

STATISTICAL SIGNIFICANCE OF DIFFERENCES MAGNESIUM DIBORIDE SUPERCONDUCTING TRANSITION TEMPERATURE MODELING

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Abstract

An extensive study has been done on a modeling approach that helps forecast the critical temperature of magnesium diboride (MgB₂) materials. To determine the statistical importance of changes in modeling techniques, investigations must be able to consistently distinguish between systematic approach impacts and mistakes caused by modeling approach variance. In this study, researchers used analysis of variance and correlation analysis to determine the statistical significance of differences in modeling method variation. The resulting results were compared to the critical temperature estimated from lattice parameter change data using gaussian process regression (GPR), support vector machine (SVM), and linear regression with natural logarithm transformation (LRNLT).

Keywords: Analysis of variance (ANOVA); Statistical significance; Magnesium diboride (MgB₂); Critical temperature; Lattice parameters

Introduction

Many areas of scientific inquiry, such as medicine, imaging, and energy, require large-scale magnets capable of producing high magnetic fields. Because of two essential properties of superconductivity: zero resistivity and perfect diamagnetism, superconducting wires may carry large current densities with no electrical resistance. Because their upper critical fields are less than 25 T at 4.2 K, low-temperature superconductors like NbTi and Nb₃Sn can only generate magnetic fields of 10.5 T and 20 T, respectively (Schwartz *et al.*, 2008). Thus, high-temperature superconductors (HTS), such as

YBa₂Cu₃O_{7-x} (YBCO) and Bi₂Sr₂CaCu₂O_x, have been developed since 1980's as promising candidates for high field magnet fabrication as they have critical temperature T_c of over 90 K and upper critical fields over 100 T (Devred *et al.*, 2005; Hazelton *et al.*, 2009; Schwartz, 2014; Zhang, *et al.*, 2016; Schwartz, *et al.*, 2017).

However, superconducting oxides have significant disadvantages, such as weak leak concerns at grain boundaries, high anisotropy, high processing temperatures, and high sensitivities to mechanical disturbances (Kajbafvala *et al.*, 2012),

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which severely limit large-scale applications of superconducting wires in high-energy physics.

The finding of superconductivity in magnesium boride (MgB_2) has opened up new possibilities for high-field magnet construction. MgB_2 superconductors have various advantages over HTS, including the absence of weak links in grain boundaries, less noticeable anisotropy, relatively straightforward powder-in-tube wire production procedures, and significantly reduced raw material costs. In addition, their upper critical field is higher than that of low-temperature superconductors, and their superconducting transition temperature is rather high (20-40 K). Additionally, different processing conditions, chemical substitutions, and irradiations might change the physical properties of the materials and induce problems in MgB_2 (X.F. Pan *et al.*, 2007; Yang *et al.*, 2008). Lattice parameters, critical temperature (T_c), normal state resistivities, higher critical fields, anisotropy, magnetic penetration depth, and GL parameters are among the factors that affect disorders.

In particular, changes in lattice parameters influence T_c . Several mechanisms are associated with changing critical temperature of MgB_2 , such as reductions of densities of the states (DOS), reductions of σ gap anisotropy, hardening of optical E_{2g} phonons, and interband scattering (Eisterer, 2007). For example, by applying isostatic pressure to compressive strain, decreases of lattice parameters lead to reductions in T_c as a result of reductions of DOS and hardening of E_{2g} phonons (Monteverde *et al.*, 2001; Deemyad *et al.*, 2003; Bud'ko *et al.*, 2005; Dhallé *et al.*, 2005; Schneider and Castro, 2005). A decrease in the cell volume by aluminum or carbon doping usually causes a reduction in T_c , mainly due to hardening of E_{2g} (Renker *et al.*, 2002). An increase in the a -axis due to lattice mismatches between superconducting films and substrates may soften E_{2g} and thus increase T_c (Hur *et al.*, 2001). These correlations observed in previous studies are obvious, in most cases, for T_c above 30 K, but they are only general tendencies and clearly not universal (Eisterer, 2007).

