Model for solidification cracking in low alloy steel weld metals

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Data on the occurrence of solidification cracking in low alloy steel welds have been analysed using a classification neural network based on a Bayesian framework. It has thereby been possible to express quantitatively the effect of variables such as the chemical composition, welding conditions, and weld geometry, on the tendency for solidification cracking during solidification. The ability of the network to express the relationship in a suitably non-linear form is shown to be vital in reproducing known experimental phenomena.

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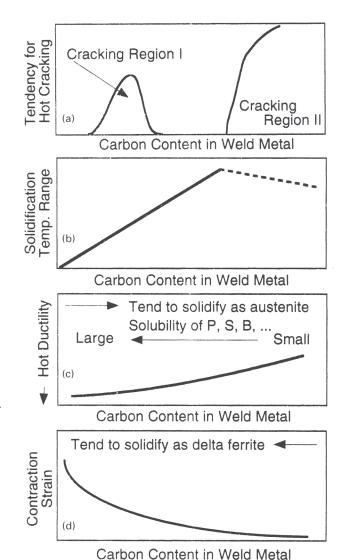
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INTRODUCTION

Solidification cracking occurs in welds during cooling from the liquidus temperature, if the density changes associated with solidification and thermal contraction can not be accommodated by fluid flow or by the motion of the solid components which constitute the weld assembly. This kind of cracking depends partly on the chemical composition of the weld metal, since that in turn determines the solidification temperature range. However, the cooling rate and weld geometry (including the extent of constraint) also control the susceptibility to solidification cracking. Modern low alloy steels for structural applications have compositions which are designed to avoid solidification cracking, for instance by minimising the sulphur concentration. Significant difficulties nevertheless remain with very high heat input welding of high tensile strength steels.

A great deal of excellent research has been reported in the published literature on the factors controlling solidification cracking in welds. 1-15 The essential phenomena are well characterised although difficulties remain with respect to the detailed mechanisms; the subject has been reviewed recently. 10,14

The results of standard tests on the tendency for solidification cracking are usually expressed in terms of the chemical composition of the weld metal.^{5,6,8,9} Relationships like these are very useful in that they help in the selection of weld metals. However, they are usually linear functions of the chemical composition and are unable to express certain known more complex effects. Unlike the proportional influence of carbon on the cold cracking susceptibility of welded steels (as evident in the famous carbon equivalent formulae), Fig. 1a shows a well established nonlinear effect of carbon on the solidification cracking susceptibility.¹² The temperature range over which solidification to delta ferrite occurs increases with the carbon concentration (Fig. 1b), but the density change on solidification decreases



a comprehensive effect of carbon on solidification cracking susceptibility; b effect of carbon on solidification temperature range; c effect of carbon on hot ductility; d effect of carbon on thermal contraction strain

Schematic diagram of the effects of carbon on the solidification cracking susceptibility in low alloy steel welds a, b and d are after Homma et al. 12

at the same time (Fig. 1c), 12 giving rise to the first peak illustrated in Fig. 1a. At even larger concentrations, the mode of solidification switches from ferrite to austenite; impurities such as sulphur and phosphorus have a lower solubility in austenite so that segregation to the residual liquid is enhanced, thereby increasing the risk of solidification cracking (Fig. 1d). As a further example of well established non-linear effects, the ability of sulphur to induce solidification cracking is greatest when the nickel concentration is large, because nickel also promotes solidification to austenite.3

All of these issues can be handled better using an artificial neural network, which has the capability of addressing complexity with relative ease. The aim of the present work was, therefore, to quantitatively model the tendency for solidification cracking using a classification neural network approach.

TECHNIQUE

Neural networks are parameterised non-linear models, used for empirical regression and classification modelling. Their flexibility makes them able to discover more complex relationships in data than traditional statistical models which assume a linear dependence of the predicted 'output' variable on the given 'input' variables. Neural networks are able to implement more general (and more complex) nonlinear relationships. When the neural network is 'trained' on empirical data, its parameters are adjusted so as to produce a non-linear interpolant which fits the data well.

