Estimating Parameters of Copper-graphene Interconnects via Machine Learning Metamodels

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***Abstract*— The accurate prediction of electrical parameters such as resistance, inductance, and ground capacitance is crucial for optimizing electronic circuit design and manufacturing processes. In this study, we explore the effectiveness of Support Vector Regression (SVR) and Decision Tree Regression models for predicting resistance, inductance, and capacitance based on the dataset. Synthetic datasets are generated from fundamental equations.**

I. Introduction

In the realm of electronic circuit design and optimization, accurate prediction of key electrical parameters such as resistance, ground capacitance, and inductance plays a pivotal role in ensuring optimal circuit performance and functionality. The ability to anticipate these parameters enables engineers and chip designers to make informed decisions during the design phase, thereby facilitating the development of efficient and reliable electronic systems.

The motivation behind this study stems from the critical need to leverage advanced computational techniques, specifically regression modeling, to forecast electrical parameters based on theoretical formulations. We aim to explore the effectiveness of Support Vector Regression (SVR) and Decision Tree Regression models in predicting resistance, ground capacitance, and inductance using synthetic datasets generated from fundamental equations governing these parameters.

The datasets are generated based on theoretical equations governing resistance, ground capacitance, and inductance, with features including width and thickness as input variables. Model performance is evaluated using Mean Squared Error (MSE) on test data, demonstrating varying performance across different parameters. Findings underscore the importance of tailored regression techniques for optimizing electronic circuit design based on specific electrical parameters.

The objectives of this investigation are twofold:

1. To assess the performance of regression models, SVR and Decision Tree Regression, in predicting resistance, capacitance, and inductance.
2. To demonstrate the applicability of synthetic datasets derived from theoretical equations as inputs for regression-based parameter prediction in electronic circuit design.

The outcomes of this study are expected to provide valuable insights into the suitability and efficacy of regression techniques for predicting electrical parameters in electronic circuits. By harnessing the power of computational modeling and synthetic dataset generation, this research contributes to the advancement of predictive design methodologies in the field of electronics.

II. Overview of Machine Learning Metamodels for Interconnects

In this section, we review the application of conventional machine learning metamodels, including Support Vector Regression (SVR) and Decision Tree Regression, for modeling and

predicting interconnect parameters in electronic circuits. The utilization of these machine learning techniques offers a promising approach to optimize interconnect design and performance by leveraging computational models derived from empirical data.

These metamodels enable the analytic calculation of the p.u.l. parameters of interconnects for different values of the design parameters free from expensive full-wave EM simulations.

2.1 Support Vector Regression

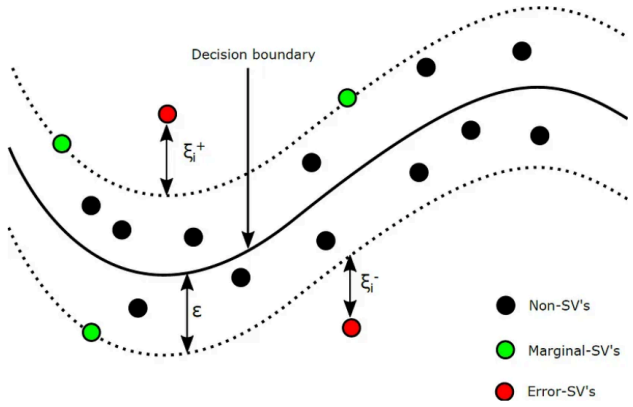

Fig 1 : SVR structure

SVR aims at reducing the error by determining the hyperplane and minimising the range between the predicted and the observed values. Minimising the value of w in the Equation given below is similar to the value defined to maximise the margin, as shown in Fig. 1.

$$\min ||w||^2 + C \sum_{i}^{n} (\xi_i^+ + \xi_i^-)$$

where the summation part represents an empirical error. Hence, to minimise this error, we use the following equation.

$$f(x) = \sum_{i}^{n} (\alpha_i^* + a_i) K(x, x_i) + B$$

where the alpha term represents the Lagrange multiplier and its value is greater than equal to 1. ***K*** represents the kernel function and ***B*** represents the bias term. In this study, we have used the Polynomial kernel given by:

$$K(x, x_i) = \gamma(x * x_i + 1)^d$$

where ***d*** is the polynomial degree and ***γ*** is the polynomial constant.

