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Neural computations of effective response of random composites

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Abstract

The effective response of disordered heterogeneous materials, in general, is not amenable to exact analysis because the phase geometry may not be completely specified. Besides the bounds for the effective moduli, most reported results are essentially approximate, may contradict each other or even violate the bounds. With increasing number of phases, and therefore increasing uncertainty inherent in the very statement of the problem, the investigation of effective response becomes less amenable to analytical treatment, in particular, by methods of boundary-value problems of mathematical physics. The present paper reports a methodology for investigating the effective response of disordered composites with the help of neural networks as well as particular results obtained for effectively isotropic and macroscopically homogeneous two-phase materials. It is shown that, after incorporating the bounds and proper training, simple neural networks may describe a wide variety of the effective response for two-phase composites, though in general more complicated networks appear necessary.

Keywords: Neural network; Random composite; Effective response; Elastic properties

1. Introduction

The present paper reports investigations into the effective response of disordered composites with the help of a neural network, which has recently become one of the main paradigms of engineering research. Though the operation of these networks resemble only superficially the brain physiology, they have proven useful in treating problems characterized by incomplete a priori given information and are difficult for exact analysis, in particular, by the methods borrowed from boundary-value problems of

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mathematical physics. This is typical of disordered materials and therefore neural networks, which are capable of discovering a 'hidden' regularity, may constitute a useful tool for specifying their effective response.

A neural network consists of mutually connected processing elements (neurons), whose weights may be adjusted so as to comply with the information available on the subject. The transfer function of the neurons is usually of a 'saturating' type. The process of specifying the weights is known as training, after which the network may acquire a generic potential, including extrapolation and interpolation capabilities. That is why the account for a priori information is critical for a successful application of a neural network. In this regard, the situation is similar to that of direct variational methods, which also require accurate account for the available information to be successful (Beltzer, 1996). Another similarity with direct variational methods is presence of a heuristic ingredient. Gallant (1994) and Hagan et al. (1996) present an extensive treatment of neural networks. Applications to identification of civil engineering structures may be found in Sato and Sato (1995, 1997). Recently Zeng (1998) published a review of applications of neural networks.

For details concerning the effective static response the reader is referred to the works by Cleary et al. (1980), Christensen (1990), Hale (1976), Hashin (1983), Watt and O'Connell (1976), Willis (1981) and the monograph by Nemat-Nasser and Hori (1993). Relevant aspects of the problem are also discussed by Beltzer (1989). The effective response of disordered heterogeneous materials is not amenable to exact analysis because the phase geometry may not be completely specified. Besides the bounds for the effective moduli, most reported results are essentially approximate, may contradict each other or even violate the bounds. Resort to a particular shape of inclusion necessary in the frameworks of such methods as the composite sphere assemblage or self-consistent schemes seems to contradict to a basic assumption of 'arbitrary' phase geometry, which should come into play through the volume concentration only. With increasing number of phases and therefore increasing uncertainty inherent in the very statement of the problem, the investigation of effective response becomes less amenable to analytical treatment, in particular, by methods of boundary-value problems of mathematical physics. That is why applications of neural networks to this problem should be useful.

This paper, which is a sequel to communication by Beltzer and Sato (1998), deals with:

1. the general methodology of application of neural networks to disordered heterogeneous materials;
2. results derived for the effective moduli of two-phase composites as a particular case.

The elastic response of isotropic composites is governed by two effective moduli. We therefore consider, as a touchstone, a problem of specifying the bulk and Young's moduli, K and E, respectively, of a two-phase elastic isotropic material of arbitrary geometry.

