

THE APPLICATION OF ANALYSIS OF VARIANCE TO DIFFERENT YTTRIUM BARIUM COPPER OXIDE SUPERCONDUCTING TRANSITION TEMPERATURE MODELING

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Abstract

Extensive research has been conducted on a modeling approach that contributes to predicting the critical temperature of Yttrium barium copper oxide (YBCO) materials. Statistical significance of differences in modeling approaches requires studies that can reliably distinguish between systematic approach effects and errors resulting from modeling approach variation. In this work, we introduce analysis of variance (ANOVA) to assess the statistical significance of differences in modeling approach variation. Comparisons of obtained results with YBCO modeling approach variation data of support vector machine (SVM) and linear regression with natural logarithm transformation (LRNLT) were presented.

Keywords: Analysis of variance (ANOVA); Critical temperature; Statistical significance; YBCO superconductors

Introduction

YBCO superconductors are of particular interest as they can be coated on a mechanically-strong Ni-alloy substrate and carry very high critical current densities (Gou and Schwartz, 2013).

Furthermore, the quality and stability of a superconducting magnet depends greatly on T_c . When temperature in the conductor rises locally near or above T_c , the superconductivity in this zone is lost and the material enters the normal state, which incurs the Ohmic heating in this normal zone. The failure to dissipate the heat results in normal

zone propagation through the entire magnet, which eventually terminates the magnet operation (Yildiz, 2013; Huang and Chen, 2015). Thus, various methods have been developed by researchers to improve T_c of YBCO superconductors, one of which is through chemical substitution and doping (Faisal and Al-Ani, 2013; Huang and Chen, 2015). Because different ions, e.g., Al, Ca, Mg, Fe, Ni, Sb, and Hf have different effects on the YBCO superconducting state and the situation becomes more complicated when multiple sites are partially or fully substituted

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(Lin *et al.*, 1991; Elsabawy, 2005; 2011; Ben Azzouz *et al.*, 2006; 2007; Mohanta and Behera, 2009; Varshney *et al.*, 2011; Faisal and Al-Ani, 2013). Therefore, the superconducting transition temperature with respect to foreign ionic substitutions, isovalent or heterovalent, carrier concentration, oxygen octahedron around Cu^{2+} , influence the charge transfer from the Cu-O chains to conducting CuO_2 planes and changing the lattice parameters a ($\text{\AA}$), b ($\text{\AA}$), c ($\text{\AA}$). Mellekh *et al.* (2006) find that the lattice parameters a ($\text{\AA}$) and c ($\text{\AA}$) increase with Al_2O_3 additions while b ($\text{\AA}$) remains almost constant, when Al is incorporated into the crystal structure and occupies both Cu(1) and Y sites. The rearrangement of oxygen in the basal plane, due to the replacement of bivalent Cu^{2+} ions by trivalent Al^{3+} ions, affects T_c in a nonmonotonic way (Mellekh *et al.*, 2006).

Shang *et al.* (2010) explain differences in T_c of Fe- and Mn- co-doped YBCO samples by correlating the incorporation of Fe and Mn cations

into the Cu-O chain with the increased Cu(2)-O(4) bond length, which causes the localization of carriers on Cu-O chains. The increase in the Cu(2)-O(4) bond length is reflected in that in the lattice parameter c ($\text{\AA}$), which is the sum of bond lengths, i.e. c ($\text{\AA}$) = $2d_{\text{Cu}(1)\text{O}4} + d_{\text{Cu}(2)-\text{Cu}(2)} + 2d_{\text{Cu}(2)-\text{O}(4)}$. Attaf *et al.* (2012) observe decreases in all lattice parameters and the orthorhombicity by adding 2% Mg, which are attributed to the reduction of the local Jahn Teller distortion and the difference in ionic radii of Mg^{2+} and Cu^{2+} . Tokura *et al.* (1988) and Buckley (1991) find that the Ca-doped YBCO, crystal structure analysis reveals that such a substitution leads to a decrease in the orthorhombicity of the system, which is correlated with an increase of the density of states and eventually the c suppression. So, it is of great importance to investigate the correlation between lattice parameters a ($\text{\AA}$), b ($\text{\AA}$), c ($\text{\AA}$) and T_c , which are much easier to determine experimentally as compared to other physical parameters. However,

Table1. The experimental $T_c(\text{K})$ data and superconducting transition temperature predictions from “SVM estimated $T_c(\text{K})$ ”, “LRNLT estimated $T_c(\text{K})$ ” and “LRNLT (C.F.) estimated $T_c(\text{K})$ ”

