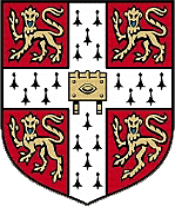
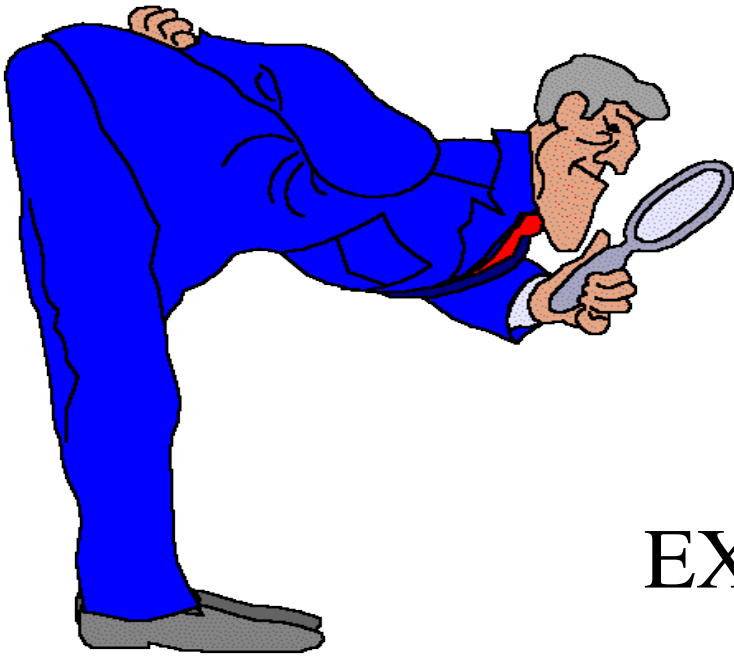


Radu Calin Dimitriu

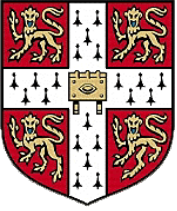
NEURAL NETWORKS,
TRICKS OF THE
TRADE



BEFORE STARTING THE TRAINING



EXAMINE THE DATA VERY
CLOSELY



AFTER A CLOSE EXAMINATION WE CAN ESTABLISH

- a)

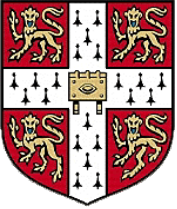
WE HAVE GOOD
DATA



- b)

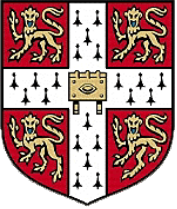
WE HAVE BAD
DATA





HOW TO DEFINE GOOD DATA?

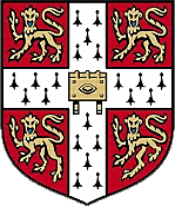
GOOD DATA ARE PHYSICALLY
MEANINGFUL AND RELEVANT
TO THE OUTPUT



FOR EXAMPLE

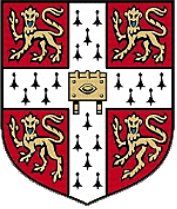
TO MODEL THE STRENGTH OF A STEEL....

- WE MUST CONSIDER THE CHEMICAL COMPOSITION, THE HEAT TREATMENT, GRAIN SIZE...
- IT WOULD BE A BAD IDEA TO INSERT THE MACHINING SPEED



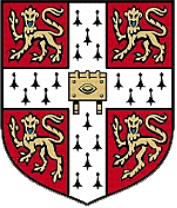
GOOD DATA

- ARE MADE OF AN OPTIMISED NUMBER OF INPUT PARAMETERS
- IT IS NOT RECOMMENDED TO HAVE AN OVER-AMBITIOUS SET OF INPUT PARAMETERS
- BECAUSE THAT WILL LIMIT THE DATA AVAILABLE FOR ANALYSIS



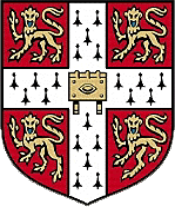
BE REALISTIC

- ALWAYS MAKE A PRAGMATIC APPROACH WHEN MAKING A DATABASE FOR A NEURAL NETWORK
- THIS WILL ENSURE SUFFICIENT DATA AND VARIABLES TO CAPTURE THE COMPLEXITY OF THE PROBLEM