The lower K_- and upper K_+ Hashin–Shtrikman bounds for the bulk modulus K for such composites are (Hashin, 1983)

$$K_- = K_1 + \frac{c_2}{1/(K_2 - K_1) + 3c_1/(3K_1 + 4G_1)}$$

$$K_+ = K_2 + \frac{c_1}{1/(K_1 - K_2) + 3c_2/(3K_2 + 4G_2)} \tag{1}$$

where K_1 and K_2 are the bulk moduli of the phases, G_1 and G_2 their shear moduli, c_1 and c_2 their volume concentrations and $K_1 < K_2$, $G_1 < G_2$, $c_1 + c_2 = 1$, Similarly, for the shear modulus, G, the bounds are

$$G_- = G_1 + \frac{c_2}{1/(G_2 - G_1) + 6c_1(K_1 + 2G_1)/5G_1(3K_1 + 4G_1)}$$

$$G_+ = G_2 + \frac{c_1}{1/(G_1 - G_2) + 6c_2(K_2 + 2G_2)/5G_2(3K_2 + 4G_2)}. \tag{2}$$

These bounds are the best ones possible as far as arbitrary geometry is concerned, and their disparity is sensitive to the shear moduli ratio, G_1/G_2, vanishing for $G_1/G_2 = 1$. The latter case, for which the exact solution does exist, is known as Hill's solid (Hale, 1976) and is naturally excluded from the present investigation. The main body of experiments available deals with the effective moduli K and E rather then K and G. The bounds for E follow from the well known relation $E = E(K, G)$ and expressions (1) and (2):

$$E_\pm = \frac{9K_\pm G_\pm}{3K_\pm + G_\pm}. \tag{3}$$

The next section deals with design and training of neural networks for evaluating K and E. In section 3 the neural computations are compared with experimental data and theoretical results. Conclusions are given in section 4.

2. Neural networks for K and E

It is assumed that:

1. the composite microstructure is not completely known and is specified in terms of K_1, K_2, G_1, G_2, c_2, (or $c_1 = 1 - c_2$) only;
2. the composite may be treated as effectively isotropic and macroscopically homogeneous.

This statement and Eqs. (1) and (2) show that the networks should incorporate the above five inputs. Besides this, the network versatility may be greatly increased by adding unit input with unknown weight, the so-called bias (Gallant, 1994). Though insufficient number of neurons may lead to problematic learning, the case of excessive neurons has difficulties of its own, as such a network would be complicated and have a tendency of 'overfitting'. One is therefore interested in a network of possibly minimal number of neurons.

We consider below a single-neuron network (perceptron) with six inputs. Fig. 1 shows the chart, where w_i, $i = 0, \ldots, 5$, are the weights of the inputs u_i, $i = 0, \ldots, 5$, to be specified by the training process. As to the transfer function, we note that the effective moduli depend on its arguments in a non-linear manner and are bounded from below and above. A sigmoid transfer function

$$-1 \le F(n) = \tanh(n) \le +1 \tag{4}$$

may incorporate this fundamental behavior. Here F is the network output (see Fig. 1) and

$$n = \sum_{i=0}^{5} w_i u_i = w_0 + w_1 K_2 + w_2 G_2 + w_3 K_1 + w_4 G_1 + w_5 c_2 \tag{5}$$

is the total (weighted) network input.

Given the value of F, the bulk modulus K follows as:

$$K = \left(\frac{F}{2} + \frac{1}{2}\right) K_+ + \left(\frac{F}{2} - \frac{1}{2}\right) K_- \tag{6}$$

and the inverse transformation

$$F = \frac{2K - (K_+ + K_-)}{K_+ - K_-} \tag{7}$$

relates $K_- \le K \le K_+$ and the network output $-1 \le F \le 1$.

Similar expressions hold for Young's modulus E. Evidently, the weights and biases can be different for the cases of K and E. This methodology enables one to inherently incorporate the bounds, which are shown below to also facilitate a proper specification of the training set.

Besides the bounds, the relevant information consists of experimental data, which are approximate because of the experimental scatter. Indeed, some experiments fall outside the bounds and must be excluded from considerations. Also, experiments with dilute mixtures or with the phases having slight mismatch of the shear moduli are of little interest, as the Hashin–Shtrikman bounds are sufficiently stringent in this case.