Index	Sample	a ($\text{\AA}$)	b ($\text{\AA}$)	c ($\text{\AA}$)	Experimental $T_c(\text{K})$	SVM estimated $T_c(\text{K})$	LRNLT estimated $T_c(\text{K})$	LRNLT (C.F.) estimated $T_c(\text{K})$
1	$\text{Y}_{1.00}\text{Ba}_2\text{Cu}_{2.76}\text{Co}_{0.21}\text{O}_{6.6}$	3.8740	3.8740	11.7250	35.00	38.69	52.28	34.68
2	$\text{Y}_{1.02}\text{Ba}_2\text{Cu}_{3.0}\text{Co}_{0.06}\text{O}_{6.3}$	3.8678	3.8678	11.7740	67.00	66.80	60.57	65.35
3	$\text{Y}_{0.99}\text{Ba}_2\text{Cu}_{3.0}\text{Co}_{0.07}\text{O}_{6.4}$	3.8684	3.8684	11.7720	67.00	67.11	59.72	63.32
4	$\text{Y}_{0.6}\text{Hf}_{0.4}\text{Ba}_2\text{Cu}_3\text{O}_z$	3.8004	3.8160	11.5631	71.60	75.56	74.26	80.82
5	$\text{Y}_{0.5}\text{Bi}_{0.5}\text{Ba}_2\text{Cu}_3\text{O}_y$	3.8610	3.8610	11.5870	77.00	76.82	72.79	80.10
6	$\text{Y}_{0.9}\text{Ca}_{0.1}\text{Ba}_2(\text{Cu}_{0.99}\text{Ni}_{0.01})\text{O}_{7-y}$	3.8289	3.8864	11.6372	81.00	81.30	82.97	83.90
7	$\text{Y}_{0.4}\text{Sb}_{0.6}\text{Ba}_2\text{Cu}_3\text{O}_z$	3.7712	3.7364	11.5127	81.60	81.90	79.24	82.69
8	$\text{Y}_{0.8}\text{Ca}_{0.2}\text{Ba}_2\text{Cu}_3\text{O}_{7-y}$	3.8369	3.8784	11.7365	82.00	79.91	78.24	82.36
9	$\text{Y}_{0.6}\text{Sb}_{0.4}\text{Ba}_2\text{Cu}_3\text{O}_z$	3.7904	3.7762	11.5131	82.70	82.64	82.27	83.67
10	$\text{Y}_{0.9}\text{Ca}_{0.1}\text{Ba}_2\text{Cu}_3\text{O}_{7-y}$	3.8328	3.8764	11.7484	83.00	83.94	83.41	84.05
11	$\text{Y}_{0.8}\text{Sb}_{0.2}\text{Ba}_2\text{Cu}_3\text{O}_z$	3.8033	3.7902	11.5591	83.10	82.80	93.40	88.66
12	$\text{YBa}_2(\text{Cu}_{0.95}\text{Zn}_{0.05-x}\text{Ga}_x)_3\text{O}_{7-y}; x=0$	3.8293	3.8864	11.6832	83.50	85.56	83.79	84.18
13	$\text{Y}_{0.9}\text{Sb}_{0.1}\text{Ba}_2\text{Cu}_3\text{O}_z$	3.8178	3.8163	11.6131	84.40	85.86	89.96	86.71
14	YBCO (0.6% of Al_2O_3 doped)	3.8370	3.8810	11.7000	85.00	80.12	75.60	81.39
15	YBCO (0.5% of Al_2O_3 doped)	3.8300	3.8830	11.6940	86.00	85.60	82.28	83.67
16	YBCO (0.4% of Al_2O_3 doped)	3.8270	3.8850	11.6940	87.00	87.25	86.28	85.09
17	$\text{Y}_{0.8}\text{Hf}_{0.2}\text{Ba}_2\text{Cu}_3\text{O}_z$	3.8133	3.8392	11.6013	87.10	82.05	77.86	82.23
18	YBCO (0.3% of Al_2O_3 doped)	3.8260	3.8850	11.6920	87.50	87.83	87.20	85.46
19	$\text{Y}_{0.9}\text{Hf}_{0.1}\text{Ba}_2\text{Cu}_3\text{O}_z$	3.8398	3.8463	11.6631	88.40	88.03	79.42	82.75
20	YBCO-un-doped	3.8273	3.8882	11.6859	88.70	86.43	87.13	85.43
21	YBCO (0.2% of Al_2O_3 doped)	3.8240	3.8850	11.6890	89.00	93.15	89.14	86.32
22	$\text{YBa}_2\text{Cu}_3\text{O}_{7-y}$	3.8067	3.8821	11.6789	89.00	88.84	105.37	99.81
23	YBCO (0.0% of Al_2O_3 doped)	3.8210	3.8840	11.6860	90.00	90.27	91.53	87.54
24	$\text{YBa}_2\text{Cu}_3\text{O}_y$	3.8230	3.8850	11.6820	91.00	89.01	89.66	86.56
25	$\text{YBa}_2\text{Cu}_3\text{O}_7$	3.8234	3.8662	11.7941	91.88	91.82	101.01	94.88
26	$\text{YBa}_2\text{Cu}_{2.955}\text{Al}_{0.045}\text{O}_{6.5+y}$	3.8354	3.8813	11.4948	92.00	95.04	92.91	88.36
27	$\text{YBa}_2\text{Cu}_3\text{O}_7$	3.8234	3.8662	11.6631	92.56	90.96	80.27	83.03
28	$\text{YBa}_2\text{Cu}_{2.97}\text{Al}_{0.03}\text{O}_{6.5+y}$	3.8203	3.8855	11.4835	95.00	104.25	106.04	100.66
29	$\text{YBa}_2\text{Cu}_{2.98}\text{Al}_{0.02}\text{O}_{6.5+y}$	3.8203	3.8855	11.4835	102.00	104.25	106.04	100.66
30	$\text{YBa}_2\text{Cu}_{2.99}\text{Al}_{0.01}\text{O}_{6.5+y}$	3.8202	3.8854	11.4837	108.00	104.12	105.94	100.54
31	$\text{YBa}_2\text{Cu}_3\text{O}_{6.5+y}$	3.8200	3.8855	11.4835	116.00	104.31	106.21	100.88
Mean		3.8261	3.8264	11.6380	85.32	85.23	85.25	84.38
Maximum		3.8704	3.8882	11.7941	116.00	104.31	106.21	100.88
Minimum		3.7712	3.7364	11.4835	35.00	38.69	52.28	34.68
Standard deviation		0.0214	0.0375	0.0968	13.67	12.72	13.61	12.65
Variance		0.0005	0.0014	0.0093	186.1925	161.8884	185.2749	160.2065
Correlation with experimental $T_c(\text{K})$		-0.470	0.196	-0.463	-	-	-	-
Root Mean Square Difference (RMSD)		-	-	-	-	4.06	8.41	6.08
Mean Bias Difference (MBD)		-	-	-	-	-0.11	-0.08	-1.11

