Modeling the $\tan\delta$ Spectrum of Rubber using Committees of Machines

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***Abstract*—Computational techniques that can improve design time, efficiency and utilize existing data are increasingly necessary in industry today. In this work we will apply these techniques to the modeling of the $\tan\delta$ spectrum, the dimensionless loss of rubber with respect to its elastic shear modulus. This measurement is diagnostic of several tire performance features associated with the tread compound. We have attempted to combine this idea, known as the Integral Rubber Concept, with artificial neural networks (ANNs) to create a front-end design tool for the engineers and scientists at Goodyear Tire and Rubber Company. In this paper we will describe the most accurate ANN structure for predicting this value. We will also discuss the statistical likelihood of our model's prediction, based on the specific ANN structure used, a committee of machines (CoM). Finally we will discuss several feature selection analysis techniques used in this application, including principal component analysis (PCA) and a network derivative based technique.**

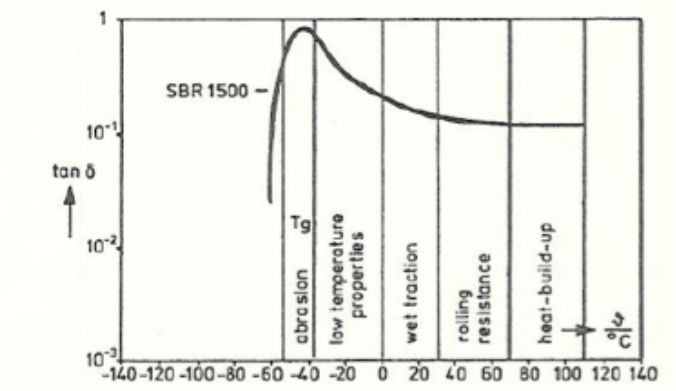

Fig. 1. Example $tan\delta$ curve for a rubber compound.

I. Introduction

HISTORICALLY the $\tan\delta$ value of rubber has been used as a tool for gaining information about the most important properties of a tire tread [1]. This information is seen in a $\tan\delta$ spectrum curve over a range of temperatures. This value at different temperatures is diagnostic of several key tire performance features. This idea is what Nordsiek referred to as the Integral Rubbers Concept. The part of the temperature spectrum that falls below 30 ^{o}C, contains the highest $\tan\delta$ values demonstrating the low level of elasticity that exists when tires are being used in the winter. This is helpful because it can indicate how a tire may perform in these conditions. At 30 ^{o}C, the tan δ values can indicate a tire treads performance in a skid or on wet road circumstance. The range above freezing level contains information about the measure of rolling resistance of a specific rubber compound. The lower $\tan\delta$ values indicate the increase in elasticity of the rubber compound as temperatures increases. Anything above the temperature of 70 ^{o}C shows how much heat and stress a tire can undergo before it can no longer be safely operated. The curve is specific to the composition of the rubber compound. Figure 1 shows an example of this type of curve.

The use of computational and optimization techniques in the design phase has shown incredible potential and increased use [2], [3], [4], [5] in recent years. Particularly in areas where experimentation is expensive and engineering design time is long, these techniques can drastically reduce time and expense. Also as discussed in [6] and [7], models that incorporate the fundamental chemistry and kinetics may be known, they are however difficult to construct and validate, computationally expensive to evaluate and often cannot take advantage of the wealth of experimental data owned by the Goodyear Tire and Rubber Company.

In order to overcome these challenges we will focus on combining the Integral Rubber Concept, with artificial neural networks (ANNs) to create a front-end design tool for the engineers and scientists at Goodyear. The remainder of this paper is arranged as follows. Section II will discuss the experimental data and the general ANN modeling problem. Section III will describe the most accurate ANN structure for predicting this value. We will also discuss the statistical likelihood of our model's prediction, based on the specific ANN structure used, a committee of machines (CoM) in Section V. Finally we will discuss several feature selection analysis techniques used in this application, primarily a network derivative based technique in Section VI.

II. Experimental Data Set Challenges

The data used for this project was created from experimentation at Goodyear's research and development center. There are 2003 experiments in this data set, each with 118 potential ingredients and preparation conditions. Each experiment also had $\tan\delta$ values at 19 discrete temperature values ($-30°$C, $-25°$C, ..., $60°$C). The ingredients and preparation conditions include various accelerants, silicones, oils, plastics, peptides, resins, silanes waxes and cure times. For this work the inputs have been given generic names to protect proprietary Goodyear rubber blends. Beyond having a high dimensional data set, most ingredients or preparation conditions are not used in each experiment, with nearly 80% of the inputs not being used in the average experiment. With this sort of data set, the primary challenge of this work was to build a consistently