A modeling method that aids in predicting the critical temperature of magnesium diboride (MgB_2) materials has been thoroughly investigated. Investigations must be able to reliably differentiate between errors brought on by modeling approach variance and systematic approach impacts in order to assess the statistical significance of modifications in modeling procedures. To ascertain the statistical

significance of variations in modeling methods, researchers employed correlation analysis and analysis of variance in this study. The outcomes were contrasted with the critical temperature calculated from lattice parameter change data using support vector machines (SVM), linear regression with natural logarithm transformation (LRNLT), and gaussian process regression (GPR).

Materials and Methods

Brief description of analysis of variance (ANOVA)

ANOVA is used to determine significance using the ratio of variance estimates from sample means and sample values (Krzywinski and Altman, 2014). Their ratio or test statistic F can be used between group mean squares (MS_B) and within group mean squares (MS_W), which are calculated from between treatment sum of squares (SS_B) and within treatment sum of squares (SS_W) weighted by degrees of freedom (d.f.). The degrees of freedom (d.f.) shows the number of independent deviations in the treatment sum of squares (SS); the deviations are not all independent because deviations of a quantity from its own mean must sum to zero. The ANOVA null hypothesis is that all samples are from the same distribution and have equal means. Under this null, between group variation of sample means and within group variation of sample values are predictably related. We introduced the idea that variance can be partitioned within group variance was interpreted as experimental error and between group variance as structural and topological parameters variation. In one way ANOVA, the relevant quantities are within group variance and between group variance. Within group variance corresponds to variance in the sample after other sources of variation have been accounted for and represents experimental error. If some sources of error are not accounted for (e.g., structural and topological parameters variation), within group variance will be inflated. Between group variance is another estimate for within group variance, additionally inflated by average squared deviation of treatment means from the grand mean. As noise within samples drops, a larger fraction variation is allocated to between group variance, and the power of the test improves (Armstrong *et al.*, 2022). This suggests that it is beneficial to decrease within group variance. We can do this through a process to identify and isolate likely sources of sample variability.

Proposed method

The uniqueness of this research work is to show that it adopts the ANOVA together with assessing the statistical significance of differences in the modeling approach will also enhance researchers that are incapacitated to acquire equipment to carry out low temperature research as well as, serving as a premise through which the full understanding of superconductivity can be grown. To demonstrate the outstanding efficiency of the ANOVA results. In this work, we compared obtained results with MgB₂ modeling between support vector machine (SVM) and adopting a simple model (linear regression) through which they developed by using natural logarithm transformation (LRNLT) and gaussian process regression (GPR).

Working principle of SVM

SVM stems from support vector machines which is derived from statistical learning theory and structural risk minimization principle (Cortes and Vapnik, 1995; Vapnik, 1995). It employs mapping function called kernel function to map non-linear regression to high dimensional feature space where linear regression is conducted. SVM adopts support vector regression (SV regression) takes some input parameters (such as hyperparameter λ , regularization factor C and kernel option) by which the chosen kernel function generates a relation between the predictor and the target. The complete regression function is presented in equation (1) with the inclusion of the mapping function $K(x_i, x)$.

$$f(x) = \sum_{i=1}^k (\lambda_i^* - \lambda_i) K(x_i, x) + b \quad (1)$$

Where $\lambda_i^* \geq 0$, $\lambda_i^* \leq C$, $K(x_i, x)$ is the polynomial kernel function, and b kernel parameters.

Working principle of LRNLT

The multiple linear regression models are built on the same simple linear regression (Lee Goldman *et al.*, 1977; Efron and Diaconis 1983); Efron and Gong, 1983). However, in addition to the concepts discussed so far for simple linear regression, which is remain applicable, a new concepts set has to be introduced. This discussion will focus on situation where there are two predictor and one outcome variable. With all three variables, three-dimensional figure can be used to visualize data. Models with more predictive variables follow the same principle, but difficult to visualize. We consider multiple regression and linear relation as follows,

$$Y = BX + W \quad (2)$$

in which,

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \dots \\ y_n \end{bmatrix}, X = \begin{bmatrix} 1 & x_{11} & x_{12} & \dots & x_{1m} \\ 1 & x_{21} & x_{22} & \dots & x_{2m} \\ \dots & \dots & \dots & \dots & \dots \\ 1 & x_{n1} & x_{n2} & \dots & x_{nm} \end{bmatrix},$$

$$B = \begin{bmatrix} b_1 \\ b_2 \\ \dots \\ b_m \end{bmatrix}, W = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \dots \\ \varepsilon_m \end{bmatrix}$$

