

# A Machine Learning-Enabled Study of Superconductivity

## Application of the XGBoost Algorithm

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# Outline

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  - Superconductivity
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# Introduction

## XGBoost

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- eXtreme Gradient Boosting
- Package for **Python**, C++, Java, R, Julia, and Scala

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- Ensemble learning [Friedman et al. 2017]

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- Ensemble learning [Friedman et al. 2017]
  - Combination of homogenous weak learners



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  - Combination of homogenous weak learners
  - End result is a weighted sum of weak learners

$$\theta_f = \sum_j w_j \theta_j$$

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$$\theta_f = \sum_j w_j \theta_j$$

- $w_j$  are determined by backpropagation via gradient descent

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## Ginzburg-Landau Theory

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## Ginzburg-Landau Theory

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- For a homogenous superconductor, the Ginzburg-Landau equation is

$$\alpha\phi + \beta|\phi|^2\phi = 0$$

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## Ginzburg-Landau Theory

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- For a homogenous superconductor, the Ginzburg-Landau equation is

$$\alpha\phi + \beta|\phi|^2\phi = 0$$

- The nontrivial solution for  $T < T_c$  is

$$|\phi|^2 = -\frac{\alpha}{\beta}(T - T_c)$$

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- The nontrivial solution for  $T < T_c$  is

$$|\phi|^2 = -\frac{\alpha}{\beta}(T - T_c)$$

- The characteristic length scale  $\xi$  is called the Ginzburg-Landau coherence length

$$\xi = \sqrt{\frac{\hbar^2}{2m^*|\alpha|}}$$

# Introduction

## Types of Superconductors

- Two types - Type 1 and Type 2

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## Types of Superconductors

- Two types - Type 1 and Type 2
- Notation

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## Types of Superconductors

- Two types - Type 1 and Type 2
- Notation
  - $H_c(T)$  is critical field as a function of temperature

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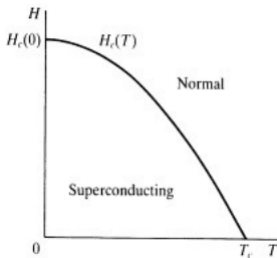
## Types of Superconductors

- Two types - Type 1 and Type 2
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  - $H_c(T)$  is critical field as a function of temperature
  - $T_c$  is critical temperature

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## Types of Superconductors

- Two types - Type 1 and Type 2
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  - $T_c$  is critical temperature



**Figure:  $H - T$  phase diagram for a Type 1 superconductor [Tinkham]**

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## Type 2 Superconductors

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## Type 2 Superconductors

- Ginzburg-Landau parameter  $\kappa > \frac{1}{\sqrt{2}}$

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## Type 2 Superconductors

- Ginzburg-Landau parameter  $\kappa > \frac{1}{\sqrt{2}}$ 
  - Definition:  $\kappa = \frac{\lambda}{\xi} = \frac{e\hbar}{m_e c} \sqrt{\frac{\beta}{2\pi}}$
  - Surface energy is negative

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## Type 2 Superconductors

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- $H_{c2} = H_{c1} \kappa \sqrt{2}$

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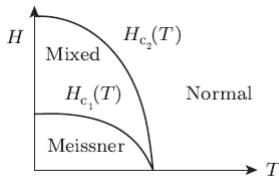
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  - Definition:  $\kappa = \frac{\lambda}{\xi} = \frac{e\hbar}{m_e c} \sqrt{\frac{\beta}{2\pi}}$
  - Surface energy is negative
- $H_{c2} = H_{c1} \kappa \sqrt{2}$
- In type 1,  $H_{c2} = H_{c1}$



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## Type 2 Superconductors

- Ginzburg-Landau parameter  $\kappa > \frac{1}{\sqrt{2}}$ 
  - Definition:  $\kappa = \frac{\lambda}{\xi} = \frac{e\hbar}{m_e c} \sqrt{\frac{\beta}{2\pi}}$
  - Surface energy is negative
- $H_{c2} = H_{c1} \kappa \sqrt{2}$
- In type 1,  $H_{c2} = H_{c1}$



**Figure:  $H - T$  phase diagram for a Type 2 superconductor [Girvin and Yang 2019]**

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## Type 2 Superconductors: Abrikosov Lattice Vortices

- For  $H_{c1} < H < H_{c2}$  in a Type 2 Superconductor, Abrikosov vortices appear in the material

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## Type 2 Superconductors: Abrikosov Lattice Vortices

- For  $H_{c1} < H < H_{c2}$  in a Type 2 Superconductor, Abrikosov vortices appear in the material
- These are flux vortices that are quantized, with

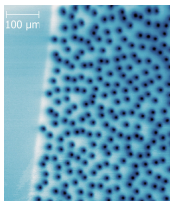
$$\Phi = \frac{nhc}{2e}, \quad n \in \mathbb{Z}$$

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## Type 2 Superconductors: Abrikosov Lattice Vortices

- For  $H_{c1} < H < H_{c2}$  in a Type 2 Superconductor, Abrikosov vortices appear in the material
- These are flux vortices that are quantized, with

$$\Phi = \frac{nhc}{2e}, \quad n \in \mathbb{Z}$$



**Figure: Abrikosov vortices in YBCO - created by Wells et al. 2015 using scanning SQUID microscopy**

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- Taken from UCI (University of California, Irvine)  
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- Taken from UCI (University of California, Irvine) Machine Learning Repository
- 21,263 examples with 81 features

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- Taken from UCI (University of California, Irvine) Machine Learning Repository
- 21,263 examples with 81 features
- Model was only trained with 11 features to prevent overfitting

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- Taken from UCI (University of California, Irvine) Machine Learning Repository
- 21,263 examples with 81 features
- Model was only trained with 11 features to prevent overfitting



Figure: UCI Machine Learning Repository



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- XGBoost library

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- XGBoost library
  - XGBClassifier class

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# Discussion

- Confusion matrix made using matplotlib library

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# Discussion

- Confusion matrix made using matplotlib library

		Actual Values	
		Positive (1)	Negative (0)
Predicted Values	Positive (1)	TP	FP
	Negative (0)	FN	TN

Figure: **Example Confusion Matrix**

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- Python training files, these slides, the dataset, etc. can be found at <https://github.com/RajeevAtla/Graphene-Research/>



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- Python training files, these slides, the dataset, etc. can be found at <https://github.com/RajeevAtla/Graphene-Research/>
- Easiest way to access is using git

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