Linear Classification

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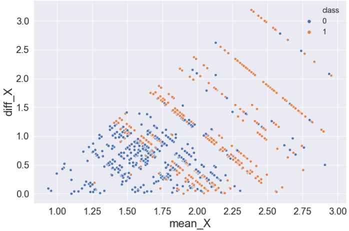
Overview

Preliminaries

- Linear methods can also be used for classification, i.e., decision boundaries are linear.
- These methods are surprisingly effective across a large spectrum of datasets, even compared to more complex ML models.

Metal vs Insulator Dataset

- To demonstrate the use of these methods, we will first discuss the "toy" dataset.
- 2000+ binary (A_xB_y) compounds with experimental band gaps.
- Class 0: metals; Class 1: insulators.
- Using pymatgen, we can generate some simple features. Here, we will create simply features based on the mean and absolute difference in electronegativity between A and B (why?).



Creating the features and classes

```python
import pandas as pd
from pymatgen.core import Composition
binaries = pd.read_csv('binary_band_gap.csv')
# We create a column holding the Composition object.
# Note the use of list comprehension in Python.
binaries['composition'] = [Composition(c) for c in binaries['Formula']]
electronegs = [[el.X for el in c] for c in binaries['composition']]
# Create the features mean and difference between electronegativities
binaries['mean_X'] = [np.mean(e) for e in electronegs]
binaries['diff_X'] = [max(e) - min(e) for e in electronegs]
# Label metals (band gap of 0. 1e-5 is used as numerical tolerance) as class 0
# Insulators are labelled as class 1.
binaries['class'] = [0 if eg < 1e-5 else 1 for eg in binaries['Eg (eV)']]}
```

Basic concepts

- If there are K classes, we have a $N \times K$ indicator response matrix. Each row is a vector $Y = (Y_1, Y_2, ..., Y_K)$ where $Y_k = 1$ if the instance belongs to the kth class and all other Ys are 0.

$$\mathbf{Y} = \begin{pmatrix} 0 & 0 & \dots & 1 \\ 1 & 0 & \dots & 0 \\ \dots & & & \\ 0 & 1 & \dots & 0 \end{pmatrix}$$

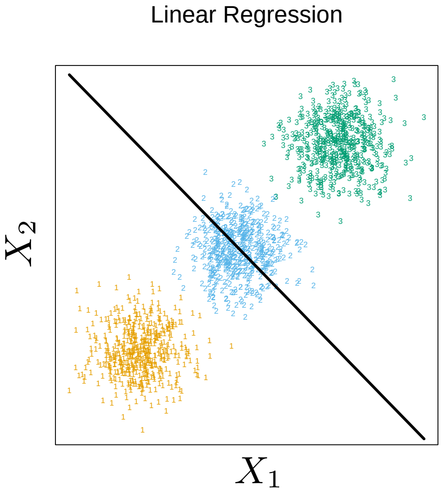
- For the kth response variable, the fitted $\hat{f}_k(x) = \hat{\beta_{k0}} + \hat{\beta_k^T} x$.
- Decision boundary between k and l class is given by $\hat{f}_k(x) = \hat{f}_l(x)$.
- Input is divided into regions.
- Similar to linear regression, we can augment the input space with polynomial (e.g., $X_1^2, X_2^s, X_1 X_2$) and other basis functions, leading to boundaries that are non-linear.

Linear regression of indicator matrix

- Treat each column of $\mathbf{Y}$ as a target. Least squares solution:

$$\hat{\mathbf{Y}} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$$

- For each new observation x, we compute $\hat{f}_k(x) = (1, x^T)(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$.
- Find the largest component, and that will result in the classification k, $G(x) = \text{argmax}_{k \in G}\, \hat{f}_k(x)$.
- Major issue: some categories may be masked for $K \geq 3$.



Discriminant Analysis

- From Bayes rule, we have:

$$P(G = k|X = x) = \frac{f_k(x)\pi_k}{\sum_{l=1}^{K} f_l(x)\pi_l}$$

- where $f_k(x)$ are the class conditional probability densities $(P(X = x|G = k))$ and π_k are the prior probabilities of being in class k.
- Most common approach - assume Gaussian class densities.

$$f_k(x) = \frac{1}{(2\pi)^{p/2}|\Sigma_k|^{1/2}} \exp -\frac{1}{2}(x - \mu_k)^T \Sigma_k^{-1}(x - \mu_k)$$

Linear Discriminant Analysis

- Assume all classes have a common covariance matrix, i.e., $\Sigma_k = \Sigma$.
- To compare two classes k and l, we can compare the log ratios.