Below use is made of experiments with sintered alumina, ceramics, tungsten carbide-cobalt alloy and KCl + Cu aggregate for a wide interval of the volume concentrations. These data should be divided into a training set used for the training of the neural network (the procedure known as the supervised learning) and a test set used for a posteriori comparison of the neural computation with experimental results. There is no precise recipe for specifying the size of a training set which is usually a matter of engineering judgment. It is essential that this set includes samples displaying the effect at hand to its maximal degree. In the present context, some of the reported data bear little information compared to the bounds, as noted earlier.

Excessive experimental data included in a training set may involve 'noisy' samples, bring about 'overfitting' and damage the generalization capability of the network. It appears that data dealing with concentrated mixtures $c_1 \approx c_2 \approx 0.5$ and possibly large mismatch of the shear moduli are most informative, as the uncertainty left over by the bounds is maximal under these conditions. Because, as the present methodology suggests, the bounds are fed into the network separately for each particular composite prior to the weight optimization process, it seems possible to adopt small training sets, which

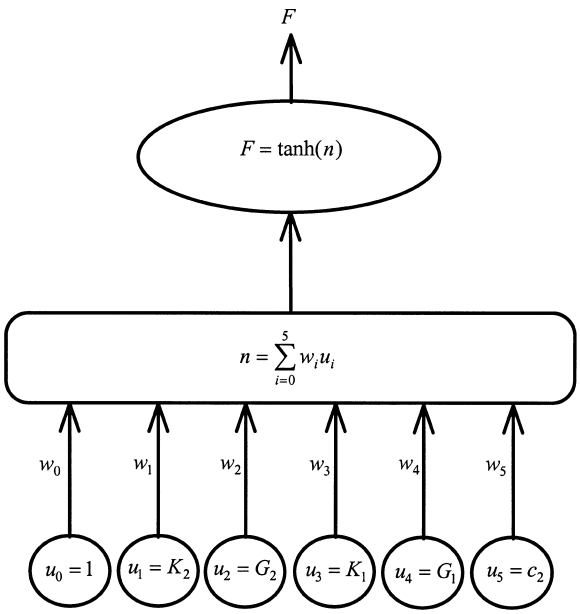

Fig. 1. Neural computation of effective moduli.

are mainly 'placed' in the region of maximal disparity between the bounds. At the same time, it is essential that the training samples should represent a possibly large variety of microstructure in agreement with the assumption (1) made in the above. A good a posteriori agreement between the neural computation and the test set suggests a well-defined neural network, which, in this sense, discovers a 'hidden' regularity.

The experimental data dealing with E and K are shown in Tables 1 and 3, respectively, and also repeated in Tables 2 and 4). For obvious experimental reasons the available data for K are considerably less than those for E. The training sets, shown by a dot, first consisted of three samples (Tables 1 and 3) and then of four samples (Tables 2 and 4. These samples have been so chosen as to comply with the above comments concerning specification of the training sets.

The Tables 1–4 also present the weights and biases arrived at by the gradient descent method chosen to perform the training. The reader is referred to Gallant (1994) and Hagan et al. (1996) for details of the numerical algorithm.

3. Analysis of results

Tables 1 and 2 show the comparison of the neural computation of Young's modulus E_N with the available experimental data for the case of three and four training samples, respectively. The column R_N presents the value of the relative error for the neural computation and the column R_A the value of the relative error if the arithmetic average of the Hashin–Shtrikman bounds would be used for prediction. It is seen that the neural computation provides a reasonable agreement with the experimental data. Except for the materials for which the gap between the bounds is narrow and any value consistent with the bounds would be acceptable from a practical point of view, the neural computation shows much better agreement with the experimental data. This is particularly true for the network trained with four samples.