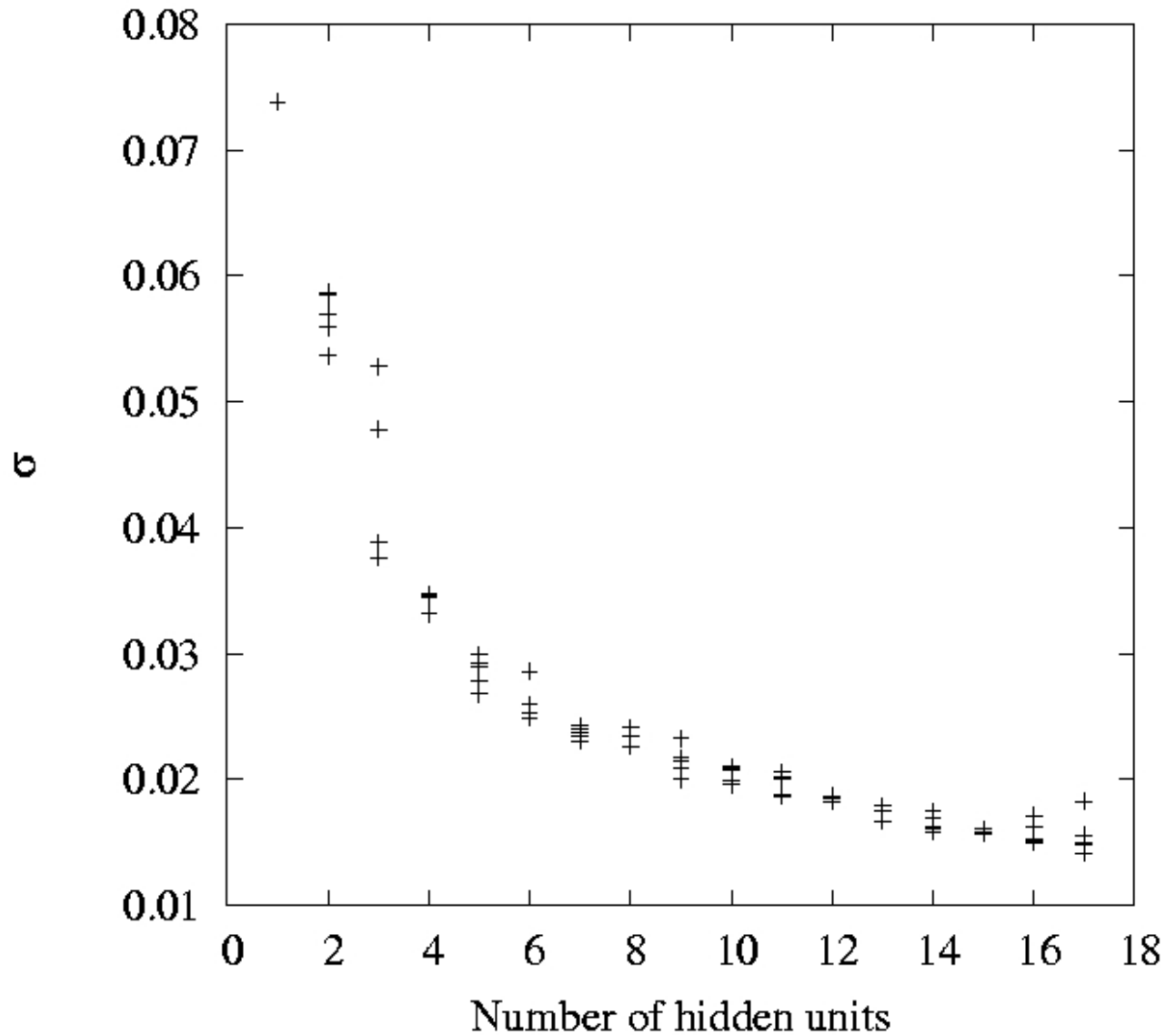
INCLUDE AS MANY MEANINGFUL PARAMETERS AS POSSIBLE

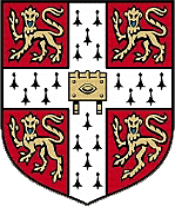
- INCLUDE MEANINGFUL PARAMETERS IN THE DATABASE
- IF YOU DO NOT KNOW HOW THEY ARE RELATED TO THE OUTPUT, THE NEURAL NETWORK MAY NEVERTHELESS CAPTURE THE RELATION