The outcome of training is a set of coefficients (called weights) and a specification of the functions which in combination with the weights relate the input to the output. The training process involves a search for the optimum non-linear relationship between the inputs and the outputs, and is computer intensive. Once the network is trained, estimation of the outputs for any given inputs is very rapid.

Because the neural network is able to implement more complex relationships than linear regression, it is also able to 'overfit' the training data; there is therefore a potential problem of obtaining a model that fits the training data well, but generalises poorly to test examples. To solve this problem, Bayesian regularisation theory can be used to control the complexity of the model. 16-22 It is then possible to identify automatically which of many possible relevant input variables are in fact important factors in the regression.

Neural networks are frequently used for regression problems in which continuous variables are modelled. In a recent example of this kind, the impact toughness of steel welds was expressed as a function of chemical compositions and temperature.²³ There are many problems where the variables to be predicted adopt discrete values. For example, the solidification cracking tests used in the assessment of welds give a result which indicates whether the weld will crack (1) or not (0). Such a problem is known as a binary classification problem, and a neural network can be made to model the probability of a crack (1) as a function of the input variables. The neural network implements a parameterised function y(x, w) where x are the input variables and w are the parameters; the output y is a real number between 0 and 1. Bayesian methods can be applied to

Table 2 The output variables used in the present study

Classification label	Value	Number
No cracks	0	95
Cracked	1	59

neural network classifiers 19,22 and have two important consequences. First, it is possible automatically to control the complexity of a neural network, and, as in MacKay ²⁰ and Bhadeshia et al.,23 to infer which input variables are most relevant in the non-linear regression. Second, Bayesian methods allow us to take into account the parameter uncertainty when making predictions by the process of marginalisation. In a classifier, the effect of marginalisation is to take the output of the best fit neural network and move it closer to 0.5 by an amount depending on the parameters' uncertainty. The value 0.5 in the output indicates the highest level of uncertainty.

This paper deals with the application of a classification neural network to the solidification cracking problem for welds.

VARIABLES

It is possible to choose a set of variables which should affect the solidification cracking susceptibility in steel welds using metallurgical experience on welding. The input and output variables considered in this study are listed in Tables 1 and 2 respectively.

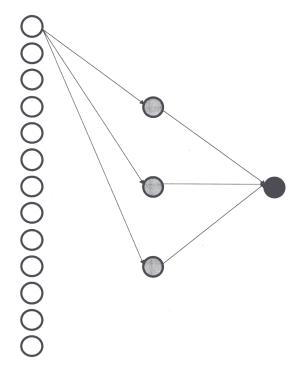
As suggested by previous work based on linear regression methods, 5,6,8,9 alloying elements such as carbon, silicon, manganese, phosphorus, sulphur, nickel, chromium, and molybdenum should all have an influence on the development of solidification cracks during welding; these elements were all included as input variables. Similarly, microalloying and impurity elements, such as niobium, vanadium, boron,¹³ and oxygen⁶ may influence cracking susceptibility, but were not included because of a lack of systematic data.

It is well known that the tendency for solidification cracking varies with the welding process parameters such as the welding conditions, joint configuration, and preheat temperature because of their influence on the solidification structure, and stress and strain development as the weldment cools. Consequently, the welding current, voltage, and travel speed were included as input variables. The joint configuration was represented by the groove angle which to a large extent controls the growth direction of solidification microstructure.

There is a significant problem in determining a uniform representation of cracking susceptibility, the output variable, because of the variety of tests used in the welding

Table 1 The input variables used in the present study

Variables	Range	Mean	Standard deviation
Carbon, wt-%	0.012-0.19	0.07492	0.009304
Silicon, wt-%	0.18 - 0.77	0.5225	0.02001
Manganese, wt-%	0.90-1.82	1.463	0.02885
Phosphorus, wt-%	0.01 - 0.10	0.01539	0.00684
Sulphur, wt-%	0.006-0.028	0.01176	0.001313
Nickel, wt-%	0.00-6.50	1.417	0.4117
Chromium, wt-%	0.00 - 0.08	0.04539	0.002798
Molybdenum, wt-%	0.00-0.22	0.07799	0.01148
Welding current, A	422-800	580.7	17.73
Voltage, V	28.0-36.5	33.23	0.2646
Travel speed, cm min ⁻¹	30-55	41.65	1.079
Groove angle, deg	0-90	43.05	3.796
Preheat temperature, °C	20-150	22.53	10.31