We develop a multiple linear regression model to predicting the critical temperature of MgB₂ from structural and topological parameters by using linear regression with natural logarithmic transformation (LRNLT). Start by considering the nonlinear regression problem is as follows,

$$y = ae^{bx}U \quad (3)$$

With the parameters a and b and the multiplication error term U . If we find the natural logarithm of both sides, this will becomes.

$$\ln(y) = \ln(a) + bx + u \quad (4)$$

in which, $u = \ln(U)$

Working principle of GPR

One kind of probabilistic model that can be applied to regression tasks is Gaussian process regression (GPR). The underlying premise of this non-parametric approach is that the function to be learned is taken from a Gaussian process. For tasks like active learning and uncertainty-aware decision-making, this assumption enables the model to produce predictions with a clearly stated degree of uncertainty.

Mathematically, the GPR model can be written as follows. Let $x_1, x_2, \dots, x_n$ be the input data points, where $x_i \in \mathbb{R}^d$ is a d -dimensional vector. Let $y_1, y_2, \dots, y_n$ be the corresponding output values, where $y_i \in \mathbb{R}$ is a scalar. The GPR model assumes that the function f that relates the inputs to the outputs is drawn from a Gaussian process with mean function μ and covariance function k . The distribution of f at a set of test points x^* is then given by

$$f(x^*) \approx \mathcal{N}(\mu(x^*), k(x^*, x^*)) \quad (5)$$

The mean function and covariance function are typically defined using kernel functions. For example, the commonly used squared exponential kernel is defined as

$$k(x_i, x_j) = \exp\left(-\frac{1}{2}\|x_i - x_j\|^2\right) \quad (6)$$

Given a set of training data (x, y) , the GPR model uses Bayesian inference to learn the distribution of f that is most likely to have generated the data.

Like k -nearest neighbors, Gaussian process regression (GPR) makes predictions using training data. It offers a prediction with quantified uncertainty and performs well with tiny data sets. It is necessary to specify the previous mean and prior covariance. A kernel object is used to specify the covariance. Using the given optimizer, the kernel hyperparameters are optimized during fitting by maximizing the log-marginal-likelihood (LML). The optimizer is restarted several times because this maximizing is a non-convex optimization (several local optima). The initial hyperparameters are used in the first iteration, and then randomly chosen hyperparameters within the permitted range are used in the following iterations.

Performance evaluation

Performance of obtained results with MgB₂ modeling approach variation data is evaluated using the root mean square difference (RMSD), mean bias difference (MBD), and Pearson's Coefficient Correlation is expressed by r_{XY} in Eq equations. (7) - (9) respectively, where N is the number of data points, T_i^{Exp} and T_i^{Model} are the i -th ($i = 1, 2, \dots, N$) experimental and model of superconducting transition temperature. $\bar{X}$ and $\bar{Y}$ are mean of a linear relationship between the X_i and Y_i variable of obtained results with MgB₂ modeling approach variation data, respectively.

$$RMSD = \sqrt{\frac{\sum_{i=1}^N (T_i^{Model} - T_i^{Exp})^2}{N}} \times 100 \quad (7)$$

$$MBD = \frac{\sum_{i=1}^N (T_i^{Model} - T_i^{Exp})}{N} \times 100 \quad (8)$$

$$r_{XY} = \frac{\sum_{i=1}^N (X_i - \bar{X})(Y_i - \bar{Y})}{\sqrt{\sum_{i=1}^N (X_i - \bar{X})^2} \sqrt{\sum_{i=1}^N (Y_i - \bar{Y})^2}} \quad (9)$$

Results and Discussion

The experimental data used, shown in Table 1 are obtained from (Zhang and Xu, 2020). This dataset contains lattice parameters obtained when dopants, are incorporated into the lattice structure of the parent compound MgB₂. Superconducting transition temperature is affected by incorporated dopants and the effects manifest through variations of lattice parameters along a , and c axes. Data visualization in Table 1 reveals nonlinear relationships, which are modeled through the SVM Estimated T_c (K), GPR Estimated T_c (K), MLR Estimated T_c (K) and LRNLTL Estimated T_c (K) as presented in Figure 1. We were used ANOVA together with correlation data to assess the statistical significance of differences in modeling approach variation in Table 2 and Table 3, respectively.