LEVEL OF PERCEIVED NOISE

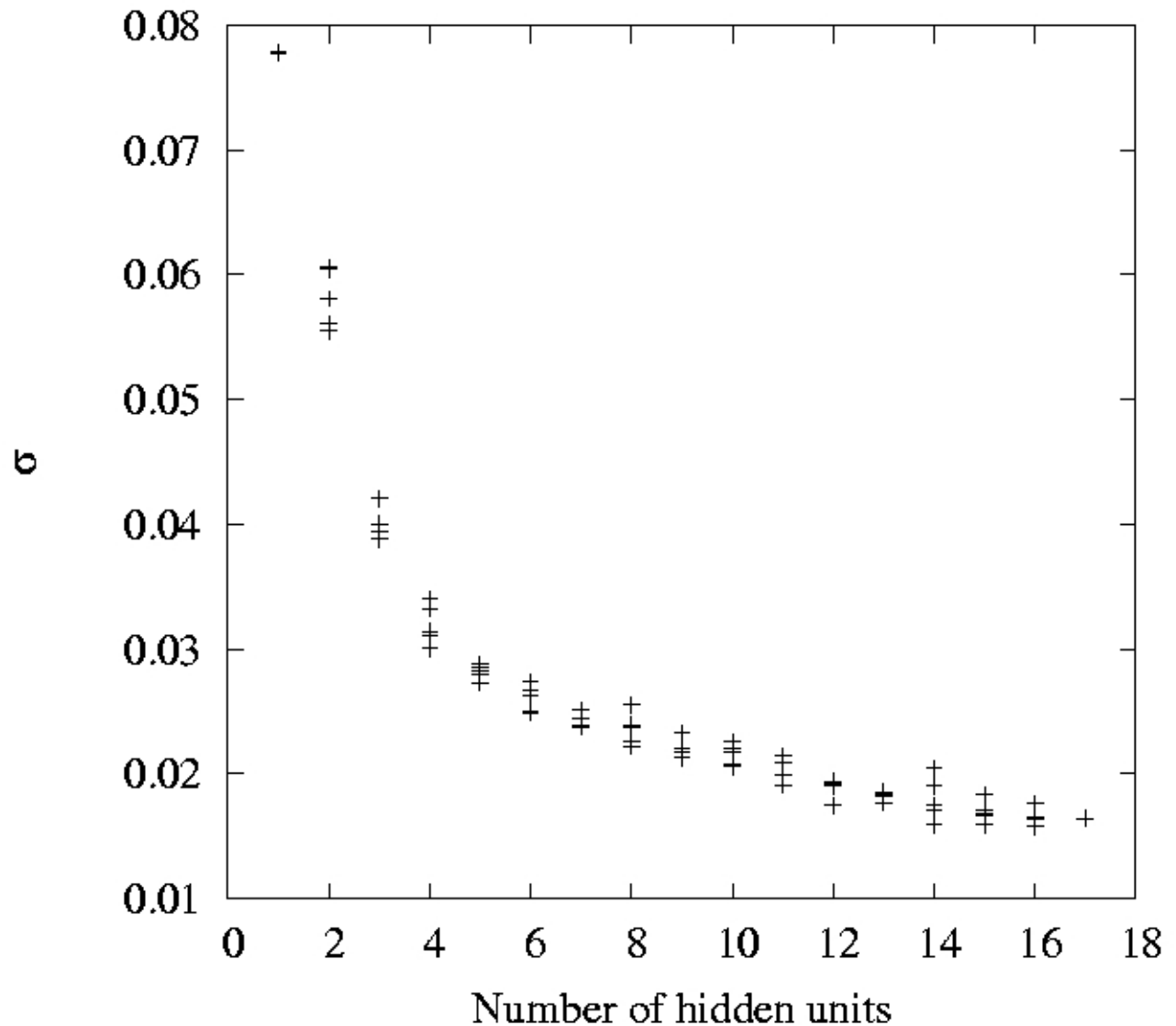
THE
LEVEL
OF NOISE
FOR
A MODEL
WITH
26
INPUTS

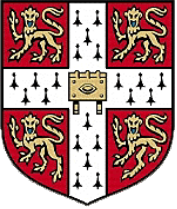




LEVEL OF PERCEIVED NOISE