SVR performs better performance prediction than other algorithms like Linear Regression, KNN and Elastic Net, due to the improved optimisation strategies for a broad set of variables. Moreover, it is also flexible in dealing with geometry, transmission, data generalisation and additional functionality of the kernel. This additional functionality enhances the model capacity for predictions by considering the quality of features. Some similar estimation work on on-chip aging estimation can be referred from .

2.2 Decision Tree Regression

We now explore the concept of decision trees in a simple and easy-to-follow manner. Each node in a decision tree represents a decision or a question about a specific feature. Based on the answer, we navigate through the corresponding branch to reach another node, ultimately leading us to a leaf node. These leaf nodes provide us with the desired outcome or prediction as shown in Fig 2.

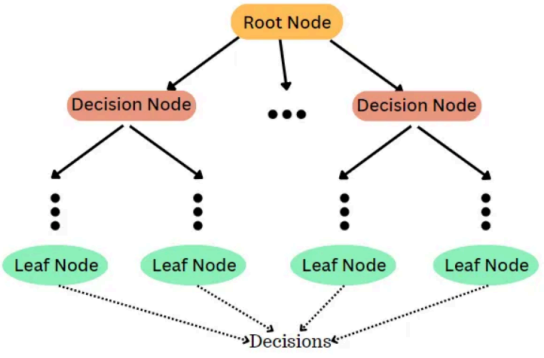

Fig. 2. Decision Tree structure.

To establish a formal definition:

1. A decision tree is a supervised machine learning algorithm that employs a tree-like structure to make decisions or predictions based on input features.
2. It recursively splits data based on different attributes and their thresholds, creating decision boundaries that divide the input space into regions associated with specific outcomes or class labels.

Classification and Regression Decision Trees:

- A classification decision tree is employed to classify data into different categories. For example, we predict whether someone will go for a run or not based on the weather conditions.
- On the other hand, a regression decision tree is used to predict numerical values. Consider predicting house prices using features like square footage, number of bedrooms, and the presence of a balcony.

Decision trees are often used in ensemble methods like random forests or gradient boosting. These methods combine multiple decision trees to enhance performance and robustness.

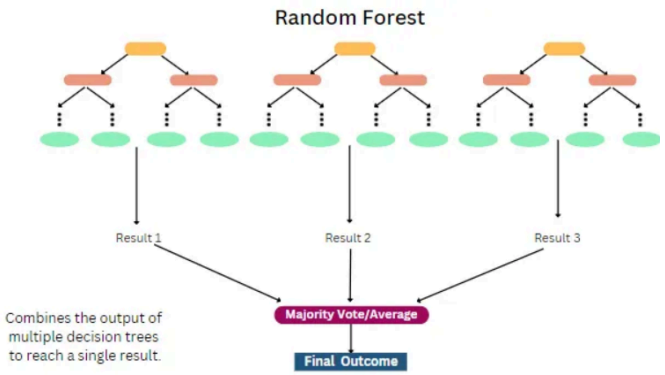

Fig. 3. Random Forest structure.

In random forests, a collection of decision trees is built using different subsets of data and features. Each tree independently makes predictions, and the final result is determined by taking the average for numerical predictions and the majority vote for categorical predictions from all the trees. This ensemble approach helps reduce overfitting and improves generalization.

In conclusion, decision trees are a powerful tool in machine learning and data analysis. They allow us to make predictions based on input features, employing decision boundaries to divide the input space and associate specific outcomes or class labels. Related work on building algorithms can be found referred from [1].

III. Dataset Simulation

The p.u.l. resistance, inductance and ground capacitance are calculated by the following equations.

3.1 For Copper Resistance

$$R_{cu} = \frac{\rho_c}{w_c \cdot t_c},$$

3.2 For Copper Inductance

$$L_{cu} = \frac{\mu_0}{2\pi}\left[In\left(\frac{2.l_c}{t_c + w_c}\right) + 0.5 + 0.22\left(\frac{t_c + w_c}{l_c}\right)\right]$$

3.3 For Copper Capacitance

$$C_{cu} = \varepsilon_i\left[\frac{w_c}{h_{gn}} + 2.22\left(\frac{d_i}{d_i + 0.7h_{gn}}\right)^{3.19} + 1.17\left(\frac{d_i}{d_i + 1.51h_{gn}}\right)^{0.76}\left(\frac{t_c}{t_c + 4.53h_{gn}}\right)^{0.12}\right]$$

where lc is interconnect length, wc is width, tc is thickness, ρc is resistivity, hgn is height above ground plane, εi is dielectric constant, di is space between the interconnects, and μ0 is the permeability. Based on ITRS 2017, the width and space between the interconnect lines, the thickness of the interconnect lines, height from the ground plane, and the interlevel dielectric medium permittivity are considered as 22, 44, 36.6, and 2.3 nm, respectively. Further, the

equations for the calculation of the p.u.l. parameters for Graphene and Copper-Graphene interconnects can also be determined.[2]