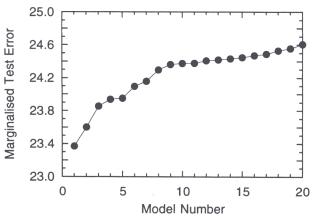
Input Units Hidden Units **Output Units**

2 Schematic illustration of the neural network model used; only the connections originating from the first input are illustrated, and two bias units are not illustrated

industry. Thus, a binary index was used, with values of 0 or 1 corresponding to a 'no cracks' or 'cracked' result respectively. In some literature, the cracking susceptibility was stated as a fractional cracking ratio rather than a binary index, in which case the outputs were defined as 1 if the ratio was greater than 0.05 and 0 if it was less than or equal to 0.05 in the neural analysis.

EXPERIMENTAL DATA

There were numerous difficulties in compiling a data set for analysis, primarily because many of the publications on the subject do not rigorously report the values of important variables. The exercise of data collection therefore had to be done pragmatically in order to collect a reasonable number of cases. Nevertheless, a positive aspect of this attempt at modelling is that it identifies for future work the variables that must be controlled in order to do reliable research.



Marginalised test error for the best 20 individual models

The database was composed using published results.3,4,7,11,12 Homma et al.12 have reported the complex effect of carbon for ultralow carbon steels to a maximum concentration of about 0.15 wt-%. They did not disclose the exact chemical composition of the steel used for each test, but published the range of concentrations; we therefore specified the composition in terms of the average of the range quoted; the chromium concentration was assumed to be zero for their data. Masumoto and Imai⁴ published data on the effects of nickel and phosphorus on solidification cracking; the chromium and molybdenum compositions, which they did not state, were again assumed to be zero. Sekiguchi et al.3 reported the complex effects of nickel and sulphur but only the sulphur and nickel concentrations of the welds were stated; the mean chemical composition of the welding electrodes they used in their study was therefore taken to represent the weld composition. In those cases where the published work did not report a preheat temperature, it was assumed that the base plate was not heated prior to welding so that the temperature was taken to

The variety of approximations stated above should, if incorrect, reflect in the perceived uncertainty in the output.

ANALYSIS

The input and variables were normalised between -0.5and +0.5, as follows

$$x_{\rm N} = \frac{x - x_{\rm min}}{x_{\rm max} - x_{\rm min}} - 0.5$$
 (1)

where x_N is the normalised value of x which has maximum and minimum values given by x_{max} and x_{min} respectively. The neural network consisted of 13 input units (one for each of the input variables), a number of hidden units, and one output unit for the crack susceptibility (Fig. 2). The network was trained using 77 randomly chosen samples from the 154 available in the assembled dataset. The remaining 77 samples were used in order to test each model for its behaviour on unseen data.

Linear functions of the inputs x_i are operated on by a hyperbolic tangent transfer function

$$h_{\rm i} = \tanh\left(\sum_{\rm j} w_{\rm ij}^{(1)} x_{\rm j} + \theta_{\rm i}^{(1)}\right)$$
 (2)

so that each input contributes to every hidden unit. The bias of each hidden unit i is designated $\theta_i^{(1)}$ and is analogous to the constant that appears in linear regression. The strength of the transfer function is in each case determined by the weight $w_{ii}^{(1)}$. The transfer to the output y is

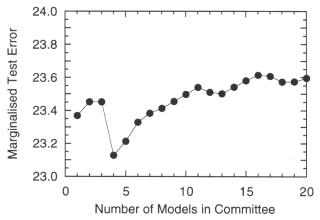
where a is linear against h_i

$$a = \sum_{i} w_{i}^{(2)} h_{i} + \theta^{(2)}$$
 (4)

