file and confirm or cancel using the OKAY or CANCEL commands.

4.2.4.3   The FITTING|SAVE Command

The FITTING|SAVE command allows you to save a fit result. This command automatically saves the test description and the data set associated to the fit. When the FITTING|SAVE command is selected, a window is displayed in which you enter a name for the fit. This name should be no longer than eight characters and should not be given an extension. (Refer to Appendix A of this document for details on the ATS file names.)

4.2.4.4   The FITTING|DELETE Command

The FITTING|DELETE command allows you to delete a previously saved fit description. When the FITTING|DELETE command is selected, the ATS displays a list of saved fit descriptions. This window allows you to select the desired fit description. You then select OKAY or CANCEL to confirm or cancel the FITTING|DELETE request. Press <ESC> to cancel from the list of fit descriptions.

4.2.4.5   The FITTING|IMPORT Command

The FITTING|IMPORT command allows you to import a fit description file. As with FITTING|NEW, a data set must be defined before a fit can be imported. When the FITTING|IMPORT command is selected, a window is displayed in which you enter the name of the fit result file to be imported. You then confirm or cancel the FITTING|IMPORT request by selecting OKAY or CANCEL. The fit description files that are imported are fit results from other sources (fits results that were generated with algorithms other than the reference algorithms of the ATS). Refer to Appendix B of this document for details on the format of the fit results.

4.2.5   The ANALYSIS Menu

The ANALYSIS menu contains the command for generating an analysis of the fit results. The only available command in this menu is ANALYSIS|NEW. This command is described in detail in section 4.2.5.1.

4.2.5.1   The ANALYSIS|NEW Command

The ANALYSIS|NEW command allows you to generate an analysis of fit results. When the ANALYSIS|NEW command is selected an ANALYSIS window is displayed. This window is divided into three sections.

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The upper left is a box listing the names of all fit result windows available for analysis. This list contains the last fit window you used together with all other fit windows associated with the same geometry type. You can select any fit for detailed analysis by clicking on it with the mouse or by highlighting it with the arrow keys and pressing *<ENTER>*. If there is more than one fit, a comparison to a reference is also done. You can select the reference fit by pressing *R* while the fit is highlighted.

The lower half of the window displays the results of a single fit analysis. The analysis displays the sum of the squares of the errors (sse), the standard deviation, the maximum and average residuals, and the gradients. The gradients are the partial derivatives with respect to x, y, and z for the location, and with respect to the size and angles where applicable. The angles describe the direction. The gradients will be very small if the fit is close to a (local) minimum.

The upper right section of the window displays comparative analysis of two fit results. The upper left section of the window lists the two fits. The imported fit is listed first. The reference fit is listed second (this is the default). The comparative analysis displays the geometry differences (axis separation and angle separation), a residual analysis (sse difference), and the gradient difference (angle and length).

The analysis window displays a different single analysis result depending on which fit is selected. If an imported fit in the upper left section of the window is selected then the single analysis displayed is of the imported fit. The comparison is of the imported fit compared to the reference fit. If the reference fit in the upper left section of the window is selected then the single analysis displayed is of the reference fit. You can make an imported fit the reference fit for the comparison analysis by pressing **R** on the selected fit.

5.   Summary

The NIST Algorithm Testing System/Version 1.1 has been distributed for beta testing to a number of potential users. These include members of the ASME B89.4.10 Working Group for CMS Software Performance Evaluation and other members of the dimensional metrology community. Users have responded favorably and have contributed useful comments and suggestions which have been considered during the development of the production ATS. One of the recommendations is the need for algorithms other than least squares in the ATS. NIST is developing additional algorithms for other fitting objectives. NIST is also developing a procedure for submitting and selecting reference algorithms. These algorithms will be the performance baseline of the ATS.

Any problems, questions, suggestions or comments regarding the NIST Algorithm Testing System should be addressed to one of the following two people.