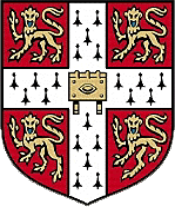
THE
LEVEL
OF NOISE
FOR
A MODEL
WITH
22
INPUTS





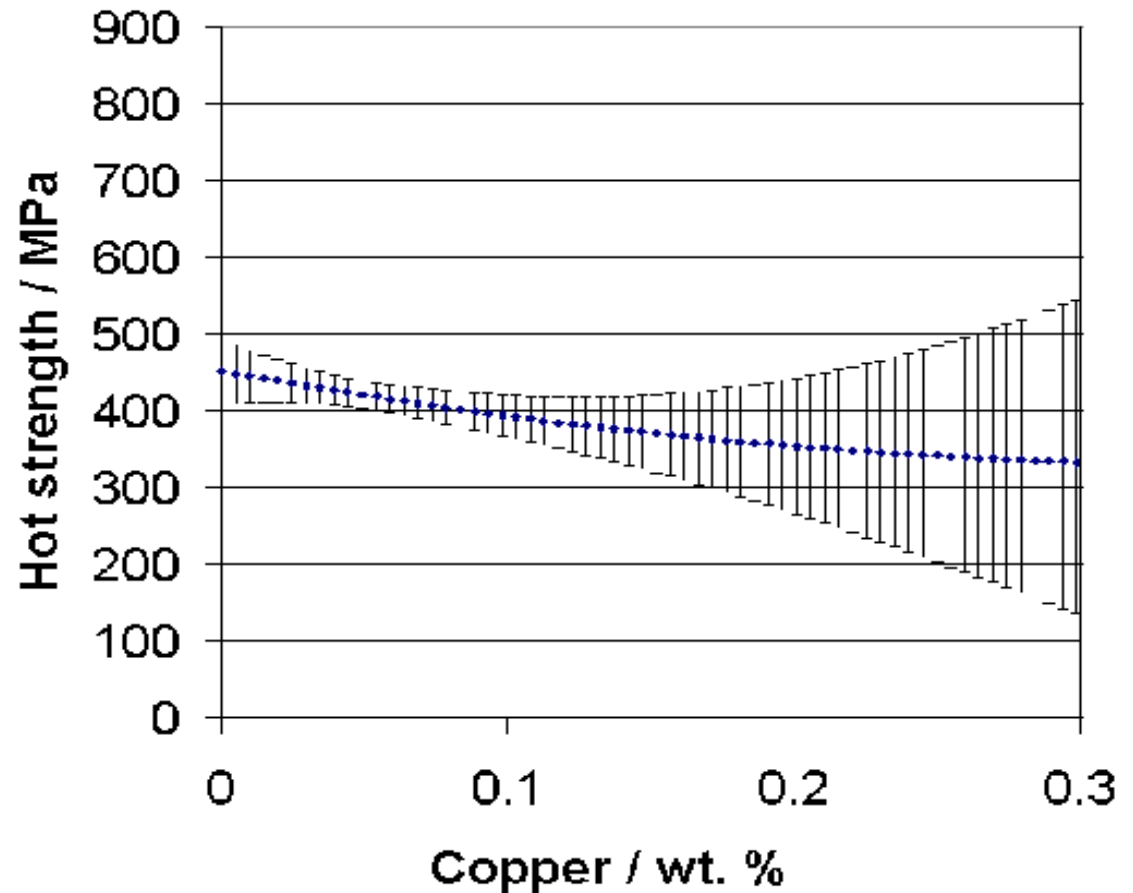
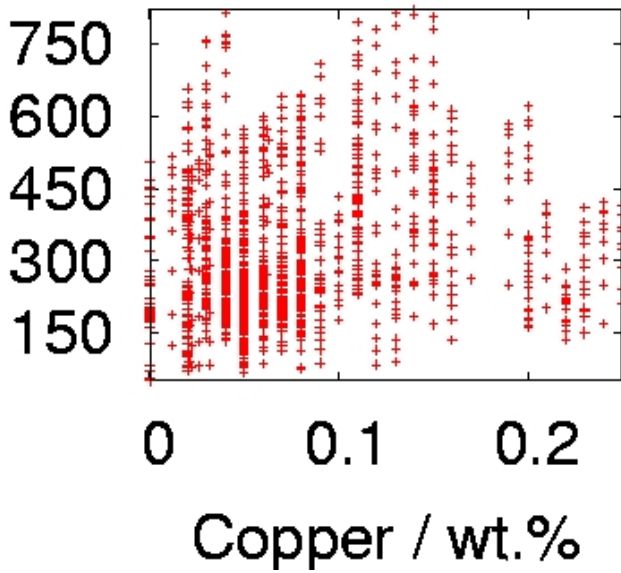
FOR A GOOD DATABASE