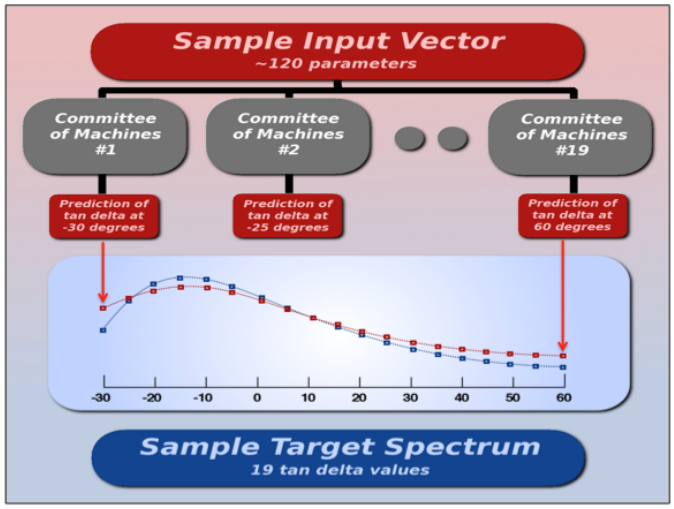

Fig. 2. The committee of machines model. 19 different CoMs

accurate ANN while understanding and identifying potential rubber designs where our model will be more or less accurate, in order to give the design engineer a level of confidence in the predictions the model makes.

III. The Committee of Machines Model

In the attempt to effectively predict the $\tan\delta$ spectrum, several different modeling techniques were used. Most of these attempts included the use of either radial basis networks, self-organizing maps, or feed-forward networks. For completeness, we mention that radial basis function networks proved only moderately successful at predicting the target spectra; and self-organizing maps failed to consistently cluster the model input space in any useful way. The true progress in the project was made in the realm of feed-forward neural networks.

When attempting to predict $\tan\delta$ values, models consisting of single feed-forward network tend to produce poor, inconsistent predictions. However, when we average the outputs of several such individual networks, prediction error is greatly reduced. Indeed, such ensembles of networks – or committees of machines (CoM) – have proven highly useful for many applications because they typically produce more accurate and stable output than single networks. For a survey of methods for combining networks into committees, as well as other related topics, see [8].

A. Model Design

The $\tan\delta$ CoM model is designed such that 19 unique CoM's predict the 19 spectrum points ($\tan\delta$ values at $-30°$C, $-25°$C, $\ldots$, $60°$C). Thus, if each CoM consists of N neural networks, then $19N$ neural networks must be selected to produce the final $\tan\delta$ CoM model.

Figure 2 illustrates the overall model structure. The first step in producing a model prediction is feeding a sample input vector to each of the 19 CoMs. This vector consists of the roughly 120 rubber measurements. Then, each of the CoMs produce a single number prediction: the first CoM predicts $\tan\delta$ at $-30°$C, the second CoM predicts $\tan\delta$ at $-25°$C, etc. Finally, the model strings the 19 predictions together to form a complete spectrum prediction. This spectrum prediction is compared to the target spectrum to assess the CoM model's reliability.

The methods used to produce each of the CoMs is fairly standard. First, the data set is randomly partitioned into a group for training and validataion (70%) and group for testing (30%). Next, for each of the 19 $\tan\delta$ spectrum targets, we train a very large number of feed-forward, back-propogation networks, using the Levenberg-Marquardt algorithm [9]. For each of the 19 batches, we choose the N networks that have the lowest mean square error on the training data. These groups of N networks become our committees. See Section IV on how the best network architecture is decided, as well as the optimal value for N.

B. Prediction Error

A model is judged by how well is makes predictions on the test partition of the data set. Thus, for each test input vector, we can calculate the MSE (mean square error) of the predicted spectrum to the target spectrum. Then, we can produce a frequency distribution of MSE values over the entire test partition. By looking at, say, the 95^{th} percentile of the distribution, we can evaluate a model's accuracy across the entire spectrum of test conditions and get a more robust view of the model's performance than simply looking at a single MSE or squared regression coefficient, R^2, number.

IV. Optimal CoM Design

In order to build an optimal CoM for $\tan\delta$ prediction we need to first figure out the most accurate ANN structure for this type of prediction and we need to find the optimal number of members in the committee.

A. Network Layer Architecture

One part of the CoM to optimize is the number of neurons to have in each of the network layers. By estimating the average test error produced by various layer-neuron combinations, we attempt to discover the optimal layer architecture. As one can see in Figure 3 the best feed-forward networks has roughly 5 neurons in first layer, around 7 in second layer. We experimented with using a larger number of layers but found that this let to over-fitting and a reduction in the robustness of the ANNs.

