

Statistical Data Analysis Project

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Introduction

- ▶ Brief overview of the data analysis project.
- ▶ Importance of the analysis: Understanding the shift in peak positions in crystals of different compositions.
- ▶ Objectives and hypotheses: Investigating if there are significant differences in peak positions among crystals.

Data Overview

- ▶ Overview of the dataset: Peaks from different crystals with compositions and varying 2 theta values.
- ▶ Key variables and their significance:
'2_theta', Condition, Value, and Cluster.

Data Preprocessing

- ▶ Cleaning and handling missing values.
- ▶ Transformation of data for analysis.

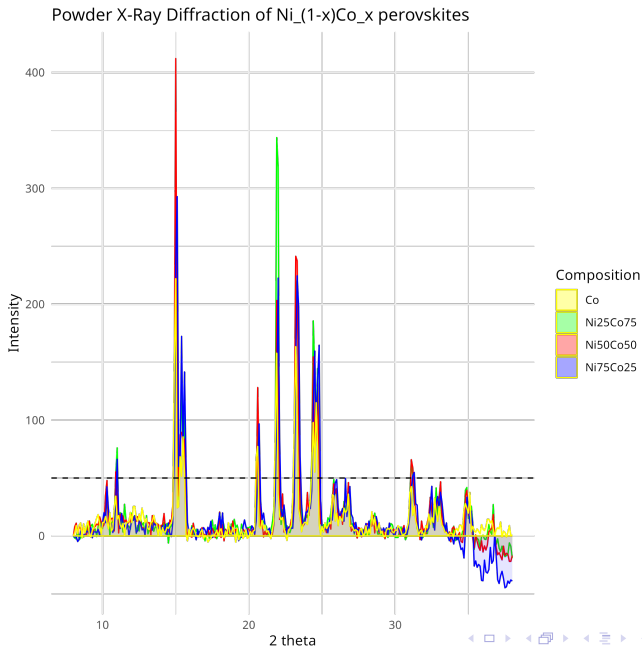
```
1 # Cleaning and transformation
2 data_clean <- na.omit(data_peaks)
3 data_long <- pivot_longer(data_clean, cols = -c('2
  _theta', Condition),
4                               names_to = "Cluster",
  values_to = "Value")
5
```

Exploratory Data Analysis

- ▶ Visualizations and summary statistics.
- ▶ Identification of patterns and trends.

```
1  # Exploratory Data Analysis (EDA)
2  ggplot(data, aes(x = '2_theta')) +
3  geom_ribbon(aes(ymin = 0, ymax = 'Ni25Co75', fill = "Ni25Co75"),
4  alpha = 0.1, color = "green"
5  ) +
6  geom_ribbon(aes(ymin = 0, ymax = 'Ni50Co50', fill = "Ni50Co50"),
7  alpha = 0.1, color = "red"
8  ) +
9  geom_ribbon(aes(ymin = 0, ymax = 'Ni75Co25', fill = "Ni75Co25"),
10 alpha = 0.1, color = "blue"
11 ) +
12 geom_ribbon(aes(ymin = 0, ymax = 'Co', fill = "Co"),
13 alpha = 0.1, color = "yellow"
14 ) +
15 labs(
16   title = "Powder X-ray Diffraction of Ni_(1-x)Co_x perovskites",
17   x = "2_theta",
18   y = "Intensity",
19   fill = "Composition"
20 ) +
21 scale_fill_manual(values = c(
22   "Ni75Co25" = "blue", "Ni50Co50" = "red",
23   "Ni25Co75" = "green", "Co" = "yellow"
24 )) +
25 theme_minimal()
26
```

Visualization of X-ray Diffraction



ANOVA Testing

- ▶ Analysis of Variance (ANOVA) to test hypotheses.
- ▶ Results and interpretation.

```
1 # ANOVA Testing
2 anova_result <- aov('2_theta' ~ Condition *
Cluster, data = data_long)
3 summary(anova_result)
4
```

Results and Discussion

- ▶ Interpretation of ANOVA results.
- ▶ Comparison of clusters: Assessing the significance of peak position variations.
- ▶ Implications of the findings: Understanding how composition affects peak positions.

Conclusion

- ▶ Summary of key findings.
- ▶ Limitations and areas for future research.

Any Questions?