Note: “ a ($\text{\AA}$)”, “ b ($\text{\AA}$)” and “ c ($\text{\AA}$)” are lattice parameters of YBCO superconductors. “Reference” shows sources of all experimental data in (Owolabi *et al.*, 2016).

Lattice parameters, processing parameters, compositions, and other physical parameters have been utilized to predict T_C of several superconducting materials, such as MgB_2 , Fe-based superconductors, $BiPbSrCaCuOF$, and YBCO films, through different computational techniques models (Cai *et al.*, 2010; 2013; Owolabi *et al.*, 2014; 2015; Hamidieh, 2018).

Therefore, the success of computational techniques directly relate to the lattice parameters a ($^\circ$), b ($^\circ$), c ($^\circ$) and the T_C paves a significant way for quick and accurate estimation of T_C of doped YBCO superconductor and eventually eases the usual highly demanding experimental procedures that involve the use of expensive cryostat (Owolabi *et al.*, 2016).

In this work, we directly relate the lattice parameters a ($^\circ$), b ($^\circ$) and c ($^\circ$) to the T_C (K) through computational techniques. Because, most of variations in T_C are reflected through or correlated with lattice distortions (Zhang and Xu, 2020). So in this research, we introduced the idea to illustrate blocking between variance of computational techniques, which can be partitioned, so-called ANOVA (Krzywinski and Altman, 2014).

For data source by (Owolabi *et al.*, 2016) in Table 1, we developed the predictor variable coefficients (lattice parameters a ($^\circ$), b ($^\circ$), c ($^\circ$)) through different modeling or computational techniques to estimate the superconducting transition temperature (T_C (K)). Under these different modeling, between group variation of modeling means and within group variation of modeling, values are predictably related.

By using analysis of variance (ANOVA) to assess the statistical significance of differences in modeling approach variation. To demonstrate the outstanding efficiency of the ANOVA results. The comparisons of obtained results with YBCO modeling approach variation data of support vector machine (SVM) and linear regression with natural logarithm transformation (LRNLT) were presented.

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.