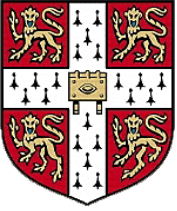
- IT IS DESIRABLE TO HAVE A GOOD SPREAD OF DATA OVER THE ENTIRE RANGE
- THAT WILL ENSURE A RELIABLE PREDICTION



DATA-SPREAD AND PREDICTIONS OF HOT-STRENGTH AS A FUNCTION OF COPPER CONTENT

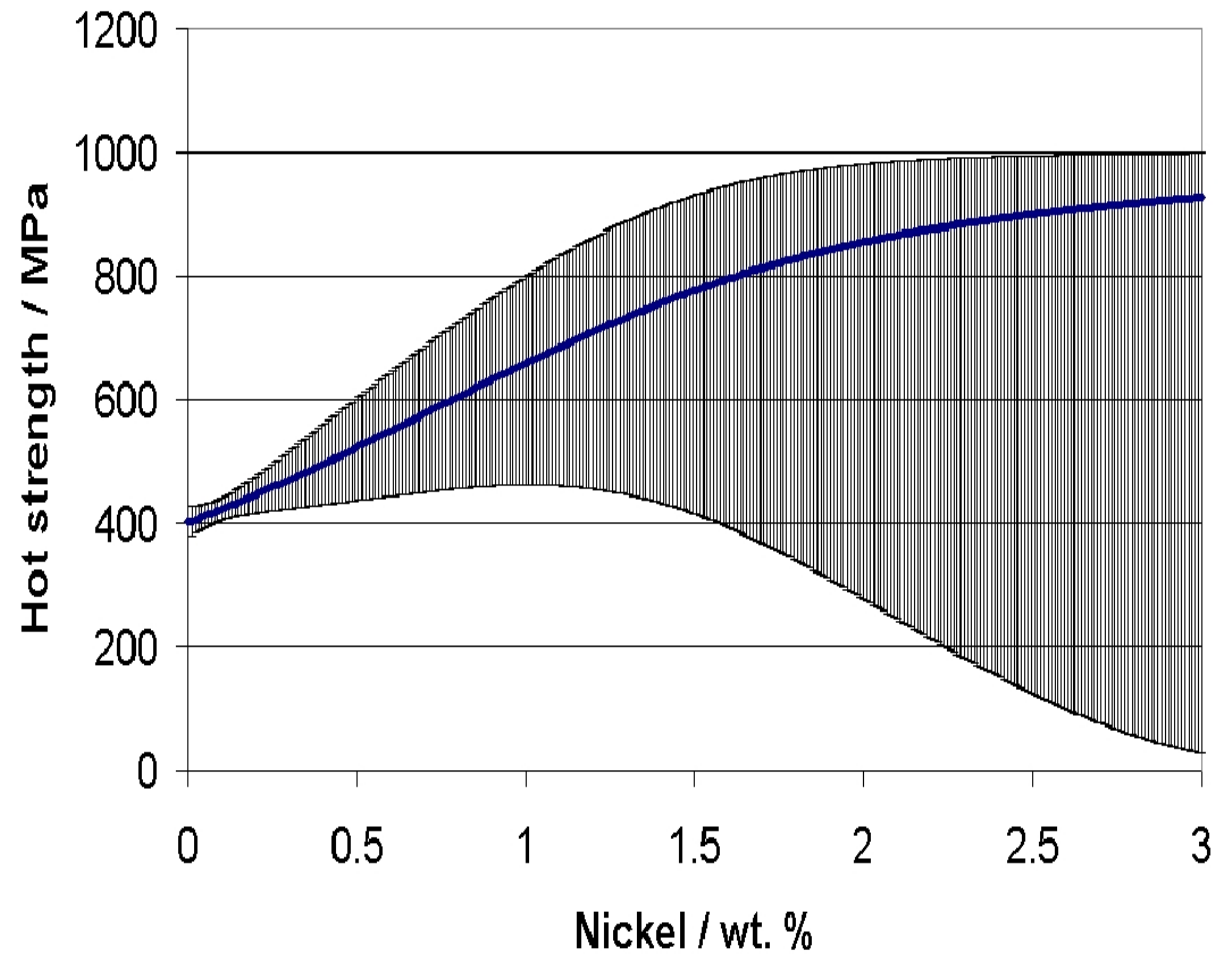
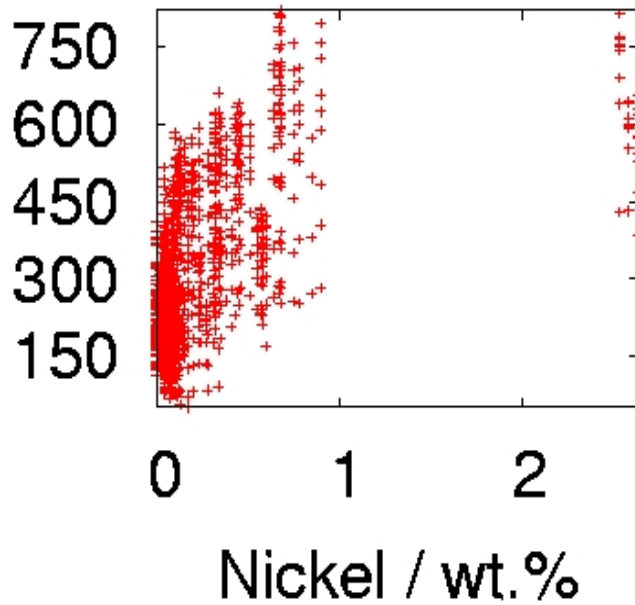
Hot strength / MPa