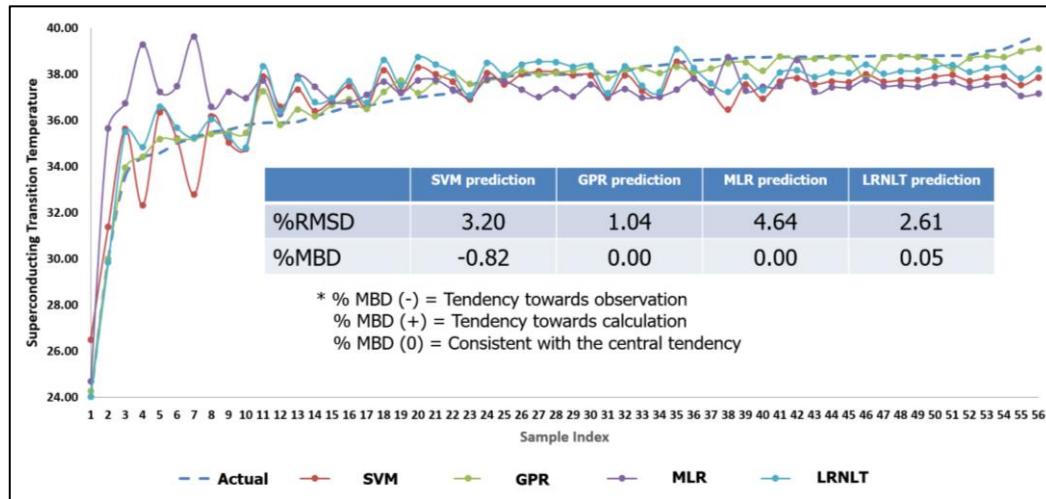


Figure 1. Superconducting transition temperature predictions by SVM, GPR, MLR and LRNLTL

Table 1. The experimental T_c (K) data and superconducting transition temperature predictions from “SVM Estimated $T_c(K)$ ”, “GPR Estimated $T_c(K)$ ”, “MLR Estimated $T_c(K)$ ” and “LRNLT Estimated $T_c(K)$ ”