3.4 For Graphene Resistance

$$R_{gr} = \left(\frac{1}{R_{grt}} + \frac{1}{R_{grb}} + \frac{1}{R_{grl}} + \frac{1}{R_{grr}}\right)^{-1}$$

where Rgrt, Rgrb, Rgrl and Rgrr are the resistance due to the thickness, breadth, length and radius of graphene respectively.

Rgrt can be calculated from the formula:

$$R_{grt} = \frac{h}{2e^2} \times \frac{1}{N_{cht}} \times \left(\frac{1}{\Lambda_{eff}}\right)$$

where Ncht is the carrier concentration for the top branch and lambda.eff is the effective mean free path of electrons in graphene.

Rgrb can be calculated from the equation:

$$R_{grb} = \frac{h}{2e^2} \times \frac{1}{N_{chb}} \times \left(\frac{1}{\Lambda_{eff}}\right)$$

where Nchb is the carrier concentration for the bottom branch.

Rgrl can be calculated from the equation:

$$R_{grl} = \frac{h}{2e^2} \times \frac{1}{N_{chl}} \times \left(\frac{1}{\Lambda_{eff}}\right)$$

where Nchl is the carrier concentration for the left branch.

Rgrr can be calculated from the equation:

$$R_{grr} = \frac{h}{2e^2} \times \frac{1}{N_{chr}} \times \left(\frac{1}{\Lambda_{eff}}\right)$$

where Nchr is the carrier concentration for the right branch.e is the elementary charge and lambda effective can be calculated from the equation:

$$\Lambda_{eff} = \frac{1}{\frac{1}{L_{ac}} + \frac{1}{L_{edge}}}$$

where Lac and Ledge are acoustic phonon mean free path and edge roughness scattering mean free path.

Acoustic phonon mean free path can be calculated as:

$$L_{ac} = \frac{1}{k_B \cdot T} \times \frac{V_s^2}{D_{ac}^2} \times \sqrt{\frac{\pi}{N_s}}$$

where, kB is the boltzmann constant, T is the temperature in Kelvin, Vs is the source velocity, Dac is the acoustic deformation potential and Ns is the electron concentration.

Furthermore, the roughness scattering mean free path can be calculated from the equation:

$$Ledge = \sum_{m=1}^{2} \left(\frac{W_{gr}}{P_{gr}}\right) \sqrt{\left(\frac{(2 \cdot W_{gr} \cdot E_F)}{(m \cdot h \cdot V_f)}\right)^2 - 1}$$

where, Wgr is the width of graphene, Pgr is a constant parameter, Ef is fermi energy, h is Planck's constant and Vf is fermi velocity. The sum is over two terms, m = 1 to 2, representing contribution from different scattering processes.

The values of the constant terms are mentioned below

h = 6.654*10^-34 J.s.

Vf = 8*10^5 m/s.

Pgr = 1.5

Ef = 1.60217657*10^-19 J.

e = 1.60217657*10^-19 C.

kB = 1.38*10^-23 J/K.

T = 300K.

Dac = 18*1.60217657*10^-19 J.

Ns = 5*10^16 /m^3.

Vs = 20*10^3 m/s.

3.5 For Graphene Capacitance

$$C_g = \left(\frac{4 \cdot e^2 \cdot N_{cht}}{V_f \cdot h} + \frac{4 \cdot e^2 \cdot N_{chb}}{V_f \cdot h} + \frac{4 \cdot e^2 \cdot N_{chl}}{V_f \cdot h} + \frac{4 \cdot e^2 \cdot N_{chr}}{V_f \cdot h}\right) \times 10^{-4}$$

where, e represents the elementary charge, Ncht, Nchb, Nchl, Nchr represent the carrier concentrations for the top, bottom, left, and right branches, respectively. Vf represents the fermi velocity and h is the planck's constant.