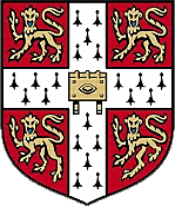




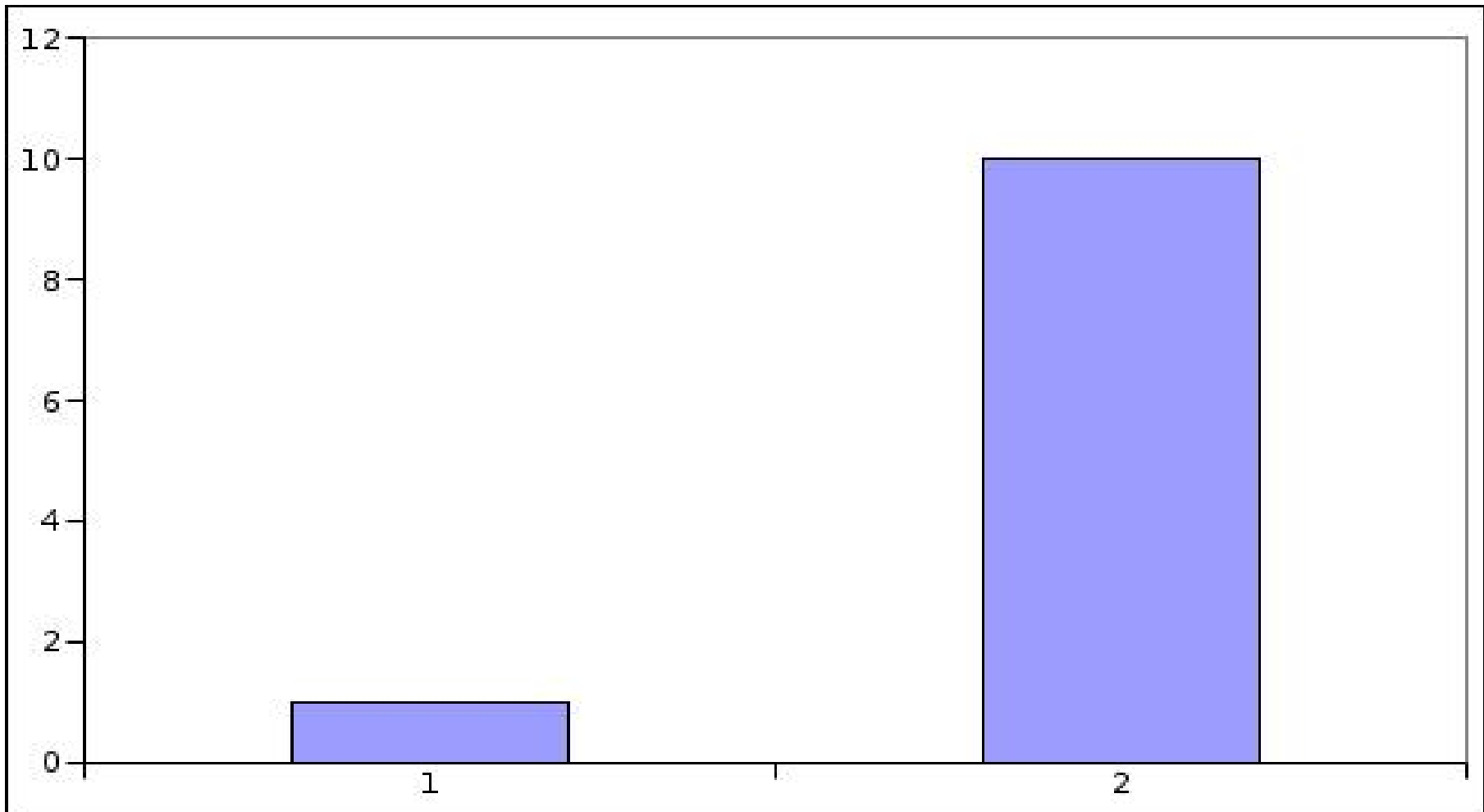
DATA-SPREAD AND PREDICTIONS OF HOT-STRENGTH AS A FUNCTION OF NICKEL CONTENT

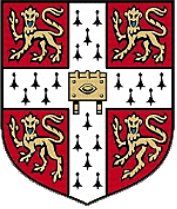
Hot strength / MPa





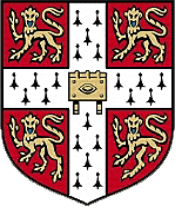
CHECKING THE MINIMUM AND MAXIMUM





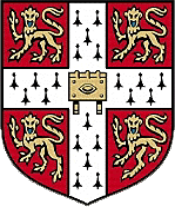
ALL THE INPUTS AND OUTPUTS

- MUST BE CHECKED BEFORE MODELLING
- TO ENSURE THAT THE LIMIT OF THE INPUTS AND OUTPUT IS MEANINGFUL



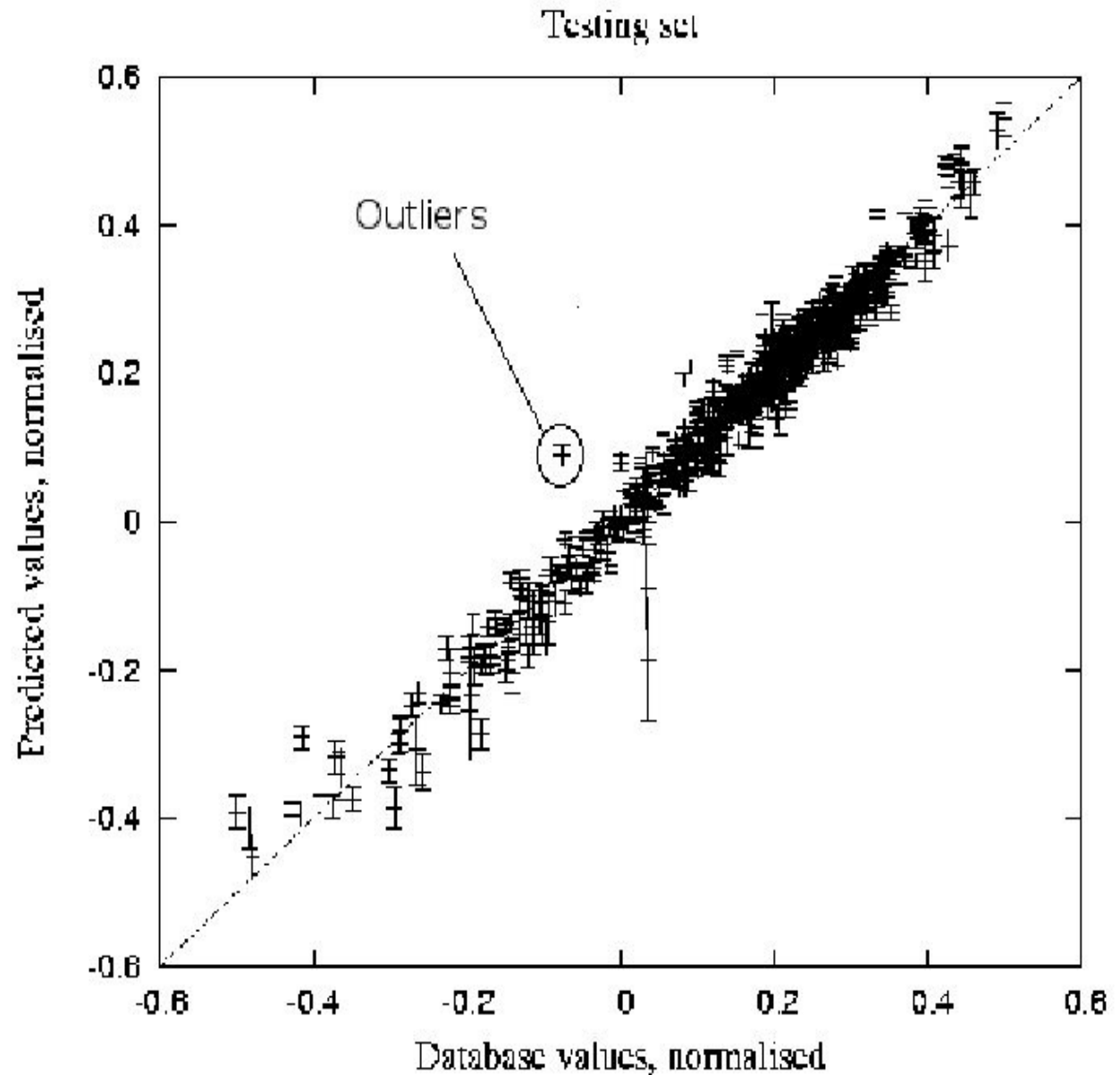
DO NOT TRUST THE EXPERIMENTS

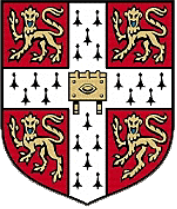
- ALWAYS MAKE AN ASSESSMENT OF THE QUALITY OF THE DATA
- QUESTION THE ACCURACY AND RELIABILITY OF THE EXPERIMENTS USED TO GENERATE THE DATA



LOOK FOR OUTLIERS

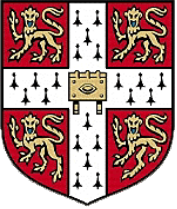
OUTLIERS
ARE POINTS
WHICH ARE
VERY
UNLIKELY





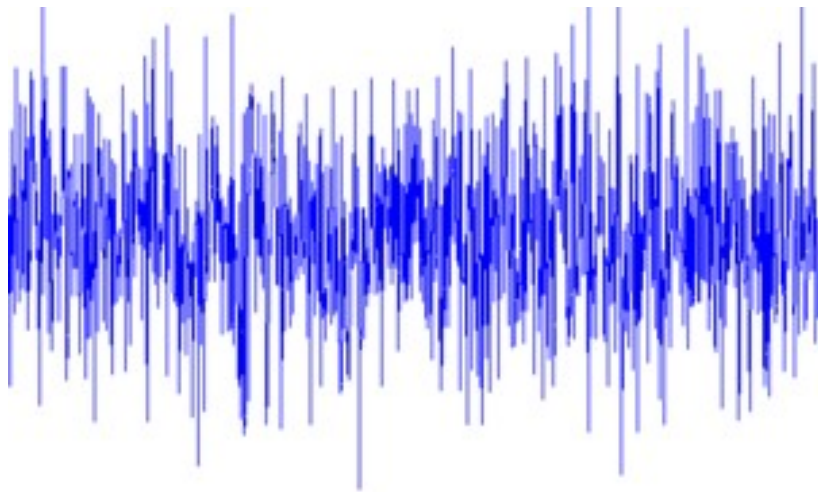
STUDY OUTLIERS

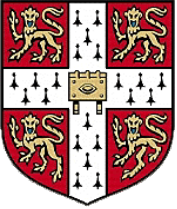
- FIRST THEY MUST BE IDENTIFIED
- TRACKED BACK TO THE ORIGIN TO LOOK FOR MISTAKES IN COLLECTING AND COMPILING THE DATABASE
- IF NO ERRORS ARE FOUND THEN SOME THINKING AND ASSUMING MUST BE DONE TO ENSURE THE CORRECTITUDE OF THE MODEL