Sample Index	a(A°)	c(A°)	$T_c(K)$	SVM prediction	GPR prediction	MLR prediction	LRNLT prediction
1	3.52240	3.05240	24.00	26.51	24.28	24.69	24.02
2	3.06410	3.52260	30.00	31.40	30.00	35.66	29.85
3	3.07601	3.52448	33.60	35.63	33.95	36.75	35.52
4	3.07270	3.55340	34.38	32.32	34.43	39.30	34.85
5	3.07898	3.52732	34.60	36.36	35.20	37.25	36.61
6	3.07600	3.53210	35.00	35.23	35.17	37.49	35.70
7	3.07540	3.55470	35.25	32.79	35.21	39.63	35.27
8	3.07760	3.52170	35.50	36.19	35.41	36.60	36.05
9	3.07500	3.53050	35.60	35.04	35.47	37.26	35.33
10	3.07382	3.52858	35.80	34.77	35.46	36.98	34.83
11	3.08574	3.52702	35.90	37.92	37.27	37.73	38.35
12	3.07879	3.51751	35.91	36.61	35.81	36.28	36.40
13	3.08397	3.53019	35.95	37.35	36.48	37.90	37.82
14	3.07960	3.52920	36.20	36.41	36.19	37.48	36.79
15	3.08016	3.52216	36.40	36.89	36.67	36.84	36.98
16	3.08235	3.52007	36.60	37.50	36.92	36.80	37.71
17	3.07950	3.52560	36.65	36.58	36.51	37.12	36.77
18	3.08677	3.52573	36.79	38.19	37.24	37.68	38.63
19	3.08190	3.52460	36.93	37.24	37.73	37.20	37.51
20	3.08746	3.52588	37.02	38.30	37.20	37.75	38.74
21	3.08620	3.52702	37.10	38.01	37.69	37.76	38.44
22	3.08390	3.52450	37.20	37.69	38.05	37.35	38.06
23	3.08054	3.52390	37.50	36.93	37.59	37.03	37.11
24	3.08657	3.52702	37.80	38.07	37.73	37.79	38.50
25	3.08430	3.52810	37.90	37.57	37.87	37.73	38.00
26	3.08520	3.52350	37.97	38.01	38.15	37.35	38.42
27	3.08520	3.52020	38.00	38.13	37.99	37.03	38.56
28	3.08570	3.52340	38.00	38.11	38.07	37.38	38.54
29	3.08450	3.52100	38.00	37.96	38.17	37.05	38.34
30	3.08550	3.52550	38.00	37.97	38.32	37.56	38.39
31	3.08082	3.52420	38.10	36.99	37.84	37.08	37.20
32	3.08500	3.52380	38.15	37.96	38.20	37.36	38.36
33	3.08180	3.52250	38.35	37.30	38.27	36.99	37.52
34	3.08098	3.52350	38.40	37.06	38.05	37.03	37.25
35	3.08770	3.52140	38.50	38.56	38.34	37.33	39.10
36	3.08570	3.52800	38.61	37.85	38.10	37.82	38.28
37	3.08220	3.52440	38.63	37.27	38.25	37.21	37.60
38	3.08380	3.53900	38.67	36.47	38.49	38.75	37.24
39	3.08330	3.52440	38.74	37.57	38.53	37.29	37.91
40	3.08140	3.52770	38.75	36.95	38.15	37.47	37.31
41	3.08420	3.52570	38.76	37.70	38.78	37.49	38.08
42	3.08890	3.53390	38.76	37.85	38.65	38.64	38.18
43	3.08320	3.52390	38.77	37.57	38.68	37.24	37.89
44	3.08410	3.52530	38.80	37.70	38.72	37.44	38.08
45	3.08400	3.52540	38.80	37.67	38.72	37.44	38.05
46	3.08620	3.52710	38.80	38.00	37.81	37.77	38.43
47	3.08400	3.52600	38.81	37.69	38.72	37.50	38.02
48	3.08450	3.52590	38.82	37.75	38.78	37.53	38.15
49	3.08440	3.52530	38.82	37.76	38.75	37.46	38.15
50	3.08530	3.52610	38.82	37.90	38.59	37.61	38.31
51	3.08580	3.52620	38.82	37.98	38.26	37.65	38.41
52	3.08420	3.52520	38.85	37.72	38.70	37.44	38.11
53	3.08500	3.52560	39.00	37.86	38.80	37.54	38.27
54	3.08520	3.52570	39.12	37.90	38.75	37.56	38.31
55	3.08286	3.52260	39.40	37.54	39.01	37.08	37.83
56	3.08429	3.52230	39.70	37.87	39.13	37.16	38.24
Root Mean Square Difference (RMSD)	-	-	-	3.20	1.04	4.64	2.61
Mean Bias Difference (MBD)	-	-	-	-0.82	0.00	0.00	0.05

Note: “a (A°)” and “c (A°)” are lattice parameters of MgB₂ superconductors. “Reference” shows sources of all experimental data in (Zhang and Xu, 2020).

