

A Machine Learning-Enabled Study of Superconductivity

Application of the XGBoost Algorithm

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- eXtreme Gradient Boosting

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

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- Ensemble learning [*Elements of Statistical Learning* Chapter 16]

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

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

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

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- The nontrivial solution for $T < T_c$ is

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

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- The characteristic length scale ξ is called the Ginzburg-Landau coherence length

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

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

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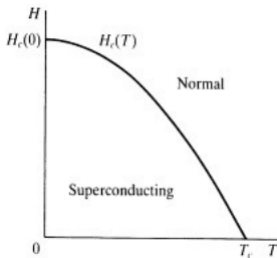


Figure: $H - T$ phase diagram for a Type 1 superconductor [Tinkham]

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Type 2 Superconductors

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

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

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

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- $H_{c2} = H_{c1} \kappa \sqrt{2}$
- In type 1, $H_{c2} = H_{c1}$

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- $H_{c2} = H_{c1} \kappa \sqrt{2}$
- In type 1, $H_{c2} = H_{c1}$

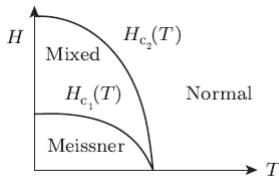


Figure: $H - T$ phase diagram for a Type 2 superconductor [Girvin and Yang 2019]

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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

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

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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

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

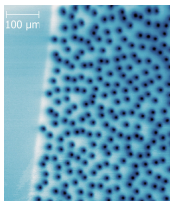


Figure: Abrikosov vortices in YBCO - created by Wells et al. 2015 using scanning SQUID microscopy

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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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- 21,263 examples with 81 features
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Figure: UCI Machine Learning Repository

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- XGBoost library

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- XGBoost library
 - XGBClassifier class

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- Confusion matrix made using matplotlib library

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- 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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