FIXING THE NOISE LEVEL

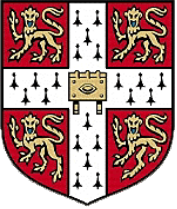
BEFORE TRAINING
WE HAVE THE
POSSIBILITY
TO FIX THE
NOISE LEVEL





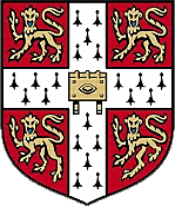
WE FIX THE LEVEL OF NOISE IF:

- WE KNOW WE HAVE A NOISY DATABASE
- AND IF WE TRAIN WITH A LOW LEVEL OF NOISE THE DATA WILL TRAIN UNTIL IT REACHES THE FIXED LEVEL (OVER-TRAIN)
- BY INCREASING THE LEVEL OF NOISE WE ENSURE A GOOD TRAINING



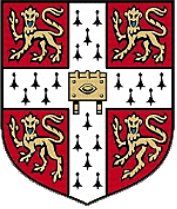
AND IF:

- WE KNOW WE HAVE A EXCELLENT DATABASE
- THEN WE LOWER THE NOISE LEVEL AND FORCE THE NEURAL NETWORK TO FIND A MORE COMPLEX SOLUTION THEN IT WOULD HAVE WITH A MEDIUM LEVEL



SO A GOOD DATABASE

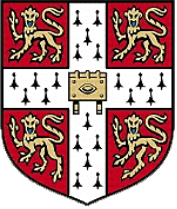
- HAS INPUTS PARAMETERS SIGNIFICANT TO THE OUTPUT PARAMETER
- AS MANY SIGNIFICANT PARAMETERS AS POSSIBLE
- UNIFORMLY DISTRIBUTED DATA
- DOES NOT HAVE OUTLIERS
- HAS A OPTIMUM LEVEL OF NOISE



INPUT PARAMETERS

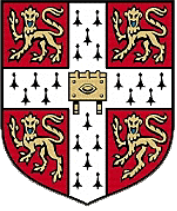
- WE CAN INSERT THE INPUT PARAMETERS AS RAW





FOR EXAMPLE

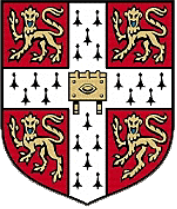
- THE CHEMICAL COMPOSITION OF A STEEL
- HEAT TREATMENT TEMPERATURE AND TIME
- GRAIN SIZE
- HARDNESS
-