YBCO Superconductors

YBCO superconductor having high T_C indicates that little effort is to be done before putting it into applications. Adequate understanding of their charge reservoir layer and the mechanism of charge transfer is required for improving their superconducting transition temperature (Behera *et al.*, 1997). Incorporation of dopants such as B, Ce, Al, Ca, Ag, and Ni among others into the CuO_2 planes weakens the antiferromagnetic ordering. The concentration of holes in CuO_2 planes as well as the level of the charge of oxygen within the plane contribute enormously to the value of the T_C of this superconducting materials (Ben Azzouz *et al.*, 2006). Meanwhile, ionic substitution has been established as one of the ways of controlling the level of the charge of oxygen within the planes (Ben Azzouz *et al.*, 2006) and affects the T_C as a result of the strain and disorder created by the dopants in the lattice (Paturi *et al.*, 2012). Variations in T_C can be caused by multiple mechanisms, most of which are reflected through or correlated with lattice distortions. Therefore, it is of great importance to investigate the correlation between T_C and lattice parameters, which are much easier to determine

experimentally as compared to other physical parameters.

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 YBCO modeling between support vector machine (SVM) and adopting a simple model (linear regression) through which they developed by using natural logarithm transformation (LRNLT) approach. In addition, the outstanding performance of ANOVA leads to the creation of an optimization correction factor (C.F.) for simple models.

Working principle of SVM

SVM stems from supporting 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 $K\langle x_i, x \rangle$.

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

where $\lambda_i^* \geq 0$, $\lambda_i^* \leq C$, $K\langle x_i, x \rangle$ 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 (Goldman *et al.*, 1977; Diaconis and Efron, 1983; Efron and Gong, 1983). However, in addition to the concepts discussed so far for simple linear regression, which remain applicable, new concepts must be introduced. This discussion will focus on situations where there are two predictors and one outcome variable. With all three variables, a three-

dimensional figure can be used to visualize data. Models with more predictive variables follow the same principle but are difficult to visualize. We consider multiple regression and linear relation as follows,

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

in which,

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

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

We develop a multiple linear regression model to predicting the critical temperature of crystal structures of YBCO materials 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, $u = \ln(U)$

Performance Evaluation

Performance of obtained results with YBCO 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 Equations (5)-(7) 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 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 YBCO modeling approach variation data, respectively.

$$RMSD = \frac{\sqrt{\sum_{i=1}^N (T_i^{Model} - T_i^{Exp})^2}}{\sum_{i=1}^N T_i^{Exp}} \times 100 \quad (5)$$

$$MBD = \frac{\sum_{i=1}^N (T_i^{Model} - T_i^{Exp})}{\frac{\sum_{i=1}^N T_i^{Exp}}{N}} \times 100 \quad (6)$$

$$r_{XY} = \frac{\sum_{i=1}^N (X_i - \bar{X})(Y_i - \bar{Y})}{\sqrt{\sum_{i=1}^N (X_i - \bar{X})^2} \sqrt{\sum_{i=1}^N (Y_i - \bar{Y})^2}} \quad (7)$$

Results and Discussion

The experimental data used, shown in Table 1 are obtained from (Owolabi *et al.*, 2016). This dataset contains lattice parameters obtained when dopants, such as aluminum, boron, calcium, cerium, cobalt, nickel, and silver, are incorporated into the lattice structure of the parent compound YBCO superconductor. Superconducting transition temperature is affected by incorporated dopants and the effects manifest through variations of lattice parameters along a, b, and c axes. Data visualization in Table 1 reveals nonlinear relationships, which are modeled through the SVM from Equation (1) and LRNLTL from Equation (4) 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 Tables 2 and 3, respectively.

In Tables 2 and 3, ANOVA and correlation coefficient between variations of lattice parameters c, a, and critical temperature T_c were highly significant at the 0.01 level. Because of parent compounds of all high T_c cuprates are antiferromagnetic insulators, where the CuO_2 plane $\text{Cu } d_{x^2 - y^2}$ orbital is exactly half filled. High T_c superconductivity occurs as a result of weakened antiferromagnetic orderings when holes are doped

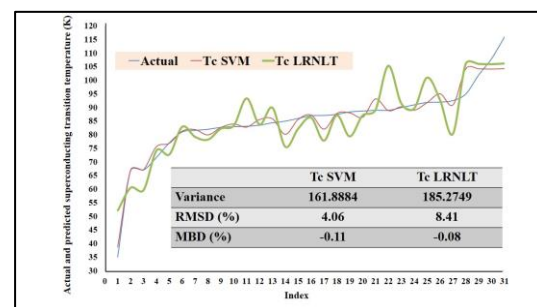


Figure 1. Superconducting transition temperature predictions by SVM and LRNLTL

Table 2. Analysis of variance (ANOVA): “experimental $T_c(K)$ ”, “SVM estimated $T_c(K)$ ” and “LRNLTL estimated $T_c(K)$ ”