This specification of the network structure, together with the set of weights is a complete description of the formula relating the inputs to the outputs. The weights are determined by training the neural network. The details are described elsewhere. 16-22 The targets are discrete binary classification labels: 'cracked' or 'no crack'. The neural network's output y is bounded between 0 and 1 and

Table 3 Chemical compositions used to predict the effects of carbon, wt-%

С	Si	Mn	P	S	Ni	Cr	Mo
0.00-0.14	0.215	1.54	0.015	0.006	0.00	0.00	0.22



4 Marginalised test error as a function of the number of models in committee

corresponds to 'cracked' and 'no crack' respectively. The value of y indicates the probability that the test will result in a cracked sample. As stated earlier, y = 0.5 indicates the highest levels of uncertainty, where the tendency for cracking is the same as that for avoiding crack.

The error function in a regression neural network model is then replaced by the logarithmic likelihood 19,23

$$G = \sum_{m} t_{m} \ln y_{m} + (1 - t_{m}) \ln(1 - y_{m})$$
 (5)

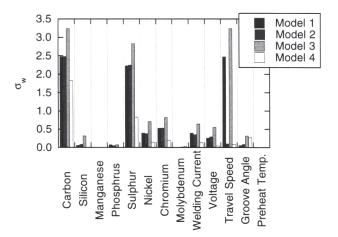
where $y_{\rm m}$ is the output for example m and $t_{\rm m}$ is the target value.

Training involves minimisation of the sum of this error function and a regulariser which penalises overcomplex models. The degree of regularisation is controlled by a set of hyperparameters denoted $\sigma_{\rm w}$.¹⁹

It is possible to have multiple classification models which are obtained by choosing different numbers of hidden units, initial values of weights, and regularisation constants $\sigma_{\rm w}$. A single prediction can then be made by a *committee* (i.e. by averaging the prediction of each model), i.e.

where N is the number of models in the committee and y_k is the estimate of a particular model k. The testing error is now obtained by replacing the y_m in equation (5) by \bar{y} .

The complexity of the model is controlled by the number of hidden units, and the value of the fifteen $\sigma_{\rm w}$, one



5 Chart showing a measure of the model perceived significance of each input variable in affecting solidification cracking in steel welds

Table 4 Process parameters used in the prediction of the carbon and molybdenum effects

Welding current, A	Voltage, V	Welding speed, cm min ⁻¹	Groove angle, deg	Preheat temperature, °C
650	31	40	60	20

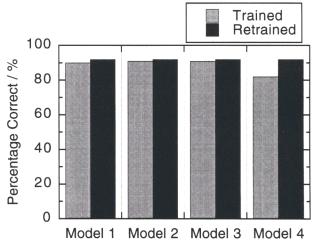
associated with each input, one for each of the biases, and one for all weights connected to the output.

Four hundred and thirty-two models were obtained by training on half the data by choosing different numbers of hidden units, different seeds, and initial values of $\sigma_{\rm w}$. The best 126 models (i.e. models with the smallest values of marginalised test error) were then examined to construct a committee model.²⁰ A 'committee' is a collection of models. It is often found that the mean prediction from a committee is more reliable than from the best individual models.

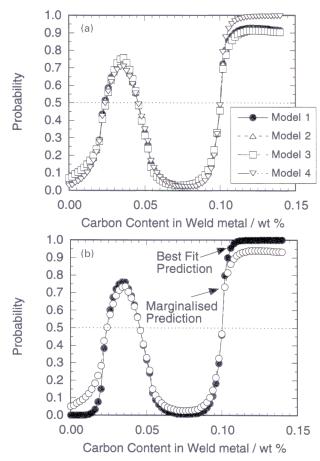
Figure 3 illustrates the marginalised test error calculated for the best 20 individual models. Figure 4 shows clearly that a committee consisting of the four best models has the minimum test error. This committee consists in fact of three models with 11 hidden units and one with just two hidden units. The four models were then retrained using all available data.