Cathleen Diaz
National Institute of Standards and Technology
Building 220 Room A127
Gaithersburg, MD 20899

email diaz@cme.nist.gov
Telephone (301) 975 - 2889
Fax   (301) 258 - 9749

Theodore H. Hopp
National Institute of Standards and Technology
Building 220 Room A127
Gaithersburg, MD 20899

email hopp@cme.nist.gov
Telephone (301) 975 - 3545
Fax   (301) 258 - 9749

Appendix A

Algorithm Testing System File Formats

A.1 INTRODUCTION

The Algorithm Testing System provides several mechanisms for bringing data into and sending data out of the system. The DATASET|IMPORT command enables you to access data sets generated outside the ATS, while the DATASET|EXPORT command enables you to save data sets generated by the ATS. This export file may be used as input to your algorithm. To bring the fit results generated by your algorithm into the ATS, use the FITTING|IMPORT command.

This appendix describes the file format requirements for importing and exporting data sets, as well as importing fit results.

A.2 DATASET IMPORT FILE FORMATS

Three types of data sets may be imported into the ATS. The formats supported are **PTB A Series**, **PTB B Series**, and **Generic** format. Both PTB A and B Series data sets are included in the ATS distribution. The **Generic** format allows you to import data from a measurement system or other source. The following three sections describe the import formats in detail.

A.2.1 PTB A Series

The files containing data sets in the **PTB A Series** have the following format:

```
<geometry type> <data set number> <time stamp>
x1-value  y1-value  z1-value
x2-value  y2-value  z2-value
x3-value  y3-value  z3-value
   .
   .
   .
```

The first line of the file contains the geometry type, the data set number, and a time stamp. The following lines list the coordinate values of the data set. An example follows:

```
LINE        1      881005
62.0007   3.5427   12.1164
69.4374   3.5504   12.1164
76.8742   3.5574   12.1164
   .
   .
   .
```

Each data set from the **PTB A Series** is in a separate file. The file name convention is **DATASET.A#** where # is the data set number and A means it is from the **PTB A Series**. For instance, the file name for the previous example is **DATASET.A1**.

A.2.2 PTB B Series

The distribution of the **PTB B Series** data includes two files for each data set. One file contains the data set, while a comment file contains detailed information about the data set. The file containing the data set has the following format:

    x1-value y1-value z1-value
    x2-value y2-value z2-value
    x3-value y3-value z3-value
    .
    .
    .

An example of a file containing a **PTB B Series** data set follows:

    746.0352 167.2775 -81.9667
    798.8503 135.0613 -127.6552
    800.1427 123.9985 -163.9518
    821.0459 168.8838 -107.2863
    .
    .
    .

The corresponding comment file indicates that the data set contains points on a cylinder. The comment file also contains details on the approximate dimensions and position of the geometric element. Each data set from the **PTB B Series** is in a separate file. Similarly, the detailed information for each data set is in a separate comment file. The files containing data set are named **DATASET.B#** where # is the data set number and B means it is from the **PTB B Series**. The files containing detailed information for a data set are name **COMMENT.B#** where # is number for the **PTB B Series** data set. For instance, the file name for the previous example is **DATASET.B20**, and its corresponding comment file is **COMMENT.B20**.

A.2.3 Generic Format

The files containing data sets in the **Generic** format have the following structure:

```
<number of points>
x1-value  y1-value  z1-value
x2-value  y2-value  z2-value
x3-value  z3-value  z3-value
    .
    .
    .
```

The first line of the file lists the number of points that are contained in the data set. The rest of the file are the x, y, and z coordinates of each point, with one point per line. An example of a data set file in the **Generic** format follows:

```
5
23.4756     3.5678     -42.9876
20.6543     3.5789     -41.9875
17.7654     3.5876     -40.6532
14.8743     3.5902     -39.8765
11.6273     3.6087     -38.4143
```

The file names for the **Generic** format can be any valid DOS file name.

A.3   DATASET EXPORT FILE FORMATS

Use the DATASET|EXPORT command to transfer ATS-generated data to the system that contains your algorithms. This export file is in **Generic** format. See Section A.2.3 for more details.