Anova : Single Factor						
SUMMARY						
Groups	Count	Sum	Average	Variance		
Experimental T _C (K)	31	2645.040	85.32387	186.8925		
SVM estimated T _C (K)	31	2642.220	85.23290	161.8884		
LRNLT estimated T _C (K)	31	2642.793	85.25140	185.2749		
ANOVA						
Source of Variation	SS	df	MS	F	P-value	F crit
Between groups	0.14332	2	0.07166	0.000403	0.999598	3.097698
Within groups	16021.68	90	178.0186			
Total	16021.82	92	174.1502			

Table 3. The correlation data of experimental T_c (K) through variations of lattice parameters “a ($^\circ$)”, “b ($^\circ$)” and “c ($^\circ$)”

		a ($^\circ$)	b ($^\circ$)	c ($^\circ$)	Experimental $T_c(K)$
a ($^\circ$)	Pearson Correlation	1	0.579**	0.533**	-0.470**
	Sig. (2-tailed)		.001	.002	.008
	N	31	31	31	31
b ($^\circ$)	Pearson Correlation	0.579**	1	0.348	0.196
	Sig. (2-tailed)	0.001		0.055	0.291
	N	31	31	31	31
c ($^\circ$)	Pearson Correlation	0.533**	0.348	1	-0.463**
	Sig. (2-tailed)	0.002	0.055		0.009
	N	31	31	31	31
Experimental $T_c(K)$	Pearson Correlation	-0.470**	0.196	-0.463**	1
	Sig. (2-tailed)	0.008	0.291	0.009	
	N	31	31	31	31

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

into planes. For YBCO 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 CuO_2 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 YBCO (Liang *et al.*, 2006). So, we can formulate an optimization correction factor of LRNLT model as follows

$$\ln(y) = \ln(a) + bx + u = A \quad (8)$$

For change in A , rewrite the optimization correction factor from LRNLT model as

$$y = e^A \rightarrow y = e^{\ln(CF \cdot A^2)} \quad (9)$$

in which $C.F.$ is the correction factor.

The creation of an optimization correction factor by using 4th degree polynomial regression forms as follows,

$$CF = -14.059x^4 + 722.1x^3 - 7875.2x^2 + 35170x - 45262 \quad (10)$$

in which, $x = A = \ln(y) = \ln(a) + bx + u$

LRNLT from the creation of an optimization correction factor LRNLT (C.F.) and ANOVA as presented in Figure 2 and Table 4, respectively.

The comparisons of obtained results with YBCO modeling approach by using t-Test as presented in Table 5.

By assigning within group variance was interpreted as experimental error causing the variations in the superconducting transition temperature, i.e. valence fluctuation in Cu ions, superexchange mechanism (O'Mahony *et al.*, 2022), oxygen vacancies, oxygen hole content, charge-transfer gap (Kowalski *et al.*, 2021), types of dopants, type of ionic dopant etc. They are not included in between group variance as predictor variable coefficients through different lattice parameters a ($\text{\AA}$), b ($\text{\AA}$), c ($\text{\AA}$) to estimate the

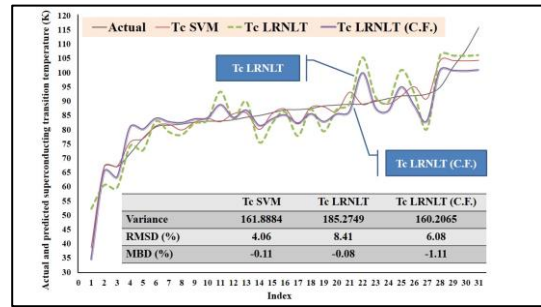


Figure 2. Superconducting transition temperature predictions by LRNLT and LRNLT (C.F.)

Table 4. Analysis of variance (ANOVA): “Experimental T_c (K)”, “SVM estimated T_c (K)” and “LRNLT (C.F.) estimated T_c (K)”

Anova : Single Factor						
SUMMARY						
Groups	Count	Sum	Average	Variance		
Experimental T _c (K)	31	2645.040	85.32387	186.8925		
SVM estimated T _c (K)	31	2642.220	85.23290	161.8884		
LRNLT (C.F.) estimated T _c (K)	31	2615.767	84.37957	160.2065		
ANOVA						
Source of Variation	SS	df	MS	F	P-value	F crit
Between groups	16.82411	2	8.412054	0.049581	0.951654	3.097698
Within groups	15269.62	90	169.6625			
Total	15286.45	92	166.1570			

Table 5. t-Test: Two-sample assuming equal variances

Two-Sample	Pooled Variance	t Stat	df	HMD	t crit
Experimental T_C (K) VS SVM estimated T_C (K)	174.3904	0.0271	60	0	1.6706
Experimental T_C (K) VS LRNLT estimated T_C (K)	186.0837	0.0209			
Experimental T_C (K) VS LRNLT (C.F.) estimated T_C (K)	173.9495	0.2822			
SVM estimated T_C (K) VS LRNLT estimated T_C (K)	173.5816	0.0055			
SVM estimated T_C (K) VS LRNLT (C.F.) estimated T_C (K)	161.0474	0.2647			

Note: t-Test: Two-Sample Assuming Equal Variances at significance level of 0.05, Hypothesized Mean Difference (HMD)

superconducting transition temperature. But these factors are included within group variation of modeling in the ANOVA approach.