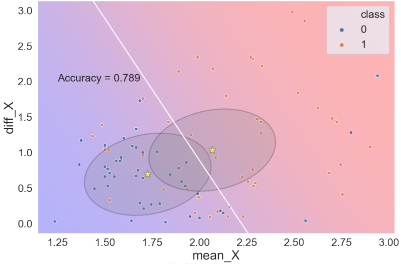
$$
\begin{aligned}
\log \frac{P(G=k|X=x)}{P(G=l|X=x)} &= \log \frac{f_k(x)}{f_l(x)} + \log \frac{\pi_k}{\pi_l} \\
&= \log \frac{\pi_k}{\pi_l} - \frac{1}{2}(\mu_k + \mu_l)^T \Sigma^{-1} (\mu_k - \mu_l) \\
&\quad + x^T \Sigma^{-1} (\mu_k - \mu_l)
\end{aligned}
$$

- At the decision boundary, $P(G=k|X=x) = P(G=l|X=x)$, which leads to a linear equation in x.
- Equivalently, we have

$$
G(x) = \operatorname*{argmax}_k \left\{ \log \pi_k - \frac{1}{2} \mu_k^T \Sigma^{-1} \mu_k + x^T \Sigma^{-1} \mu_k \right\}
$$

Linear Discriminant Analysis, contd.

- In general, we do not know the prior distributions and covariance matrix. These are estimated from the data.
  - $\hat{\pi}_k = N_k/N$
  - $\hat{\mu}_k = \sum_{g_i=k} x_i/N$
  - $\hat{\Sigma} = \sum_{k=1}^{K} \sum_{g_i=k} (x_i - \hat{\mu}_k)^T (x_i - \hat{\mu}_k)/(N-K)$
- Avoids masking problem of linear regression classification.
- For the example data,

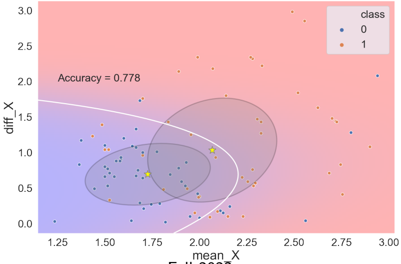


Quadratic Discriminant Analysis

- Covariances are not assumed equal.

$$G(x) = \underset{k}{\operatorname{argmax}} \left\{ \log \pi_k - \frac{1}{2}(x-\mu_k)^T \Sigma_k^{-1}(x-\mu_k) - \frac{1}{2}\log|\Sigma_k| \right\}$$

- No cancellation of terms and decision boundaries are quadratic.
- Covariances must be estimated for each category.
- For the same metal-insulator example,



Discriminant analysis in scikit-learn

```
from sklearn.discriminant_analysis import LinearDiscriminantAnalysis,
    QuadraticDiscriminantAnalysis
lda = LinearDiscriminantAnalysis(solver="svd", store_covariance=True)
X = binaries[["mean_X", "diff_X"]]
y = binaries["class"]
model = lda.fit(X, y)
y_pred = model.predict(X)

qda = QuadraticDiscriminantAnalysis(store_covariance=True)
y_pred = qda.fit(X, y).predict(X)
\end{minted}
```

Logistic regression

- Model posterior probabilities with linear function.

$$\begin{aligned}
\log \frac{P(G=1|X=x)}{P(G=K|X=x)} &= \beta_{10} + \beta_1^T x \\
\log \frac{P(G=2|X=x)}{P(G=K|X=x)} &= \beta_{20} + \beta_2^T x \\
&\dots \\
\log \frac{P(G=K-1|X=x)}{P(G=K|X=x)} &= \beta_{(k-1)0} + \beta_{k-1}^T x
\end{aligned}$$

- Results in the following posterior probabilities:

$$\begin{aligned}
P(G=1|X=x) &= \frac{\exp\left(\beta_{10} + \beta_1^T x\right)}{1 + \sum_{l=1}^{K-1} \exp\left(\beta_{l0} + \beta_l^T x\right)} \\
P(G=K|X=x) &= \frac{1}{1 + \sum_{l=1}^{K-1} \exp\left(\beta_{l0} + \beta_l^T x\right)}
\end{aligned}$$

Solving for the Logistic Regression Coefficients

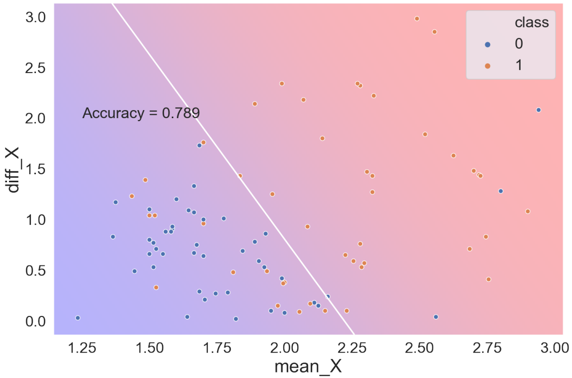
- Typically fitted using *maximum likelihood*.

$$l(\beta) = \sum_{i=1}^{N} \log P(G = k | X = xi; \beta)$$

- Differentiation and setting $\frac{\partial l}{\partial \beta} = 0$ leads to equations that are non-linear in β.
- These equations are solved using some optimization algorithm (e.g., Newton-Raphson, BFGS, etc.).

Logistic regression on metal/insulator dataset

```
from sklearn.linear_model import LogisticRegression
clf = LogisticRegression(penalty='none', random_state=0)
model = clf.fit(X, y)
y_pred = model.predict(X)
```



The End