The similar conclusions follow from Tables 3 and 4, which show the results for the bulk modulus K. Once again the accuracy of neural computation K_N is much better than that of the arithmetic average of the Hashin–Shtrikman bounds and the prediction further improves when four samples are used for the training instead of three. A particular experiment with porous Mg Al_2O_4, $c_2 = 0.61$, appears inconsistent and may be considered as outlier. The generalization capability of the networks seems fairly impressive, particularly in view of their extreme simplicity and the small training sets.

Going over to comparison of the neural computation with analytical techniques such as the self-consistent scheme and the differential method, we note that even though the results associated with these techniques employ the phase concentration c_2 as the only phase geometry parameter, their derivation essentially assumes a particular phase geometry (spherical inclusions embedded in a homogeneous matrix). On the other hand, the above neural computation is solely based on the Hashin–Shtrikman bounds and experiments which incorporate a variety of microstructures in agreement with the assumption made. Therefore any comparison between these approaches should not be taken literally. This comparison would be more meaningful if the training and test sets consist only of the samples of spherical inclusions in a purely homogeneous matrix. Presently, to the best knowledge of these authors, the available experimental data of this type are too limited to allow for such a procedure.

Nevertheless, it would be of interest to appreciate the difference between these analytical models and the neural computation in case of composite with a particularly large gap between the Hashin–Shtrikman bounds. Figs. 2 and 3 show the effective moduli E and K, respectively, as functions of the volume concentration, c_2, for a composite with the following values of elastic moduli: $K_2 = 30$ GPa, $G_2 = 22$ GPa, $K_1 = 1$ GPa, $G_1 = 0.375$ GPa. The values, which correspond to the differential scheme and

Table 1
Young's modulus (training set of 3 samples). The neural weights are: $w_1 = 0.00482\ (\mathrm{GPa})^{-1}$, $w_2 = -0.00591\ (\mathrm{GPa})^{-1}$, $w_3 = -0.00042\ (\mathrm{GPa})^{-1}$, $w_4 = -0.00224\ (\mathrm{GPa})^{-1}$, $w_5 = 2.3608$, $w_0 = -1.7375$

	K_2 (GPa)	G_2 (GPa)	K_1 (GPa)	G_1 (GPa)	c_2	E_+ (GPa)	E_- (GPa)	E_{exp} (GPa)	E_N (GPa)	R_N (%)	R_A (%)	Material	Source
•	193.6	148.1	44.3	33.6	0.50	184.5	154.4	161	161.4	0.3	5.2	Tungsten in borosilicate glass	Zimmerman (1991)
					0.40	159.9	134.6	136	138.6	1.9	8.3		
•	418	288	172	79.3	0.50	403.2	362.9	374	373.8	0.0	2.4	Tungsten carbide + cobalt alloy	Nishimatsu and Gurland (1959)
					0.35	336.2	305.0	314	309.8	1.3	2.1		
	180	108	0	0	0.84	195	0	165	140.6	15.0	41.0	Porous Mg Al_2O_4	Ramakrishnan and Arunachalam (1993)
	267	160	0	0	0.95	362	0	340	305.8	10.0	47.0	Porous $Al_2\ O_3$	Ramakrishnan and Arunachalam (1993)
					0.90	327	0	280	265.2	5.3	42.0		
•					0.85	296	0	230	228.6	0.6	36.0		
					0.80	266	0	190	193.7	1.9	30.0		
					0.75	240	0	150	162.9	8.6	20.0		
					0.70	215	0	120	134.5	12.0	10.0		
					0.65	192	0	100	109.2	9.2	4.0		
					0.60	171	0	80	87.2	9.0	6.9		
	137	47.7	18.2	9.4	0.8	97.4	82.2	87.0	93.3	7.3	3.2	KCl + Cu aggregate	Watt and O'Connell (1980)
					0.6	73.2	57.6	62.3	65.6	5.3	5.0		
					0.4	53.6	42.2	46.4	45.5	1.9	3.2		
					0.2	37.5	31.7	35.5	32.5	8.4	2.5		