The contribution of the block effect to illustrate blocking of variances is shown in Tables 2 and 4, now a substantial component of the variance in each computational technique. ANOVA owing to computational technique by LRNLTL (C.F.) estimated T_C (K) has distribution of variance lower LRNLTL estimated T_C (K) correspond with decreased of RMSD. This result explains that the development of the LRNLTL estimated T_C (K) became LRNLTL (C.F.) estimated T_C (K) with the ANOVA makes the model more accurate near to the famous model, as SVM estimated T_C (K).

The reason ANOVA makes the model more accurate is because the result of ANOVA leads to the analysis contribution of the block effect to the deviations. By using correlation analysis and multiple regression analysis with block effect of the deviations in Table 3, it leads to a correlation factor (C.F.) of LRNLTL (C.F.) estimated T_C (K) in Equation (10), which causes a decrease in RMSD. To confirm the efficiency of ANOVA, it can reduce the distribution of variance, leading to the model being more accurate for development of the LRNLTL model, corresponding with a decrease in RMSD until near to the famous model. ANOVA can be used to test the efficiency between two models from different computational techniques, which can be done using test statistic t as shown in Table 5. The (pooled) variance is the lowest when compared to both the experimental T_C (K) and SVM estimated T_C (K), respectively, at a significant level of 0.05.

Although the application of ANOVA to develop a simple model (LRNLTL) with similar performance to a complex model (SVM) succeeds in reducing the value of RMSD. But the superconducting transition temperature mean (average) between experimental T_C (K) and LRNLTL (C.F.) estimated T_C (K) is more than different compared to the superconducting transition temperature mean between experimental T_C (K) and SVM estimated T_C (K). We assume that such a difference may cause the RMSD of LRNLTL (C.F.) estimated T_C (K) to deviate from experimental T_C (K) rather than SVM estimated T_C (K).

Since, in the view of parametric statistics, ANOVA uses means as representative of the raw data set to analyze variance. Such methods may cause the analysis of variance to be influenced by raw data with very large or very small value. Therefore, we propose to combine the median together with ANOVA under the concept of nonparametric statistics. To reduce the influence of extreme raw data and increase the likelihood of

RMSD has decreased, until it is close to SVM for next times.

Conclusions

The application of ANOVA to assess the statistical significance of differences in modeling approach variation is developed to predict doped yttrium barium copper oxide 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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References

- Armstrong, R.A., Eperjesi, F., and Gilmartin, B. (2002). The application of analysis of variance (ANOVA) to different experimental designs in optometry. *Ophthalmic and Physiological Optics*, 22:248-256. <https://doi.org/10.1046/j.1475-1313.2002.00020.x>.
- Attaf, S., Mosbah, M.F., Fittipaldi, R., Zola, D., Pace, S., and Vecchione, A. (2012). Effect of double substitution on structural and magnetic properties of $Y_{1-x}Ca_xBa_2(Cu_{1-y}Mg_y)_2O_{7-\delta}$. *Physica C: Superconductivity*, 477:36-42. <https://doi.org/10.1016/j.physc.2012.02.031>.
- Behera, D., Mishra, N.C., and Patnaik, K. (1997). Ag-Doping-Induced Coordination Inco patibility and Its Effect on SupercenductMty in YBCO. *Journal of Superconductivity*, 10(1):27-32. <https://doi.org/10.1007/BF02763947>.
- Ben Azzouz, F., Zouaoui, M., Mani, K.D., Annabi, M., Van Tendeloo, G., and Ben Salem, M. (2006). Structure, microstructure and transport properties of B-doped YBCO system. *Physica C: Superconductivity and its Applications*, 442(1):13-19. <https://doi.org/10.1016/j.physc.2006.03.135>.
- Ben Azzouz, F., Zouaoui, M., Mellekh, A., Annabi, M., Van Tendeloo, G., and Ben Salem, M. (2007). Flux pinning by Al-based nanoparticles embedded in YBCO: A transmission electron microscopic study. *Physica C: Superconductivity and its Applications*, 455(1-2):19-24. <https://doi.org/10.1016/j.physc.2007.01.033>.
- Buckley, R.G., Pooke, D.M., Tallon, J.L., Presland, M.R., Flower, N.E., Staines, M.P., Johnson, H.L., Meylan, M., Williams, G.V.M., and Bowden, M. (1991). Ca- and La-substitution in $YBa_2Cu_3O_{7-\xi}$, $Y_2Ba_4Cu_7O_{15-\xi}$ and