3.6 For Graphene Inductance

$$L_g = \left(\frac{h}{4 \cdot e^2 \cdot V_f \cdot N_{cht}} + \frac{h}{4 \cdot e^2 \cdot V_f \cdot N_{chb}} + \frac{h}{4 \cdot e^2 \cdot V_f \cdot N_{chl}} + \frac{h}{4 \cdot e^2 \cdot V_f \cdot N_{chr}}\right) \times 10^{-3}$$

where the unknown parameters are assumed to be the same as those used in the calculation for the capacitance of graphene.

IV. Cu-Mlg Interconnect

4.1 For Resistance

Using the resistance of copper and graphene, we can calculate the equivalent resistance of CuMlg according to the equation given below.

$$R_{Esc} = \left(\frac{1}{R_{cu}} + N \times \frac{1}{R_{gr}}\right)^{-1}$$

where, Rcu is the resistance of copper and Rgr is the resistance of graphene.

4.2 For Capacitance

Based on the values of capacitance of copper and graphene generated from the equations, we can calculate the capacitance of CuMlg interconnect according to the equation given below.

$$C_{Esc} = \left(\frac{1}{C_g} + \frac{1}{C_e}\right)^{-1}$$

where, Cg is the capacitance of graphene and Ce is the capacitance of copper.

4,3 For Inductance

Similarly, based on the values of inductance of copper and graphene we can calculate the inductance of our interconnect from the equation below.

$$L_{Esc} = \left(\frac{1}{L_g} + L_e\right)^{-1}$$

where Lg is the inductance of graphene and Le is the inductance of copper.

V. COMPARISON TABLE

1. CuMlg INDUCTANCE

Slno	Cu_In(H)	Gr_In(H)	Act(H)	Pred(H)
1.	4.4e-7	2.95e-7	1.768e-7	1.762e-7
2.	2.95e-7	3.08e-7	1.507e-7	1.596e-7
3.	3.00e-7	3.16e-7	1.541e-7	1.567e-7
4.	6.00e-7	2.05e-7	1.530e-7	1.594e-7

2. CuMlg RESISTANCE

Slno	Cu_res(ohm)	Gr_res(ohm)	Act (ohm)	Pred (ohm)
1	323670.0	1696545.62	205851.72	207471.64
2	162690.0	1660102.76	125726.44	125861.27
3	43591.0	1656701.52	40401.84	40377.08
4	62369.0	1661261.03	56055.49	56058.49

3. CuMlg CAPACITANCE

Slno	Cu_cap(F)	Gr_cap(F)	Act(F)	Pred(F)
1	6.40e-11	6.45e-11	3.2e-11	3.17e-11
2	6.60e-11	6.77e-11	3.3e-11	3.24e-11
3	7.9e-11	9.43e-11	4.3e-11	3.5e-11
4	7.1e-11	7.85e-11	3.72e-11	3.16e-11

VI. CONCLUSION

Model Performance: Both SVR and Decision Tree Regression demonstrated promising performance in predicting electrical parameters. SVR, leveraging advanced optimization strategies and the flexibility of kernel functions, outperformed traditional algorithms like Linear Regression, KNN, and Elastic Net. Decision Tree Regression, with its intuitive tree-like structure, provided accurate numerical predictions suitable for our parameter forecasting needs.

Dataset Generation: The use of synthetic datasets derived from theoretical equations proved effective as inputs for regression-based parameter prediction. This approach demonstrated applicability in electronic circuit design, allowing engineers to anticipate critical electrical parameters during the design phase.

Parameter Relationships: Our study highlighted the complex relationships between interconnect dimensions (width, thickness), material properties (resistivity, dielectric constant), and electrical parameters (resistance, inductance, capacitance). By incorporating these factors into regression models, we achieved valuable insights into parameter behaviors and dependencies.

Enhanced Circuit Design: Accurate prediction of resistance, inductance, and capacitance enables engineers and chip designers to optimize electronic circuit performance and reliability. By leveraging regression modeling techniques, circuit designs can be refined and tailored to meet specific operational requirements.

Computational Modeling in Electronics: The utilization of machine learning metamodels like SVR and Decision Tree Regression offers a promising approach to enhance interconnect design and performance. These techniques complement traditional empirical methods, providing efficient alternatives for parameter prediction.

Further Model Exploration: Exploring additional regression techniques and ensemble methods could further enhance predictive accuracy and robustness. Techniques such as Random Forests or Gradient Boosting could be investigated for their suitability in predicting complex electrical parameters.

Real-World Validation: Validating our models with experimental data from real-world electronic circuits would strengthen the applicability and reliability of our predictive approach. Incorporating diverse datasets and scenarios can provide comprehensive insights into model generalization.

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