The committee model was then tested extensively to examine how well it represents metallurgical experience. There is a lot of research which indicates that carbon, sulphur, and nickel should be prominent in controlling the tendency for solidification cracking. Figure 5 shows the models' perceived role of each of the inputs in explaining the variations in the experimental data on the tendency for solidification cracking. These models are therefore consistent with metallurgical experience. Figure 6 shows the reasonable accuracy obtained for the predictions for both the training and test data. It was therefore decided to choose this committee consisting of four individual models, both because it gave reasonable statistical accuracy and because it reproduced metallurgical expectation rather well.

The calculated influence of the carbon concentration on the tendency for solidification cracking represented by the marginalised probability for the data listed in Tables 3 and 4 using the retrained four models is illustrated in Fig. 7a. All the models, in this case, correctly reproduce the fact that solidification cracking does not occur at intermediate concentrations, as illustrated schematically in Fig. 1.



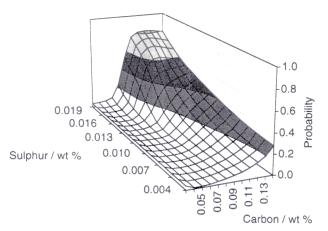
6 Percentage of correct answers on the test data set after training on the training data set, then after retraining on all the data



a marginalised predictions of effect of carbon on solidification cracking probability in steel welds by the four individual retrained models; b best fit and marginalised predictions of effect of carbon on solidification cracking probability in steel welds using the retrained committee model

Figure 7b shows the best fit and marginalised predictions by the committee model. It can be found that marginalised prediction is moderated from the best fit one. Figure 7a and b also show a significant tendency towards reduced cracking when the carbon concentration decreases towards zero (see Fig. 1).

Figure 8 shows results of prediction of the effect of carbon and sulphur for the hypothetical input data listed in Tables 5 and 6 using the retrained model. The behaviour illustrated is expected since there should be an increase in the solidifi-



Predicted effect of sulphur and carbon on solidification cracking in steel welds

Table 5 Chemical compositions used to predict the combined effects of carbon and sulphur, wt-%

С	Si	Mn	P	S	 Cr	
				0.004-0.020	 	

Table 6 Process parameters used to predict the combined effects of carbon and sulphur

Welding current, A	Voltage, V	Welding speed, cm min ⁻¹	Groove angle, deg	Preheat temperature, °C
422	34	32.5	45	20

cation cracking probability as a function of suphur content, particularly at higher carbon concentrations.

The weights for the retrained models which constitute the committee are listed in the appendix. This list, together with the minimum and maximum values in the input data and output values given in Tables 1 and 2, is sufficient to reproduce the necessary equations and predictions described in this study.

USE OF THE MODEL

A number of further tests were carried out using the retrained model in order to ensure that the selected model predicts in a way consistent with metallurgical experience.

It is widely accepted that sulphur and phosphorus are harmful impurities with respect to the solidification cracking of steel welds. Sekiguchi et al.3 reported that the effect of sulphur is exacerbated by the presence of nickel as an alloying element. Calculations using the input data listed in Tables 7 and 8 were done to confirm this trend. Any reduction in the sulphur concentration should increase the resistance to solidification cracking. An increase in the nickel concentration promotes austenitic solidification and therefore should promote solidification cracking, the effect being exaggerated when both the nickel and sulphur concentrations are large. The model reproduces this behaviour rather well, as illustrated in Fig. 9a and consistent with the published experimental data presented in Fig. 9b.

Molybdenum is a ferrite former and empirical data suggest that it reduces tendency for solidification cracking. 1,2,6 Calculations were carried out for the hypothetical input data listed in Tables 9 and 4 where the molybdenum concentration is varied in the range 0 to 0.6 wt-% which is

Table 7 Chemical compositions used to predict the combined effects of sulphur and nickel, wt-%

С	Si	Mn		S	Ni	Cr	Mo
0.064	0.77	1.48	0.01	0.005-0.020	0.50-3.50	0.08	0.01

Table 8 Process parameters used to predict the combined effects of sulphur and nickel

Welding current, A	Voltage, V	Welding speed, cm min ⁻¹	Groove angle, deg	Preheat temperature, °C
500	36	40	45	20