B. Committee Size

The second way we optimize the CoM model is by determining the optimal number of committee members. Figure 4 compares committee size to overall MSE and R^2 values. We can see that increasing committee size from 1 to 10 improves error and R^2 considerably, after which, error and R^2 seem to level off. These results suggest that committee should have 10 members.

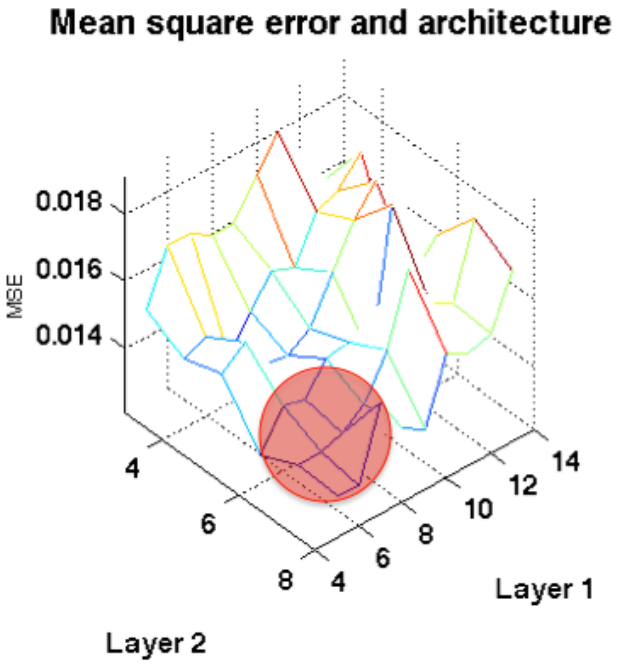

Fig. 3. MSE for various numbers of neurons in each layer.

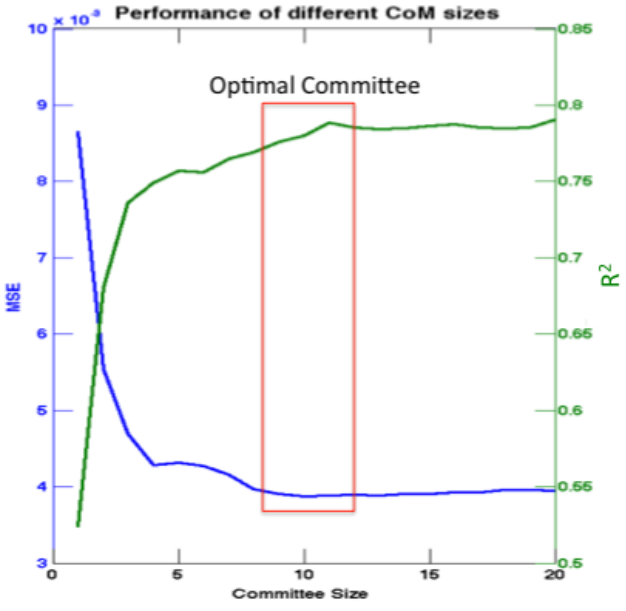

Fig. 4. MSE and R^2 value for various numbers of committee members.

C. Prediction Error

The results of our optimal CoM analysis suggest that a CoM with 10 members and with five neurons in the first layer and 7 in the second architecture is an optimal design. By implementing the optimized model, we find that 95% of error is less than 0.0084 MSE, a substantial improvement over the rest of the design methodologies we tried. For a full analysis of the accuracy of all models tried see [10]

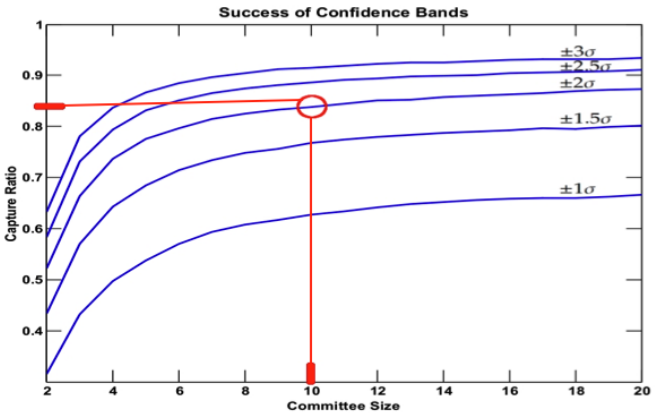

Fig. 5. Summary of confidence intervals for optimal model.

V. Confidence Intervals

The current model provides a convenient way of placing a confidence interval around a prediction. Since the CoM for each of the 19 $\tan\delta$ targets consists of n different neural networks, where y_i is the tanδ prediction for the i^{th} committee member. We can place upper and lower bands around the CoM's prediction $\hat{y}$ by finding the standard deviation of the n predictions, where $\hat{y}$ represents the mean, $\hat{y} = (1/n)\sum_{i=1}^{n} y_i$. Once we have the standard deviation, we can produce bands to suit our needs.