A.4   FITTING IMPORT FILE FORMATS

Fit results from test algorithms are imported by using files. Each file contains a single fit result that is comprised of an appropriate number of fit parameters according to the type of geometry. These parameters vary among the different geometry types. Table A.1 specifies the parameters to be reported for each geometry. Within the import file for fit results, the parameter values are separated by white space (such as spaces, tabs, or end-of-line characters). Any other separation characters (such as commas) will cause unpredictable results. These parameter values may be expressed by decimal floating point or exponential notation. The ATS ignores information or comments in the file beyond the last parameter.

GEOMETRY	FILE FORMAT		
	PARAMETER NUMBER	PARAMETER NAME	PARAMETER DESCRIPTION
LINE	1, 2, 3	$<x>$ $<y>$ $<z>$	coordinates of a point on line
	4, 5, 6	$<a>$ $<b>$ $<c>$	direction numbers of line
CIRCLE	1, 2, 3	$<x>$ $<y>$ $<z>$	coordinates of center
	4, 5, 6	$<a>$ $<b>$ $<c>$	direction numbers of the normal
	7	$<d>$	diameter
PLANE	1, 2, 3	$<x>$ $<y>$ $<z>$	coordinates of a point on plane
	4, 5, 6	$<a>$ $<b>$ $<c>$	direction numbers of plane normal
SPHERE	1, 2, 3	$<x>$ $<y>$ $<z>$	coordinates of center
	4	$<d>$	diameter
CYLINDER	1, 2, 3	$<x>$ $<y>$ $<z>$	coordinates of a point on axis
	4, 5, 6	$<a>$ $<b>$ $<c>$	direction numbers of axis
	7	$<d>$	diameter
CONE	1, 2, 3	$<x>$ $<y>$ $<z>$	coordinates of a point on axis
	4, 5, 6	$<a>$ $<b>$ $<c>$	direction numbers of axis
	7	$<d>$	diameter at perpendicular cross section through point specified by parameters 1-3.
	8	$<\psi>$	full cone angle

Appendix B

Algorithm Testing System File Names

B.1   INTRODUCTION

The Algorithm Testing System accesses data files when saving, deleting, importing, and exporting data. There are test description files, data set description files, and fit description files. You can give each of these files a file name or you can let the ATS give each one a default file name. Each window that is displayed in the ATS has a default name from which the default file name is generated. This appendix describes the different file names in the ATS.

B.2   DEFAULT FILE NAMES

A default name is given to any new window displayed in the ATS. Following is a list of these types of file names:

        (TST000)
        (DSD000)
        (FIT000)
        (ANA000)
        (TST001)

The test description window is denoted with (TST###). The window that allows you to generate the data set for the test description is denoted (DSD###). The fitting window is denoted with (FIT###) and the analysis window is denoted with (ANA###). The ### symbol is a number in each of the file names. All numbers are used to distinguish open windows of the same type. Windows corresponding to saved objects have as window names, the name of the saved object.

If a test description, a data set, or a fit result is saved and you do not provide the ATS with a file name, the ATS will generate a default file name. Following is an example of the default file names:

        (TST000).TSD
        (DSD000).DSD
        (FIT000).FD
        (TST001).TSD

You can choose any valid DOS name for the file being saved. The ATS will add the appropriate extension. In other words, the ATS will always automatically add an extension to the file name.

B1

The following table summarizes default file names.

	display name	default saved name	saved name
test descriptions	(TST###)	(TST###).TSD	NAME.TSD
data sets	(DSD###)	(DSD###).DSD	NAME.DSD
fit results	(FIT###)	(FIT###).FD	NAME.FD
analysis	(ANA###)	N/A	N/A

TABLE 1: Default File Names

B.3   DATA SETS

Data sets are imported and exported in three file formats: **PTB A, PTB B,** and **Generic.** In this distribution of the ATS we have included some files with data sets in the **PTB A Series** and the **PTB B Series.** The file names in the **PTB A Series** are denoted **DATASET.A#.** The name itself tells you that it is a data set. The **A** in the extension means it is from the **PTB A Series** and the number is a unique identifier. The file names in the **PTB B Series** are denoted **DATASET.B#.** The name itself tells you that it is a data set. The **B** in the extension means it is from the **PTB B Series** and the number is a unique identifier. The files in the **PTB B Series** have associated comment files. These comment files are denoted **COMMENT.B#.** Following is a list with examples of these types of file names.