- YBa₂Cu₄O₈. *Physica C: Superconductivity*, 174(4-6):383-393. [https://doi.org/10.1016/0921-4534\(91\)91574-N](https://doi.org/10.1016/0921-4534(91)91574-N).
- Cai, C.Z., Xiao, T.T., Tang, J.L., and Huang, S.J. (2013). Analysis of process parameters in the laser deposition of YBa₂Cu₃O₇ superconducting films by using SVR. *Physica C: Superconductivity*, 493:100-103. <https://doi.org/10.1016/j.physc.2013.03.038>.
- Cai, C.Z., Zhu, X.J., Wen, Y.F., Pei, J.F., Wang, G.L., and Zhuang, W.P. (2010). Predicting the superconducting transition temperature T_c of BiPbSrCaCuOF superconductors by using support vector regression. *Journal of Superconductivity and Novel Magnetism*, 23(5):737-740. <https://doi.org/10.1007/s10948-010-0732-x>.
- Cortes, C. and Vapnik, V. (1995). Support-vector networks. *Machine Learning*, 20:273-297. <https://doi.org/10.1007/BF00994018>.
- Diaconis, P. and Efron, B. (1983). Computer-intensive methods in statistics. *Scientific American*, 248:116-130. <https://doi.org/10.1038/scientificamerican0583-116>.
- Efron, B. and Gong, G. (1983). A leisurely look at the bootstrap, the jackknife, and cross-validation. *The American Statistician*, 37:36-48. <https://doi.org/10.1080/00031305.1983.10483087>.
- Elsabawy, K.M. (2005). Raman spectra, microstructure and superconducting properties of Sb (III)-YBCO composite superconductor. *Physica C: Superconductivity*, 432(3-4):263-269. <https://doi.org/10.1016/j.physc.2005.09.005>.
- Elsabawy, K.M. (2011). Superconductivity, structure visualization, mechanical strength promotion and Raman spectra of hafnium-doped-123-YBCO synthesized via urea precursor route. *Cryogenics*, 51(8):452-459. <https://doi.org/10.1016/j.cryogenics.2011.05.004>.
- Faisal, W.M. and Al-Ani, S.K. (2013). The influence of aluminum doping and oxygenation on the properties of YBa₂Cu_{3-x}Al_xO_{6.5-δ} (0 ≤ x ≤ 0.045) HTSC. *International Journal of Nanoelectronics and Materials*, 6:1-8.
- Goldman, L., Debra, M.P.H., Caldera, D.L., Nussbaum, S.R., Southwick, F.S., Krogstad, D., Murray, B., Burke, D.S., O'Malley, T.A., Goroll, A.H., Caplan, C.H., Nolan, J., Carabello, B., and Slater, E.E. (1977). Multifactorial index of cardiac risk in noncardiac surgical procedures. *The New England Journal of Medicine*, 297:845-850. <https://doi.org/10.1056/NEJM197710202971601>.
- Gou, X. and Schwartz, J. (2013). Fractal analysis of the role of the rough interface between Bi₂Sr₂CaCu₂O_x filaments and the Ag matrix in the mechanical behavior of composite round wires. *Superconductor Science and Technology*, 26(5):055016. <https://doi.org/10.1088/0953-2048/26/5/055016>.
- Hamidieh, K. (2018). A data-driven statistical model for predicting the critical temperature of a superconductor. *Computational Materials Science*, 154:346-354. <https://doi.org/10.1016/j.commatsci.2018.07.052>.
- Huang, H.-C. and Chen, Y.-C. (2015). Survey of bio-inspired computing for information hiding. *Journal of Information Hiding and Multimedia Signal Processing*, 6(3):430-443.
- Kowalski, N., Dash, S.S., Sémon, P., and Tremblay, A.-M. (2021). Oxygen hole content, charge-transfer gap, covalency, and cuprate superconductivity. *PNAS*, 118(40):e2106476118. <https://doi.org/10.1073/pnas.2106476118>.
- Krzywinski, M. and Altman, N. (2014). Analysis of variance and blocking. *Nature Methods*, 11(7):699-700. <https://doi.org/10.1038/nmeth.3005>.
- Liang, R., Bonn, D.A. and Hardy, W.N. (2006). Evaluation of CuO₂ plane hole doping in YBa₂Cu₃O_{6+x} single crystals. *Physical Review B*, 73(18):180505. <https://doi.org/10.1103/PhysRevB.73.180505>.