Table 9 Chemical compositions used to predict the effect of molybdenum, wt-%

C	Si	Mn	P	S	Ni	Cr	Mo
0.04-0.14	0.215	1.54	0.015	0.006	0.00	0.00	0.0-0.6

Table 10 Chemical compositions used to study the effect of voltage, wt-%

C	Si	Mn	Р	S	Ni	Cr	Mo
0.10	0.215	1.54	0.02	0.01	0.00	0.00	0.22

typical for low alloy steel welds. Figure 10 shows that the addition of molybdenum decreases the risk of solidification cracking in general for the steel analysed here. This agrees with published regression equations. 1.2.6

As well as the chemical compositions of welds, welding conditions, such as the current, voltage, and groove configuration, also influence the solidification cracking susceptibility. Figure 11a and b shows the predictions of effect of voltage on the solidification cracking probability for the data shown in Tables 10 and 11. At the lower voltages, predictions by the two hidden unit model (model 4) do not agree very well with those by the other three models and predictions are much uncertain. In fact, marginalised predictions are close to 0.5 in Fig. 11b. Figure 12a and b shows the predicted effect of groove angle on the solidification cracking probability for the data listed in Tables 12 and 13. For the effects of groove angle, predictions by the different constituents of the committee model do not agree very well (Fig. 12a). Also, the committee model does not give many decisive predictions by using the marginalised predictions (Fig. 12b). This is due to the insufficient data on the effect of these welding conditions.

CONCLUSIONS

A classification neural network model has been successfully used to represent experimental data on the tendency for solidification cracking during the solidification of low alloy

Table 11 Process parameters used to study the effect of voltage

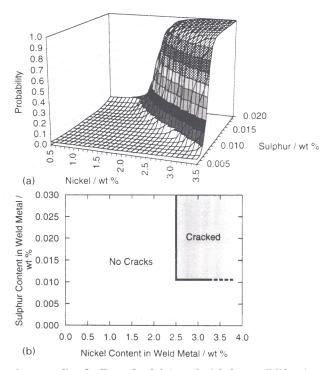
Welding current,	Voltage, V	Welding speed, cm min ⁻¹	Groove angle, deg	Preheat temperature, °C
650	25-40	40	60	20

Table 12 Chemical compositions used to study the effect of groove angle, wt-%

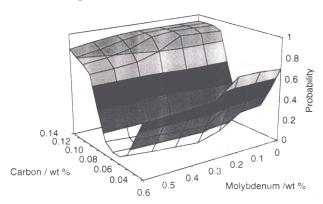
С	Si	Mn	P	S	Ni	Cr	Mo
0.08	0.77	1.48	0.01	0.02	1.5	0.08	0.01

Table 13 Process parameters used to study the effect of groove angle

Welding current,	Voltage, V	Welding speed, cm min ⁻¹	Groove angle, deg	Preheat temperature, °C
422	34	32.5	0-90	20



9 a predicted effect of sulphur and nickel on solidification cracking in steel welds; b predicted effects of nickel and sulphur contents on solidification cracking in steel welds after Sekiguchi et al.³



10 Predicted effect of molybdenum and carbon on solidification cracking in steel welds

steel welds. The model has been demonstrated to reproduce known metallurgical experience and will be updated as more data become available.

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APPENDIX

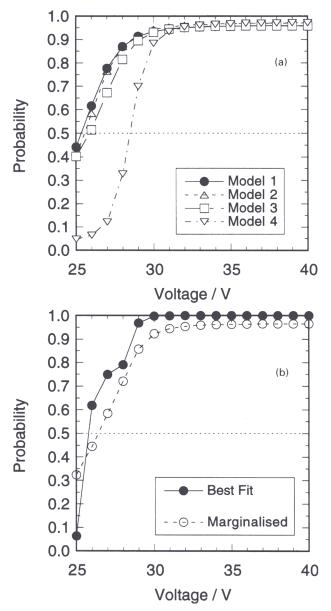
The values for the weights obtained by the training with all the data listed in Tables 1 and 2 are shown in Table 14a-d. Best fit predictions of solidification cracking in steel welds can be made using these data and the data in Tables 1 and 2 together with equations (1)–(4) and (6).