Table 2
Young's modulus (training set of 4 samples). The neural weights are: $w_1 = 0.00533\ (\mathrm{GPa})^{-1}$, $w_2 = -0.00779\ (\mathrm{GPa})^{-1}$, $w_3 = 0.00139\ (\mathrm{GPa})^{-1}$, $w_4 = -0.00292\ (\mathrm{GPa})^{-1}$, $w_5 = 2.5336$, $w_0 = -1.7427$

	K_2 (GPa)	G_2 (GPa)	K_1 (GPa)	G_1 (GPa)	c_2	E_+ (GPa)	E_- (GPa)	E_{exp} (GPa)	E_N (GPa)	R_N (%)	R_A (%)	Material	Source
•	193.6	148.1	44.3	33.6	0.50	184.5	154.4	161	161.0	0.0	5.2	Tungsten in borosilicate glass	Zimmerman (1991)
					0.40	159.9	134.6	136	138.3	1.7	8.3		
•	418	288	172	79.3	0.50	403.2	362.9	374	374.0	0.0	2.4	Tungsten carbide + cobalt alloy	Nishimatsu and Gurland (1959)
					0.35	336.2	305.0	314	309.7	1.4	2.1		
	180	108	0	0	0.84	195	0	165	142.8	13.0	41.0	Porous Mg Al_2O_4	Ramakrishnan and Arunachalam (1993)
	267	160	0	0	0.95	362	0	340	305.2	10.0	47.0	Porous Al_2O_3	Ramakrishnan and Arunachalam (1993)
					0.90	327	0	280	263.8	5.8	42.0		
•					0.85	296	0	230	226.2	1.7	36.0		
					0.80	266	0	190	190.3	0.2	30.0		
					0.75	240	0	150	158.7	5.8	20.0		
					0.70	215	0	120	129.5	7.9	10.0		
					0.65	192	0	100	103.7	3.7	4.0		
•					0.60	171	0	80	81.6	2.0	6.9		
	137	47.7	18.2	9.4	0.8	97.4	82.2	87.0	94.1	8.2	3.2	KCl + Cu aggregate	Watt and O'Connell (1980)
					0.6	73.2	57.6	62.3	66.4	6.6	5.0		
					0.4	53.6	42.2	46.4	45.9	1.1	3.2		
					0.2	37.5	31.7	35.5	32.6	8.3	2.5		

Table 3
The bulk modulus (training set of 3 samples). The neural weights are: $w_1 = -0.00459$ (GPa)$^{-1}$, $w_2 = 0.00877$ (GPa)$^{-1}$, $w_3 = -0.00765$ (GPa)$^{-1}$, $w_4 = -0.00769$ (GPa)$^{-1}$, $w_5 = 0.6800$, $w_0 = 0.5564$

	K_2 (GPa)	G_2 (GPa)	K_1 (GPa)	G_1 (GPa)	c_2	K_+ (GPa)	K_- (GPa)	K_{exp} (GPa)	K_N (GPa)	R_N (%)	R_A (%)	Material	Source
•	418.5	288.2	172.0	79.3	0.63	305.4	288.9	294.5	294.5	0.0	0.9	Tungsten carbide + cobalt alloy	Nishimatsu and Gurland (1959)
	180	108	0	0	0.84	126.0	0	119.2	116.6	2.3	47.0	Porous Mg Al_2O_4	Ramakrishnan and Arunachalam (1993)
					0.69	89.5	0	74.7	81.3	8.8	40.0		
					0.61	73.8	0	19.5	66.3	240.0	90.0		
	267	160	0	0	0.9	214	0	210	200	4.6	49.0	Porous Al_2O_3	Ramakrishnan and Arunachalam (1993)
•					0.8	171	0	161	159	1.4	47.0		
					0.7	136	0	119	125	4.9	43.0		
					0.6	107	0	88	97	10.0	39.0		
					0.5	82	0	62	73	18.0	34.0		
	137	47.7	18.2	9.4	0.6	63.3	46.2	60.3	59.0	2.2	9.2	KCl + Cu aggregate	Watt and O'Connell (1980)
•					0.4	43.6	32.5	40.1	40.2	0.2	5.1		