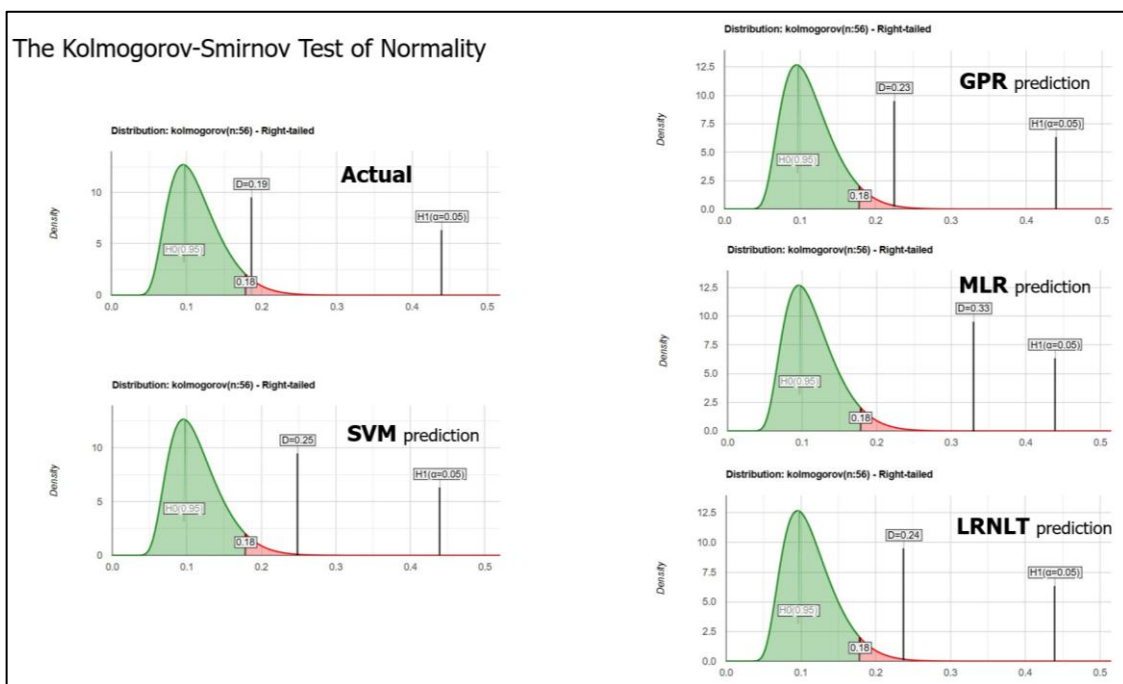


Figure 2. Superconducting transition temperature predictions by SVM, GPR, MLR and LRNL

Table 2. The correlation data of experimental T_c (K) through variations of lattice parameters “a ($\text{\AA}$)” and “c ($\text{\AA}$)”

		Lattice a	Lattice c	T_c	SVM	GPR	MLR	LRNL
Lattice_a	Pearson Correlation	1	-.994**	-.671**	-.649**	-.687**	-.931**	-.728**
	Sig. (2-tailed)		.000	.000	.000	.000	.000	.000
	N	56	56	56	56	56	56	56
Lattice_c	Pearson Correlation	-.994**	1	.695**	.657**	.712**	.965**	.754**
	Sig. (2-tailed)	.000		.000	.000	.000	.000	.000
	N	56	56	56	56	56	56	56
T_c	Pearson Correlation	-.671**	.695**	1	.892**	.988**	.721**	.921**
	Sig. (2-tailed)	.000	.000		.000	.000	.000	.000
	N	56	56	56	56	56	56	56
SVM	Pearson Correlation	-.649**	.657**	.892**	1	.924**	.644**	.966**
	Sig. (2-tailed)	.000	.000	.000		.000	.000	.000
	N	56	56	56	56	56	56	56
GPR	Pearson Correlation	-.687**	.712**	.988**	.924**	1	.740**	.953**
	Sig. (2-tailed)	.000	.000	.000	.000		.000	.000
	N	56	56	56	56	56	56	56
MLR	Pearson Correlation	-.931**	.965**	.721**	.644**	.740**	1	.782**
	Sig. (2-tailed)	.000	.000	.000	.000	.000		.000
	N	56	56	56	56	56	56	56
LRNL	Pearson Correlation	-.728**	.754**	.921**	.966**	.953**	.782**	1
	Sig. (2-tailed)	.000	.000	.000	.000	.000	.000	
	N	56	56	56	56	56	56	56

** . Correlation is significant at the 0.01 level (2-tailed).

Table 3. Analysis of variance (ANOVA): “SVM Estimated TC (K)”, “GPR Estimated TC(K)”, “MLR Estimated TC(K)” and “LRNLT Estimated TC(K)”