- Lin, C.T., Li, S.X., Zhou, W., Mackenzie, A., and Liang, W.Y. (1991). Cobalt-doped YBCO single crystals and their accurate characterisation. *Physica C: Superconductivity*, 176(1-3):285-294. [https://doi.org/10.1016/0921-4534\(91\)90725-E](https://doi.org/10.1016/0921-4534(91)90725-E).
- Mellekh, A., Zouaoui, M., Ben Azzouz, F., Annabi, M., and Salem, M.B. (2006). Nano-Al₂O₃ particle addition effects on YBa₂Cu₃O_y superconducting properties. *Solid State Communications*, 140(6):318-323. <https://doi.org/10.1016/j.ssc.2006.08.008>.
- Mohanta, A. and Behera, D. (2009). Effect of Ga and Zn doping on coherent transition of YBCO superconductor. *Indian Journal of Pure & Applied Physics*, 47:676-680.
- O'Mahony, S.M., Ren, W., Chen W., Chong, Y.X., Liu, X., Eisaki, H., Uchida, S., Hamidian, M.H., and Davis, J.C.S. (2022). On the electron pairing mechanism of copper-oxide high temperature superconductivity. *PNAS*, 119(37):e2207449119. <https://doi.org/10.1073/pnas.2207449119>.
- Owolabi, T.O., Akande, K.O. and Olatunji, S.O. (2014a). Prediction of superconducting transition temperatures for Fe-based superconductors using support vector machine. *Advances in Physics Theories and Applications*, 35:12-26.
- Owolabi, T.O., Akande, K.O. and Olatunji, S.O. (2015). Estimation of superconducting transition temperature T_c for superconductors of the doped MgB₂ system from the crystal lattice parameters using support vector regression. *Journal of Superconductivity and Novel Magnetism*, 28(1):75-81. <https://doi.org/10.1007/s10948-014-2891-7>.
- Owolabi, T.O., Akande, K.O. and Olatunji, S.O. (2016). Application of computational intelligence technique for estimating superconducting transition temperature of YBCO superconductors. *Applied Soft Computing*, 43:143-149. <http://dx.doi.org/doi:10.1016/j.asoc.2016.02.005>.
- Owolabi, T.O., Akande, K.O., and Olatunji, S.O. (2014b). Support vector machines approach for estimating work function of semiconductors: addressing the limitation of metallic plasma model. *Applied Physics Research*, 6(5):122-132. <https://doi.org/10.5539/apr.v6n5p122>.
- Paturi, P. Palonen, H., and Huhtinen, H. (2012). Properties of Pr- and BZO-doped YBCO multilayers. *Physics Procedia*, 36(100):661-664. <https://doi.org/10.1016/j.phpro.2012.06.263>.
- Shang, M., Feng, Q., Jiao, Y.L., Xiao, L., Zheng, M.H., Yan, Q.Z., and Ge, C.C. (2010). Optimization of the properties of codoped single-domain Y-Ba-Cu-O bulk superconductors. *Physica C: Superconductivity*, 470(11-12):491-495. <https://doi.org/10.1016/j.physc.2010.04.005>.
- Tokura, Y., Torrance, J.B., Huang, T.C., and Nazzari, A.I. (1988). Broader perspective on the high temperature superconducting YBa₂Cu₃O_y system: the real role of the oxygen content. *Physical Review B*, 38(10):7156-7159. <https://doi.org/10.1103/PhysRevB.38.7156>.
- Vapnik, V.N. (1995). *The Nature of Statistical Learning Theory*. 1st Ed. Springer New York, NY., 188p. <https://doi.org/10.1007/978-1-4757-2440-0>.
- Varshney, D., Yogi, A., Dodiya, N., and Mansuri, I. (2011). Alkaline earth (Ca) and transition metal (Ni) doping on the transport properties of Y_{1-x}Ca_xBa₂(Cu_{1-y}Ni_y)₃O_{7-δ} superconductors. *Journal of Modern Physics*, 2(08):922. <https://doi.org/10.4236/jmp.2011.28109>.
- Yildiz, A.R. (2013). Optimization of cutting parameters in multi-pass turning using artificial bee colony-based approach. *Information Sciences*, 220:399-407. <https://doi.org/10.1016/j.ins.2012.07.012>.
- Zhang, Y. and Xu, X. (2020). Yttrium barium copper oxide superconducting transition temperature modeling through gaussian process regression. *Computational Materials Science*, 179:109583. <https://doi.org/10.1016/j.commatsci.2020.109583>.