Table 4
The bulk modulus (training set of 4 samples). The neural weights are: $w_1 = 0.01383\ (\mathrm{GPa})^{-1}$, $w_2 = -0.01736\ (\mathrm{GPa})^{-1}$, $w_3 = -0.00502\ (\mathrm{GPa})^{-1}$, $w_4 = -0.00277\ (\mathrm{GPa})^{-1}$, $w_5 = 2.2884$, $w_0 = -1.4774$

	K_2 (GPa)	G_2 (GPa)	K_1 (GPa)	G_1 (GPa)	c_2	K_+ (GPa)	K_- (GPa)	K_{exp} (GPa)	K_N (GPa)	R_N (%)	R_A (%)	Material	Source
•	418.5	288.2	172.0	79.3	0.63	305.4	288.9	294.5	294.5	0.0	0.9	Tungsten carbide + cobalt alloy	Nishimatsu and Gurland (1959)
	180	108	0	0	0.84	126.0	0	119.2	112.5	5.6	47.0	Porous Mg Al_2O_4	Ramakrishnan and Arunachalam (1993)
					0.69	89.5	0	74.7	72.2	3.3	40.0		
					0.61	73.8	0	19.5	54.9	181.0	90.0		
	267	160	0	0	0.9	214	0	210	204	2.9	49.0	Porous Al_2O_3	Ramakrishnan and Arunachalam (1993)
•					0.8	171	0	161	158	1.6	47.0		
					0.7	136	0	119	121	1.6	43.0		
					0.6	107	0	88	89	1.5	39.0		
•					0.5	82	0	62	62	0.8	34.0		
	137	47.7	18.2	9.4	0.6	63.3	46.2	60.3	60.6	0.6	9.2	KCl + Cu aggregate	Watt and O'Connell (1980)
•					0.4	43.6	32.5	40.1	40.1	0.0	5.1		

