# Critical Temperature Prediction for a Superconductor: A Bayesian Neural Network Approach


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## Background

Much research in recent years has focused on using empirical machine learning approaches to extract useful insights on the structure-property relationships of superconductor material. Notably, these approaches are bringing extreme benefits when superconductivity data often come from costly and arduously experimental work. However, this assessment cannot be based solely on an open black-box machine learning, which is not fully interpretable, because it can be counter-intuitive to understand why the model may give an appropriate response to a set of input data for superconductivity characteristic analyses, e.g., critical temperature. The purpose of this study is to describe and examine an alternative approach for predicting the superconducting transition temperature $T_c$ from SuperCon database obtained by Japan's National Institute for Materials Science. We address a generative machine-learning framework called Variational Bayesian Neural Network using superconductors chemical elements and formula to predict $T_c$.

## Objectives

- **First,** to improve the interpretability, we adopt a variational inference to approximate the distribution in latent parameter space for the generative model. It statistically captures the mutual correlation of superconductor compounds and; then, gives the estimation for the $T_c$ .
- **Second**, a stochastic optimization algorithm, which embraces a statistical inference named Monte Carlo sampler, is utilized to optimally approximate the proposed inference model, ultimately determine and evaluate the predictive performance.

## Model and Preliminaries

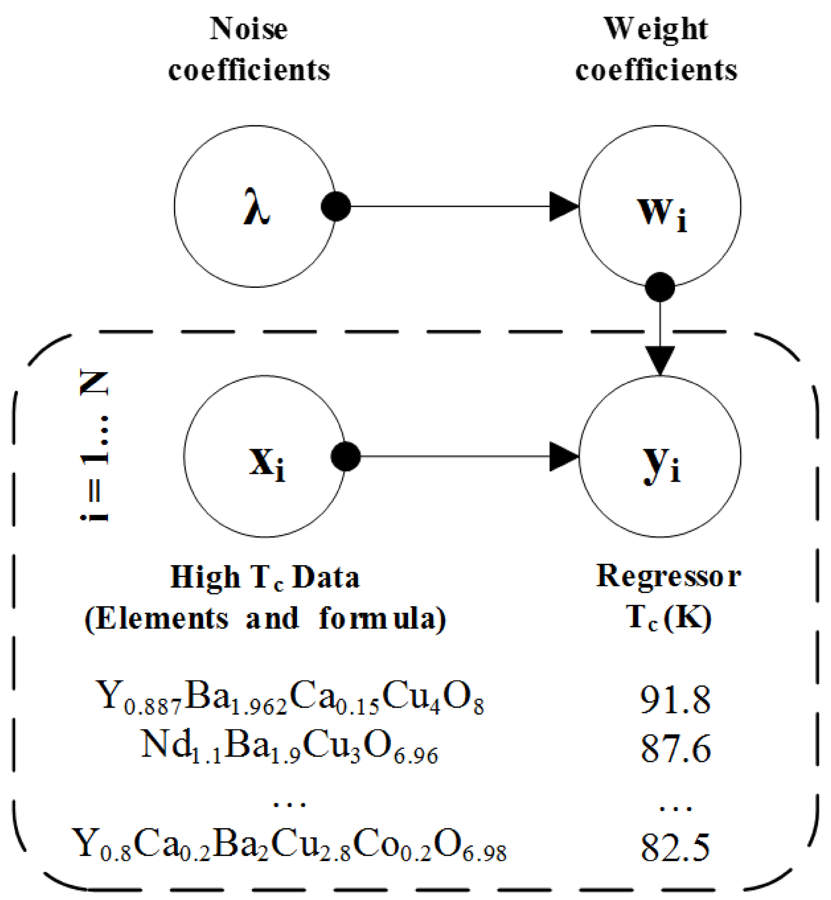


Fig. 1. Probabilistic graphical model of the VBNN model to predict

### Bayesian Neural Network Regression Model

$$p(\mathbf{y}|\mathbf{X},\mathbf{w}) = \prod_{i=1}^{I} \mathcal{N}\left(y_i|\mathbf{w}^T\mathbf{x}_i, \lambda^{-1}\right)$$

$$p(\mathbf{y},\mathbf{w}|\mathbf{X}) = p(\mathbf{y}|\mathbf{X},\mathbf{w})p(\mathbf{w})$$