Figure 5 illustrates that a confidence interval of $\hat{y} \pm 2\sigma$, placed around the predicted $\tan\delta$ value $\hat{y}$, has a roughly a 85% chance of capturing the true $\tan\delta$ value, y when you use 10 CoM members. Likewise, a $\hat{y} \pm 2.5\sigma$ interval is successful 90% of the time. One can also see several different sizes of confidence bands and how the success rate relates to CoM size.

Without confidence intervals, models just provide predictions, without any measure of how confident the user can be in those predictions. The idea of confidence bands allows the users to have a sense for how accurate the model prediction output is likely to be.

VI. Feature Selection

We attempted several methods to analyze both the data and our CoM model, including Principal Component Analysis (PCA), Self Organizing Maps (SoMs) and a derivative based technique. As the unsupervised methods, PCA and SoMs, did not give us a consistent way to group our data, particularly with respect to building more accurate models, we will focus on the derivative based analysis here.

A. Derivative Analysis

The derivative based approach to feature selection allows one to understand the influence of the different inputs on a neural network. Fundamentally what we do is vary the input to the model from an average value by a small amount and look at how much the prediction for the $\tan\delta$ value changes. The higher the absolute value of the derivative of the network

for an input, the more influence the input has on the output of the network. If the derivative is zero, then this means the input has no influence. It is quite similar to saliency measure in [11]. The derivatives were approximated with the centered difference formula:

$$y'_k(x_{ij}) \approx \frac{y_k(x_{ij}+h) - y_k(x_{ij}-h)}{2h} \quad (1)$$

where $h = 10^{-6}$ is a common difference increment, x_{ij} is the i^{th} ingredient for the j^{th} experiment, y_k is the model for the k^{th} temperature and $y_k(x_{ij})$ is the $\tan\delta$ value at the k^{th} temperature for the particular recipe.

For the networks created, the derivatives were found for the different temperatures using the approximation shown by equation 1. In order to accumulate results for the different inputs at the different temperatures we used the 2-norm of the derivative for each input at each temperature was calculated. This is calculated with the following equation

$$N_{ik} = \sqrt{\sum_{j=1}^{2003} (y'(x_{ij}))^2} \quad (2)$$

where N_{ik} is the 2-norm for the i^{th} ingredient at the k^{th} temperature. For each temperature the inputs were sorted in descending order according to influence.

Table 1 below shows the top 5 ingredients obtained using derivative analysis, recall that the names of the specific ingredients have been given generic names. In this table, in the positive temperature range, it appears that Filler 05 and Filler 15 were more influential. Overall, Filler 05 was quite influential frequently. Also the polymers were highly influential in the negative temperature range. In the range of $-25°$C to $-15°$C cure time seems to have some importance. These results match the physical understanding of how influential certain ingredients are in certain temperature ranges and increase the confidence of the design engineers in this model.

TABLE I
Table of top 4 ingredients according to the derivative analysis.

Temp (°C)	Ingredients			
	#1	#2	#3	#4
-30	Filler05	Poly23	Oil07	Filler15
-25	Poly30	cure time	Filler05	Silane01
-20	Poly21	Poly04	Filler05	Filler22
-15	Poly03	Poly06	Poly04	cure time
-10	Poly04	Poly24	Poly03	Poly06
-5	Poly03	Cure05	Poly04	Poly24
0	Filler05	Poly04	Poly03	Poly24
5	Filler05	Poly03	Poly04	Filler15
10	Filler05	Poly03	Filler15	Filler14
15	Filler05	Filler15	Filler14	Poly03
20	Filler15	Filler05	Filler14	Filler22
25	Filler05	Race04	Filler15	NR02
30	Filler15	Filler05	Race04	Filler14
35	Filler05	Filler15	Filler22	Oil05
40	Filler15	Filler05	Race04	Filler14
45	Filler05	Filler15	Filler14	Race04
50	Filler05	Race04	Filler15	Filler09
55	Filler05	Filler15	Filler22	Acc11
60	Filler05	Filler15	Race04	Filler14

VII. Summary

With increasing demand in performance and developmental expenses it is important to take advantage of computational techniques that can reduce design time, improve performance, reduce cost and take advantage of existing experimental data. We have demonstrated an accurate, efficient way to do this using a CoM framework. This paper demonstrates a way to optimize this CoM in the case where the input data is high dimensional and sparse. Our confidence interval work provides an additional tool to the design engineer who will use this model to design potential rubber compounds. Finally, not only does our derivative analysis give us insight into the key ingredients in these designs but it also can help inform first principle chemical studies that seek to better understand the underlying physical mechanisms at work in this process.

Acknowledgment

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