Materials Algorithms Project
Program Library

Program MAP_STEEL_THERMAL10

Provenance of Source Code

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Added to MAP: September 2010

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Purpose

Prediction of the thermal conductivity for steels as a function of the chemical composition and operation temperature.

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Specification

Language:	FORTRAN / C
Product form:	Source code / Executable files
Operating Systems:	Linux, Solaris 5.5.1 & Windows 95/98

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Description

MAP_NEURAL_Thermal contains a suite of programs which enables the user to estimate the thermal conductivity for any steel as a function of chemical composition. It makes use of a neural network program called **generate44**, which was developed by David MacKay and is part of the **bigback5** program. The network was trained using a large database of experimental results [1]. 6 different models are provided, which differ from each other by the number of hidden units and by the value of the seed used when training the network. It was found that a more accurate result could be obtained by averaging the results from all the models [2]. This suite of programs calculates the results of each model and then combines them, by averaging, to produce a *committee result* and error estimate, as described by MacKay [page 387 of reference 2]. The source code for the neural network program can be downloaded from David MacKay's website; the executable files only are available from MAP. Also provided are FORTRAN programs (as source code) for normalising the input data, averaging the results from the neural network program and unnormalising the final output file, along with other files necessary for running the program.

Programs are available which run on PC under Windows or Linux. A set of program and data files are provided for the model, which calculate the thermal conductivity in $Wm^{-1}K^{-1}$ for steel.

readme.txt
: A text file containing instructions for running the program.

labels.txt
: A text file containing a list of input variables, as used in training, these do not include units which are documented in this web page.

MINMAX

A text file containing the minimum and maximum limits of each input and output variable. This file is used to normalise and unnormalise the input and output data.

test.dat
An input text file containing the input variables used for predictions.

install.sh
This is a unix shell file containing the command steps required to run the module. It can be executed by typing `sh install.sh` at the command prompt. This shell file compiles all the programs necessary for using the model.

model.gen
This is a unix shell file containing the command steps required to run the module. It can be executed by typing `sh model.gen` at the command prompt. This shell file runs all the programs necessary for normalising the input data, executing the network for each model, unnormalising the output data and combining the results of each model to produce the final *committee* result.

spec.t1
A dynamic file, created by **spec.ex/spec.exe**, which contains information about the module and the number of data items being supplied. It is read by the program **generate44/generate55.exe**.

norm_test.in
This is a text file which contains the normalised input variables. It is generated by the program **normtest.for** in subdirectory **s**.

generate44
This is the executable file for the neural network program. It reads the normalised input data file, **norm_test.in**, and uses the weight files in subdirectory **c**. The results are written to the temporary output file **_out**.

_ot, _out, _res, _sen
These files are created by **generate44** and can be deleted.

result
Contains the final un-normalised committee results for the predicted thermal conductivity.

SUBDIRECTORY s

spec.c
The source code for program **spec.ex**.

normtest.for
Program to normalise the data in **test.dat** and produce the normalised input file **norm_test.in**. It makes use of information read in from **no_of_rows.dat** and **committee.dat**.

gencom.for
This program uses the information in **committee.dat** and combines the predictions from the individual models, in subdirectory **outprdt**, to obtain an averaged value (*committee prediction*). The output (in normalised form) is written to **com.dat**.

treatout.for
Program to un-normalise the committee results in **com.dat** and write the output predictions to **unnorm_com**. This file is then renamed **Result**.

committee.dat
: A text file containing the number of models to be used to form the committee result and the number of input variables. It is read by **gencom.for**, **normtest.for** and **treatout.for**.

SUBDIRECTORY c

_w*f
: The weights files for the different models.

***.lu**
: Files containing information for calculating the size of the error bars for the different models.

_c*
: Files containing information about the perceived significance value [1] for each model.

_R*
: Files containing values for the noise, test error and log predictive error [1] for each model.

SUBDIRECTORY d

outran.x
: A normalised output file which was created when developing the model. It is accessed by **generate44** via **spec.t1**.

SUBDIRECTORY outprdt

out1, out2 *etc.*
: The normalised output files for each model.

com.dat
: The normalised output file containing the committee results. It is generated by **gencom.for**.

Detailed instructions on the use of the program are given in the README files. Further information about this suite of programs can be obtained from reference 1.

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References

1. D.J.C. MacKay, 1997, *Mathematical Modelling of Weld Phenomena 3*, eds. H. Cerjak & H.K.D.H. Bhadeshia, Inst. of Materials, London, pp 359.
2. D.J.C MacKay, Information Theory, Inference, and Learning Algorithms, 2003. Book details
3. Bigback5 Code, D.J.C MacKay's website http://www.inference.phy.cam.ac.uk/mackay/SourceC.html
4. Smithall metals Reference Book Ed: W.F. Gale, T.C. Totmeier Eight Edition Publisher Elsevier/ASM 2004.
5. P. Karditítas, M-J Baptiste, Thermal and structural properties of fusion related Materials, http://www-ferp.ucsd.edu/LIB/PROPS/PANOS/ss.html.

6. MATWEB, Material property Data, http://www.matweb.com/
7. J.P.Holman, Heat Transfer, 8th Edition 1997 McGraw-Hill Companies.

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Parameters

Input parameters

Column 1 - 15
"C", "Mn", "Ni", "Mo", "V", "Cr", "Cu", "Al", "Nb", "Si", "W", "Ti", "Co", "P", "S".
Elements Carbon, Manganese, Nickel, Molybdenum, Vanadium, Chromium, Copper, Aluminium, Niobium, Silicon, Tungsten, Titanium, Cobalt, Phosphorous, Sulphur in weight percent.
Column 16
"TC"
Temperature in degrees Celcius.

The inputs are also listed in `labels.txt`. The maximum and minimum values for each variable are given in the file **`MINMAX`**.

Output parameters

These program gives the thermal conductivity in $Wm^{-1}K^{-1}$. The corresponding output files is called **`Model_RESULT.dat or Result`**. The format of the output file is:

```
Prediction     Error bar      Lower-limit      Upper-limit

    (Wm-1K-1)                      (Wm-1K-1)              (-1K-1)
```

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Error Indicators

None.

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Accuracy

A full calculation of the error bars is presented in reference 2.

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Further Comments

None.

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Example

1. Program text

```
Complete program.
```

2. Program data

See sample data file: **`test.dat`**.

3. Program results

See sample output file: R**`esult or Model_RESULT.dat`**.

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Auxiliary Routines

None

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Keywords

neural network, thermal conductivity, steel, properties.

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Linux / UNIX:

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Tested on Debian Linux, please report sucess on other sytems to Mathew Peet.

PC Software:

Available for testing on request from Mathew Peet - consider using cygwin

or virtual machine in windows.

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MAP Website administration / map@msm.cam.ac.uk

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