### Variational Inferece Model

$$p_\theta(w|x) = \frac{p_\theta(x|w)p(w)}{p_\theta(x)} = \frac{p_\theta(w,x)}{p_\theta(x)} = \frac{p_\theta(w,x)}{\int_w p_\theta(x,w)}$$

$$\mathrm{KL}\left(q_\phi \| p_\theta\right) = \left(\mathbb{E}_{q_\phi} \log \frac{q_\phi(w|x)}{p_\theta(w,x)}\right) + \log p_\theta(x) = -\mathcal{L}(x;\theta,\phi) + \log p_\theta(x)$$

$$\mathcal{L}(x;\theta,\phi) = -\mathbb{E}_{q_\phi}\left[\log \frac{q_\phi(w|x)}{p_\theta(w,x)}\right] = \mathbb{E}_{q_\phi}\left[\log p_\theta(x|w) + \log p(w) - \log q_\phi(w|x)\right]$$

### Optimization

$$\nabla_\phi L(\phi,\theta) = \mathbb{E}_{\epsilon\sim\mathrm{N}(0,I)} \nabla_\phi \left[\log p_\theta(x, w(\epsilon;x,\phi)) - \log q_\phi(w(\epsilon;x,\phi)|x)\right.$$
$$\approx \frac{1}{k}\sum_{i=1}^{k} \nabla_\phi \left[\log p_\theta\left(x, w\left(\epsilon_i;x,\phi\right)\right) - \log q_\phi\left(w\left(\epsilon_i;x,\phi\right)|x\right)\right.$$

where $\epsilon_i \sim \mathrm{N}(0,I)$

## Evaluation and Results

### Model Evaluation

Root Mean Square Error (RMSE):

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(\hat{y}_i - y_i)^2}$$

R-squared ($R^2$):

$$R^2 = 1 - \frac{\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{N}(y_i - \bar{y}_i)^2}$$

Log-likelihood:

$$LL = \log p(y|x,D) \simeq \log \int_w p(y|x,w)q(w)$$

### Numerical Results

$$\hat{y} = \mathbb{E}_{p(y|x,D)}y \simeq \frac{1}{M}\sum_{i=1}^{M}\mathbb{E}_{p(y|x,w)}y$$

TABLE I
NUMERICAL RESULT COMPARISON

| ML Approaches | $R^2$ | RMSE (K) |
|---|---|---|
| Random Forest [6] | 0.85 | N/A |
| Random Forest & XGboost [11] | 0.74 | 17.6 |
| Support Vector Machine [12] | 0.96 | N/A |
| Convolutional Neural Network [13] | 0.93 | N/A |
| Atom Table Convolutional Neural Network [14] | **0.97** | 8.14 |
| Variational Bayesian Neural Network | 0.94 | **3.83** |

**Note:** The reproducibile predictions and evaluations, the implementation code and results are available at GitHub repository: https://github.com/ltdung/VBNN_HighTc

## Conclusion

The presented Bayesian regression approach can also directly be applied to predict the critical temperature of a superconductor, as shown in Table I. Our confidence scores $R^2$ have strong overall concordance with previous predictions (**$R^2$ = 0.94**). Besides, a significant improvement was obtained in the **RMSE at 3.83 K**. The result is a striking illustration of VBNN performance compared with other techniques. Although there are not any results for log-likelihood from existing approaches, it is evident that the **log-likelihood value at -2.75** will give a comparable estimation of the regression task for future researches. In short, to the knowledge of the authors, the generative approach for superconductors $T_c$ prediction is the first of its kind. This finding is promising and should be investigated with other advanced predictive models.

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