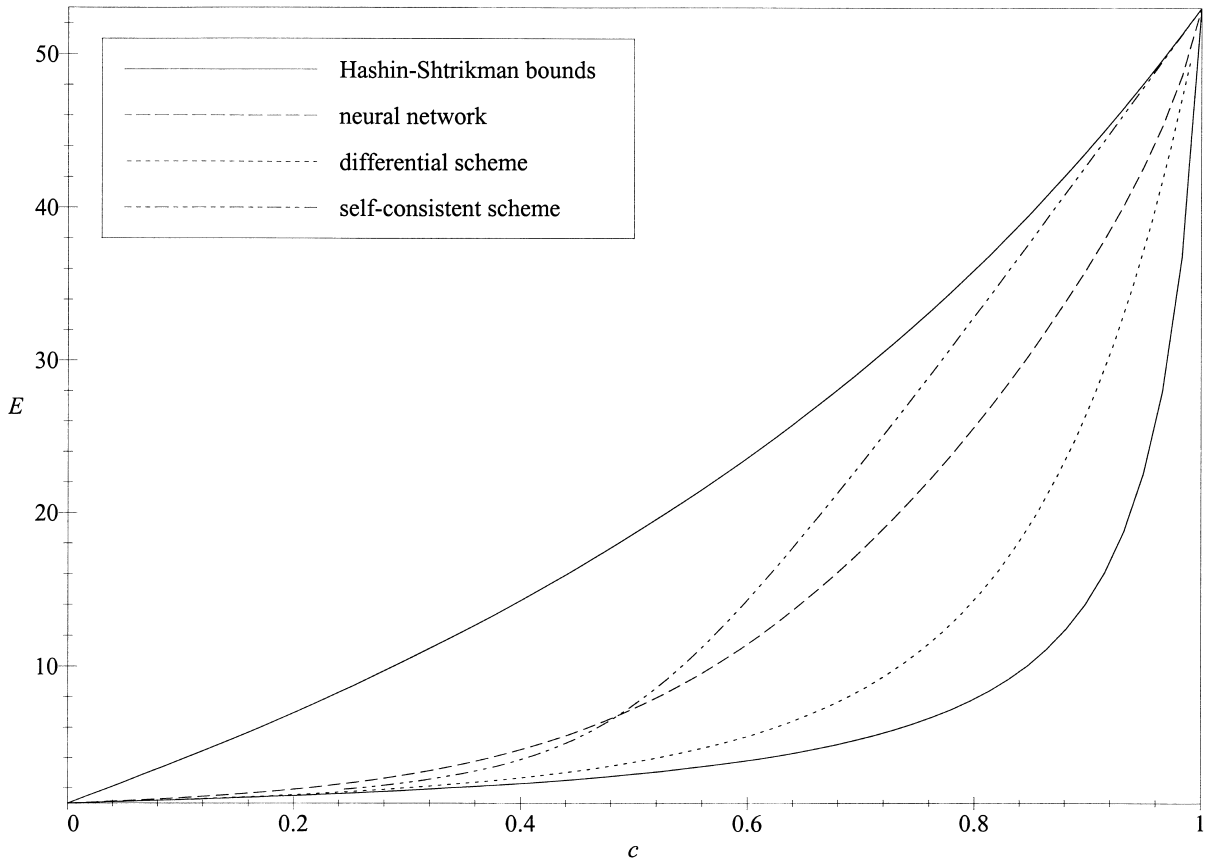

Fig. 2. Effective Young's modulus, E (GPa) vs volume concentration c_2: $K_1 = 1$ GPa, $G_1 = 0.375$ GPa, $K_2 = 30$ GPa, $G_2 = 22$ GPa.

to the self-consistent method, have been computed according to expressions discussed in detail by Christensen (1990) and Zimmerman (1991).

If, contrary to the assumption (1) of Section 2, the inclusion shape is known, the training set should be reformulated so as to include proper samples, say, disk-like inclusions. The Hashin–Shtrikman bounds still hold, though, in general, they may be replaced by more stringent bounds because of the specific geometry involved. This would allow for incorporating the effect of inclusion shape.

Further, since the Hashin–Shtrikman bounds do not distinguish between phases in the form of matrix or particles, in order to investigate yet another effect of 'which component is the matrix phase and which is the inclusion phase', one should design two networks trained on two different sets. One of these sets should contain only the samples with much stiffer matrix phase and the second with much stiffer particles phase. A single network may also be designed, if one employs additional input parameter, say, -1 for the first case and 1 for the second. Unfortunately, the experimental data presently available do not seem sufficient for such investigations.

It is well-known that engineering problems may be amenable to solutions by various methods, which is also the case at hand: instead of neural networks the problem may be treated by traditional statistical methods, which also deal with the treatment of experimental data. The general discussion on the advantages and drawbacks of each of these two approaches is outside of the scope of this work, which is focused on the prediction of the effective response of composites. Nevertheless, the simplicity of the