    DATASET.A12
    DATASET.B1
    COMMENT.B1
    DATASET.B30
    COMMENT.B30
    DATASET.A5

There are also **Generic** data set files. These file names are denoted with any valid DOS name. For example:

    TESTDATA.DAT
    NEWDATA

are file names for data sets of the **Generic** format. In the **Generic** format, one line has the number of points in the file and the rest of the file contains the points.

B.4   OTHER FILE NAMES

The ATS executable is denoted ATS.EXE. The *.DAT file names denote files with data sets in the **Generic** format. The **Generic** format is the default file type when a data set is exported. The file contains a line with the number of points in the data set and the data set itself. Each value is separated by a white space. Files in the **Generic** format can also be imported.

Appendix C

Algorithm Testing System Data Generator

Geometry Types, Form Errors, Sampling Patterns, and Measurement Errors

C.1   INTRODUCTION

The Algorithm Testing System allows you to generate data for your tests using the Data Generator. This Appendix describes the **Data Generator** in detail. The **Data Generator** allows you to generate data based on geometry types, form errors, sampling patterns, and measurement errors. The following sections describe the specifics of the **Data Generator**.

C.2   GEOMETRY TYPES

The ATS Data Generator supports the following geometry types: lines, circles, planes, spheres, cylinders, and cones. Each geometry is defined by a set of parameters which describes, when applicable, the geometry's location, direction, size, angle, and extent. Table C.1 lists the parameters necessary for describing each geometry type. Note that the size parameters are radii, not diameters, and the angle of a cone is the half-angle. These parameters are different from the corresponding parameters in the import format for fits, where diameters and full cone angle are expected. (See Appendix A.)

Geometry definitions are specified relative to a world coordinate system. Each geometry has a local coordinate system determined by the geometry definition. The local coordinate system for each geometry type is defined relative to the world coordinate system. This is done by defining a local x and a local z axis as shown in the following table.

geometry type	local x	local z
line	line direction	projected world z (or x)[†]
circle	projected world x (or y)[†]	normal to plane of circle
plane	projected world x (or y)[†]	normal to plane
sphere	world x	world z
cylinder	projected world x (or y)[†]	axis direction
cone	projected world x (or y)[†]	axis direction

[†]The world axis is projected into a plane perpendicular to the other local axis to obtain the indicated local axis. The alternate world axis is used when the other local axis is close to the default world axis. ("Close to" means that the dot product has magnitude at least 0.9.)

The local y axis is defined so that the local coordinate system is right-handed.

C.3   FORM ERRORS

The ATS can simulate any one of a number of form errors. The types of form errors available vary among the different geometry types. The types of form errors, and the geometry types to which they apply, are shown in Table C.2. The ATS will not allow you to define a form error until a geometry type has been specified. Detailed information about the parameters that define each form error type can be found in the report *Form Error Models of the NIST Algorithm Testing System*.[1] That report is included in the ATS distribution.

C.4   SAMPLING PATTERNS

The ATS supports four types of sampling: random, equispaced with end points, equispaced without end points, and stratified. All four sampling patterns are supported for all geometries, although they mean slightly different things for each geometry type. The ATS will not allow you to define a sampling pattern until a geometry type has been specified.

In the description below, geometry extents are based on Table C.1. In particular, for circles, spheres, cylinders, and cones, if $u_{min}=u_{max}$, u_{max} is treated as having the value $u_{min}+360°$.

Random sampling means that each data point is selected at random from within the extent of the geometry. For circles and lines, a uniformly-distributed random number is generated between u_{min} and u_{max}. For surfaces, two random numbers are generated, one for u and one for v.