Anova: Two-Factor						
Source of Variation	SS	df	MS	F	P-value	F crit
Rows (different types of dopants)	1201.3407	55	21.8425575	29.849994	4.499E-76	1.39312079
Columns (different types of models)	4.3624235	4	1.09060587	1.4904197	0.2060519	2.41268204
Error	160.98371	220	0.73174412			
Total	1366.6868	279				

t-Test: Paired Two Sample for Means			t-Test: Paired Two Sample for Means		
	SVM	Actual		GPR	Actual
Mean	36.895	37.20178571	Mean	37.20178571	37.20178571
Variance	4.06481818	6.315887662	Variance	5.751076753	6.315887662
Observations	56	56	Observations	56	56
Pearson Correlation	0.89187119		Pearson Correlation	0.98848401	
Hypothesized Mean Difference	0		Hypothesized Mean Difference	0	
df	55		df	55	
t Stat	-1.9812098		t Stat	4.87026E-15	
P(T<=t) one-tail	0.02628804	Non-Sign.	P(T<=t) one-tail	0.5	Non-Sign.
t Critical one-tail	1.67303397		t Critical one-tail	1.673033965	
P(T<=t) two-tail	0.05257608		P(T<=t) two-tail	1	
t Critical two-tail	2.00404478		t Critical two-tail	2.004044783	

	MLR	Actual		LRNLT	Actual
Mean	37.20178408	37.20178571	Mean	37.22069591	37.20178571
Variance	3.277638671	6.315887662	Variance	5.360112753	6.315887662
Observations	56	56	Observations	56	56
Pearson Correlation	0.720382954		Pearson Correlation	0.921102146	
Hypothesized Mean Difference	0		Hypothesized Mean Difference	0	
df	55		df	55	
t Stat	-7.03457E-06		t Stat	0.144632233	
P(T<=t) one-tail	0.499997206	Non-Sign.	P(T<=t) one-tail	0.442764972	Non-Sign.
t Critical one-tail	1.673033965		t Critical one-tail	1.673033965	
P(T<=t) two-tail	0.999994413		P(T<=t) two-tail	0.885529943	
t Critical two-tail	2.004044783		t Critical two-tail	2.004044783	

Figure 3. t-Test: Paired Two Sample for Means of “SVM Estimated T_c(K)”, “GPR Estimated T_c(K)”, “MLR Estimated T_c(K)” and “LRNLT Estimated T_c(K)”

To determine the statistical importance of changes in modeling techniques, investigations must be able to consistently distinguish between systematic approach impacts and mistakes caused by modeling approach variance. In this study, we use analysis of variance (ANOVA) to determine the statistical significance of differences in modeling technique variation.

Data visualization in Table 1 reveals relationships, which are modeled through the magnesium bromide modeling technique variation data as presented in Figure 1. Before the analysis of variance, we used the Kolmogorov-Smirnov test to check the normality of the set of raw data, which comes from each modeling approach in Figure 2.

The graph in Figure 2 shows the test maximum statistic D of “SVM Estimated T_c(K)”, “GPR Estimated T_c(K)”, “MLR Estimated T_c(K)” and “LRNLT Estimated T_c(K)” equals 0.25, 0.23, 0.33 and 0.24, respectively, which had a trend lower than the critical test maximum statistic D, which equals 0.18. In those results, it was assumed that the data distribution was normal. In other words, the

difference between the raw data sample and the normal distribution was big enough to be statistically significant. For this reason, the raw data sample was the ANOVA under elements of the parametric statistical model Siegel, 1956).

In Table2 and Table3, ANOVA and correlation coefficient between variations of lattice parameters c, a and critical temperature T_c were highly significant at the 0.01 level. For MgB₂ without foreign ions, the lattice parameter c is of great interest as it is very sensitive to the change in the oxygen content and both electron and hole concentration. This reason correspond with Liang *et al.* (2006) evaluate both electron and hole concentration p in the CuO₂ planes by using the lattice parameter c, with a simple estimation of p in the chain oxygen-ordered phases. In other words, the empirical relationship between c and p allows for the calculation of p from c for the entire doping range of MgB₂ (Liang *et al.* 2006).

The comparisons of obtained results with MgB₂ modeling approach by using t-Test: Paired Two Sample for Means as presented in Figure 3.

Conclusions

The application of ANOVA to assess the statistical significance of differences in modeling approach variation is developed to predict doped MgB_2 superconductor transition temperature based on lattice parameters. The high correlation coefficient between the predicted and experimental superconducting transition temperature, the low prediction root mean square difference and mean bias difference, and the outstanding efficiency of the ANOVA results suggest the usefulness of the ANOVA for modeling and understanding the relationship between lattice parameters and superconducting transition temperature.

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