Table 14 Weights and biases describing the trained network with all the data in Tables 1 and 2: a model 1, b model 2, c model 3, d model 4.

The data are arranged in a continuous horizontal sequence in the following order in a, b, and c, and d.

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a, b, and c
\begin{array}{l} \theta_1^{(1)}, \theta_2^{(1)}, \theta_3^{(1)}, \dots, \theta_{11}^{(1)}, \theta^{(2)} \\ w_{1:1}^{(1)}, w_{2:1}^{(1)}, w_{3:1}^{(1)}, \dots, w_{11:1}^{(1)}, w_{12}^{(2)} \\ w_{1:2}^{(1)}, w_{1:2}^{(1)}, w_{3:2}^{(1)}, \dots, w_{11:2}^{(1)}, w_{2}^{(2)} \\ w_{1:3}^{(1)}, w_{1:3}^{(1)}, w_{3:3}^{(1)}, \dots, w_{11:3}^{(1)}, w_{3}^{(2)} \end{array}
                                                                                                                           \begin{array}{c} \theta_1^{(1)}, \theta_2^{(1)}, \theta_2^{(2)} \\ w_{1:1}^{(1)}, w_{2:1}^{(1)}, w_1^{(2)} \\ w_{1:2}^{(1)}, w_{1:2}^{(1)}, w_2^{(2)} \\ w_{1:3}^{(1)}, w_{2:3}^{(1)} \end{array}
\begin{array}{c} w_{1:1}^{(1)}, w_{1:1}^{(1)}, w_{3:11}^{(1)}, \dots, w_{11:11}^{(1)}, w_{11}^{(2)}\\ w_{1:12}^{(1)}, w_{1:12}^{(1)}, w_{3:12}^{(1)}, \dots, -w_{11:12}^{(1)}\\ w_{1:13}^{(1)}, w_{2:13}^{(1)}, w_{3:13}^{(1)}, \dots, w_{11:13}^{(1)} \end{array}
                                                                                                                           w_{1\cdot11}^{(1)}, w_{2\cdot11}^{(1)}

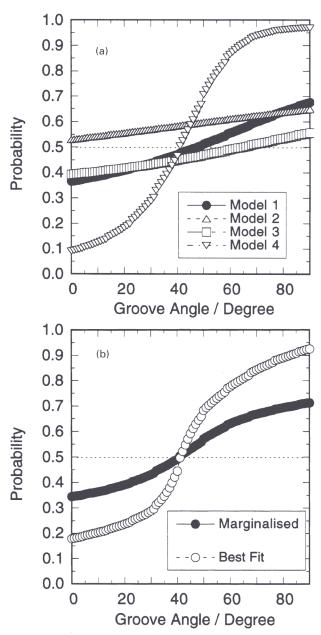
w_{1\cdot12}^{(1)}, w_{2\cdot12}^{(1)}
-0.0091755
                   -0.032463
                                       -0.0118383
                                                           0.0115176
                                                                             0.0113844
                                                                                             -0.0120524
                                                                                                                -0.0096163
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                     3.10162
                                       -0.326395
                                                           0.324679
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                                        0.00729347
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                    -0.126957
                                       -0.109805
                                                           0.108029
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  0.165749
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                                                                             -0.188032
                                                                                               0.193882
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  6.29E - 06
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                                                          7:61E-06
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  -0.496351
                    -0.522203
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-0.751424
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 -0.131658
                                      0.314876
  0.00288703
                                      0.000938893
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11 a marginalised predictions of effect of voltage on solidification cracking in steel welds by the four individual retrained models; b best fit and marginalised predictions of effect of voltage on solidification cracking in steel welds by the retrained committee model

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12 a marginalised predictions of effect of groove angle on solidification cracking in steel welds by the four individual retrained models; b best fit and marginalised predictions of effect of groove angle on solidification cracking in steel welds by the retrained committee model

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