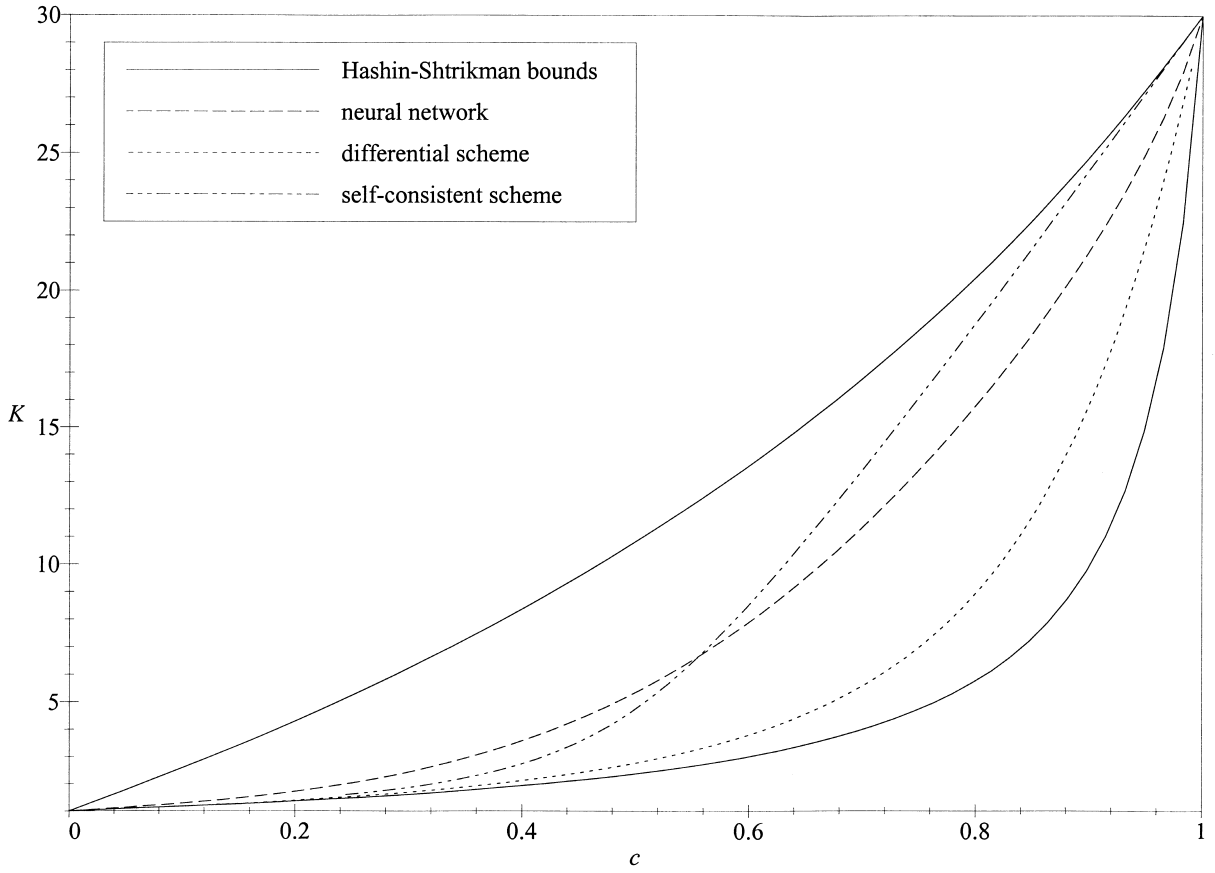

Fig. 3. Effective bulk modulus, K (GPa) vs volume concentration c_2 for the same composite as in Fig. 1.

results obtained herein and a possibility of their extension to more complicated cases in the frameworks of the modern paradigm of neural networks seems attractive.

4. Conclusions

The uncertainty typical of disordered heterogeneous materials increases in case of multiphase and incompletely specified microstructure. This further complicates their analysis by the conventional methods borrowed from boundary-value problems of mathematical physics and neural networks may serve as a useful alternative.

The bounds play an essential role in the present methodology of applications of neural networks to the effective response of disordered composites. Since the experimental data concerning dilute mixtures and/or slight mismatch of elastic moduli bear little information compared to the bounds, they may be put aside while specifying a training set. Then the bounds are fed into the neural network separately for each particular composite as an integral part of the training. The generalization capability of the designed networks appears substantial, particularly in view of their extreme simplicity and the small

training sets employed. Though the simple perceptrons show a wide variety of the effective response for two-phase composites, in general a more complicated network appears necessary.

It seems that neural networks, which incorporate the relevant bounds and are trained on small but properly selected experimental sets, may provide a useful insight into the effective behavior of heterogeneous materials.

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