OR

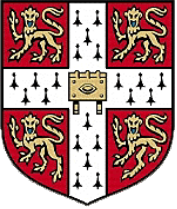
- WE CAN INSERT THE INPUTS IN A FUNCTIONAL FORM





FOR EXAMPLE

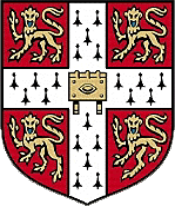
- THERMAL ACTIVATION
- LOGARITHM OF TIME
- A COMBINATION OF INPUT PARAMETERS
- NORMALISATION



THERMAL ACTIVATION

THE FORMULA DESCRIBES THE
DEPENDENCE OF THE OUTPUT UPON AN
ACTIVATION ENERGY

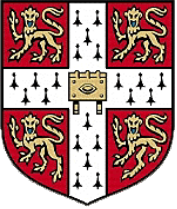
$$\exp\left(-\frac{Q}{RT}\right)$$



LOGARITHM OF TIME

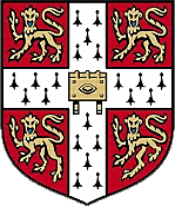
IT IS WISE TO INCORPORATE THE
LOGARITHM OF TIME IN THE DATABASE
WHEN THE EXTENT OF REACTION IS
EXPECTED TO VARY WITH

$\ln \{ \text{time} \}$



A COMBINATION OF INPUT PARAMETERS

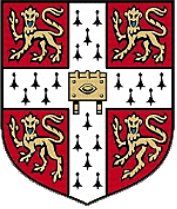
IF A COMBINATION OF ONE OR MORE
PARAMETERS HAS A PARTICULAR
SIGNIFICANCE THAN THAT
COMBINATION SHOULD BE INSERTED IN
THE DATABASE



FOR EXAMPLE

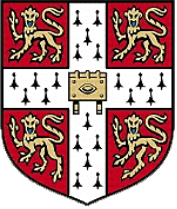
- THE FOLLOWING PRODUCT CAN BE USED TO AS AN INPUT FROM KINETIC THEORY, A FUNCTION OF TIME AND TEMPERATURE

$$time * exp\left(-\frac{Q}{RT}\right)$$



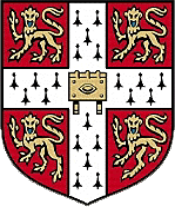
NORMALISATION OF INPUTS

- USUALLY IT IS GOOD TO NORMALISE THE INPUTS IN ORDER TO MAKE COMPARISON BETWEEN THEM EASIER
- FROM THE COMPARISON WE CAN SEE WHICH INPUT PARAMETER HAS A BIGGER INFLUENCE ON THE MODEL



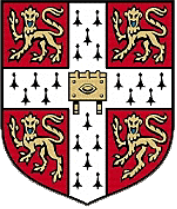
FOR EXAMPLE

- IF WE WANT TO COMPARE THE EFFECT OF CARBON WHICH VARIES BETWEEN 0.1-1 wt% AND CHROMIUM WHICH CAN VARY BETWEEN 0-13 wt%.
- IT IS EASY TO SEE THEIR EFFECT ON THE MODEL WHEN THEY ARE NORMALISED



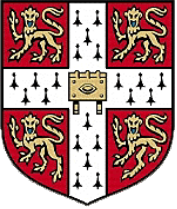
BUT

- IT IS SENSITIVE THAT ALONG THE RAW DATA THE DATA THAT WAS TRANSFORMED AS A FUNCTIONAL FORM TO BE KEPT IN THE DATABASE
- IF WE DO NOT KEEP ALL THE DATA WE RUN THE RISK OF BIASING THE MODEL



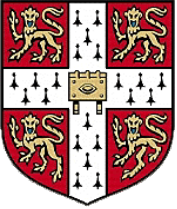
THE OUTPUTS

- THE OUTPUTS CAN ALSO BE INSERTED IN A RAW FORM IN THE MODEL



OR

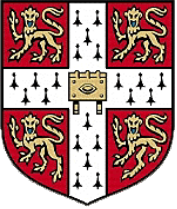
- AS A MATHEMATICAL FUNCTION FOR THE MODELS THAT HAVE THE TENDENCY TO PREDICT UNPHYSICAL VALUES



FOR EXAMPLE

WE HAVE THE STRENGTH AS AN OUTPUT
AND AS A MATHEMATICAL FUNCTION
THE STRENGTH CAN GO BELOW ZERO,
THAT IS PHYSICALLY IMPOSSIBLE SO WE
CAN GUIDE TO OUTPUT NOT TO REACH
ZERO

$$f_{strength} = \ln\left(-\ln\left(1 - \frac{X_{max} - X}{X_{max} - X_{min}}\right)\right)$$



ACKNOWLEDGEMENTS

- MANY THANKS TO PROFESSOR H. K. D. H. BHADESHIA
- DEPARTMENT OF MATERIAL SCIENCE AND METALLURGY
- UNIVERSITY OF CAMBRIDGE
- EUROPEAN COMMISSION UNDER THE MARIE CURIE EARLY STAGE RESEARCH TRAINING PROGRAMME