Equispaced sampling can be done with or without endpoints. In both cases, the surface is divided into a grid by dividing the extent into bins according to the number of points indicated in u (and v for surfaces). Equispaced sampling with end points means that a sample point is generated at each grid intersection point. Equispaced sampling without end points means that a sample point is generated in the center (in u-v space) of each box in the grid.

Stratified sampling is similar to equispaced sampling without end points. Rather than sampling at the center of each box, however, each sample point is obtained by generating a uniformly-distributed random number (or two numbers, for surfaces) between the limits of the grid box.

For spheres and cones, it may happen that several grid points in u-v space correspond to the same x-y-z coordinates. For instance, if v=-90° on a sphere, all values of u correspond to the south pole. A similar problem occurs at the other pole of the sphere and at the apex of a cone. This

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[1]Algeo, M. E. A. and Hopp, T. H., *Form Error Models of the NIST Algorithm Testing System*, NISTIR 4740, National Institute of Standards and Technology, Gaithersburg, MD, January 1992.

problem only arises for spheres when using equispaced sampling with end points. It can occur in cones for either type of equispaced sampling. In all cases where the sampling pattern defines multiple points at the same x-y-z coordinates, the ATS will generate only one point at that position. This means that the actual number of points generated in a data set may be less than the number defined in the sampling plan.

C.5   MEASUREMENT ERROR

Measurement error is a displacement of a sampled point. The ATS adds a measurement error to each sample point after it is generated. The measurement error at a point is independent of the error at any other point, and is also independent of the geometry. All measurement errors are random. You can control whether measurement errors are to be added, and you can define the distribution for the magnitude of the measurement error. Two distributions are supported: uniform and normal. Each error is added in a random direction, with approximately uniform distribution.

Table C.1 Geometries and parameters

	LINE	CIRCLE	PLANES	SPHERE	CYLINDER	CONE
LOCATION	point on line	center point	point on plane	center point	point on axis	point on axis
DIRECTION*	line direction	normal to plane of circle	plane normal		axis direction	axis direction away from apex
SIZE		radius		radius	radius	radius in plane through location
ANGLE						half angle
EXTENT	u: start & end points $-\infty < u_{min} \le u_{max} < \infty$	u: start & end angles $0 \le u_{min} \le u_{max} \le 360$ $u_{min} = u_{max}$ implies full circumference	u: start & end points v: start & end points $-\infty < u_{min} \le u_{max} < \infty$ $-\infty < v_{min} \le v_{max} < \infty$	u: start & end angles v: start & end angles $0 \le u_{min} \le u_{max} \le 360$ $-90 \le v_{min} < v_{max} \le 90$ $u_{min} = u_{max}$ implies full circumference	u: start & end angles v: start & end points $0 \le u_{min} \le u_{max} \le 360$ $-\infty < v_{min} < v_{max} < \infty$ $u_{min} = u_{max}$ implies full circumference	u: start & end angles v: start & end points $0 \le u_{min} \le u_{max} \le 360$ $-\infty < v_{min} < v_{max} < \infty$ $u_{min} = u_{max}$ implies full circumference

*Direction numbers do not have to be unit magnitude, but they cannot be all zero.

Table C.2 Application of form errors

	LINE	CIRCLE	PLANE	SPHERE	CYLINDER	CONE
SINE	X	X	X	X		
STEP	X	X	X			
BEND	X		X			
RANDOM	X	X	X	X	X	X
AXIAL SINE					X	X
RADIAL SINE					X	X
AXIAL RADIUS SINE					X	X
AXIAL STEP					X	X
RADIAL STEP					X	X
AXIAL RADIAL STEP					X	X

Appendix D

Algorithm Testing System Analysis Results

D.1 INTRODUCTION

The Algorithm Testing System allows you to analyze and compare fit results. This appendix describes the details displayed in the analysis window of the ATS.

D.2 FIT RESULTS LIST

The upper left section of the analysis window displays the names of the fits computed. This list contains the name of the last window you used together with the names of all other fit windows associated with the same geometry type. Each fit can have a single analysis done, one at a time. You do this by selecting a fit with the mouse or by highlighting it. Any two fits can be compared and any one of the two can be the reference. You select the reference fit by pressing *R* while the fit is highlighted.

D.3 SINGLE ANALYSIS

The lower half of the window displays the results of a single fit analysis. The analysis displays the sum of the squares of the errors (sse), the standard deviation, the maximum and average residuals, and the gradients. The gradients are the partial derivatives with respect to x, y, and z for the location, and with respect to the size and angles where applicable. The angles describe the direction. The gradients will be very small if the fit is close to a (local) minimum.

The following table lists the parameters that describe the details in the single analysis.

Sum of the Squares of Errors (sse)	$\sum \varepsilon^2$
Standard Deviation	$\sqrt{\dfrac{\sum \varepsilon^2}{N}}$
Maximum Residual	$Max_i \lvert \varepsilon_i \rvert$
Average Residual	$\dfrac{1}{n} \sum \varepsilon_i$

TABLE 1: Single Analysis Parameters

The following table lists the equations that describe the gradients in the single analysis. Note that sse is the sum of the squares of errors.

Gradient with respect to x	$\dfrac{\partial sse}{\partial x}$
Gradient with respect to y	$\dfrac{\partial sse}{\partial y}$
Gradient with respect to z	$\dfrac{\partial sse}{\partial z}$
Gradient with respect to size	$\dfrac{\partial sse}{\partial size}$
Gradient with respect to the angle	$\dfrac{\partial sse}{\partial angle}$
Angle from z axis	$\dfrac{\partial sse}{\partial \alpha}$
Angle from z-x plane	$\dfrac{\partial sse}{\partial \beta}$

TABLE 2: Single Analysis Gradient Parameters

D.4   COMPARATIVE ANALYSIS

The comparative analysis is presented by computing the geometry differences between the test fit and the reference fit. The computations displayed for the geometry difference is dependent upon the geometry type.

The following table lists the specific details that are displayed for each geometry type. The X's in the table indicate which details are listed for each geometry type.

	line	circle	plane	sphere	cylinder	cone
separation	X	X	X	X	X	X
angle	X	X	X		X	X
size		X		X	X	X
form						X

TABLE 2: Geometry Difference Specifics

D.4.1 Geometry Difference

The separation difference is the perpendicular distance from the point that locates the test fit to the different points on the reference. This location varies with the geometry type.

The following table lists where the point on the reference lies.

geometry	reference
line	line
circle	center
plane	plane
sphere	center
cylinder	axis
cone	axis

TABLE 3: Separation Difference in Geometry

The angle difference is the angle that is formed between the two geometry fits. For example in the case of a cone, the angle is the one formed between the axis of the test fit and the axis of the reference fit. The size difference is the difference between the test fit radius and the reference fit radius $(r_1 - r_0)$ (if applicable to the geometry type). The form difference is the difference in angles between the two forms, the reference fit and the test fit.

D.4.2 Residual Analysis

The residual analysis in the comparative section of the window displays the sum of the errors difference and the gradient difference between the two geometries.

Following is a table containing the equations that represent the comparative parameters in the residual analysis.

Sum of the Squares of Errors Difference (sse)	$\left(\sum \varepsilon^2\right)_T - \left(\sum \varepsilon^2\right)_R$
Gradient of the Test Fit (V_T)	$\nabla\left(\sum \varepsilon^2\right)_T$
Gradient of the Reference Fit (V_R)	$\nabla\left(\sum \varepsilon^2\right)_R$
Gradient Difference: angle	$\cos^{-1}\left(\dfrac{V_T V_R}{|V_T||V_R|}\right)$
Gradient Difference: length	$|V_T| - |V_R|$

TABLE 4: Residual Analysis Equations

The sse difference is the difference between the sse's of each fit, the test fit and the reference fit. The gradient difference between the geometries is computed with respect to the angle and to the length. The gradient of the sse is computed for the test fit and the reference fit. These results are used to calculate the gradient differences with respect to the angle and to the length.

D4