Introduction to Machine Learning

Lecture 11 Classification - Introduction (Linear Classification)

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Outline

Review

- Bayesian inference of Gaussian mixture model and MCMC
- Nonparametric clustering and kernel density estimation
- Mean shift algorithm

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- Bayesian inference of Gaussian mixture model and MCMC
- Nonparametric clustering and kernel density estimation
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Today

- Classification, definition, evaluation
- Linear classifiers (Naïve Bayes, Linear discriminant analysis, Logistic regression)

Classification Problems

- Object recognition and detection
- Face recognition
- ....

A Viewpoint of Statistical ML

- Given a set of labeled data $\{\boldsymbol{x}_n \in \mathcal{X}, y_n \in \mathcal{C}\}_{n=1}^{N}$
- Train a model (a.k.a. a classifier) $f : \mathcal{X} \mapsto \mathcal{C}$

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Special Cases of Classification Problems

Outlier Detection (One-class Recognition):

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Constrastive Learning:

- Given a pair of samples, judge whether they are in the same class or not.

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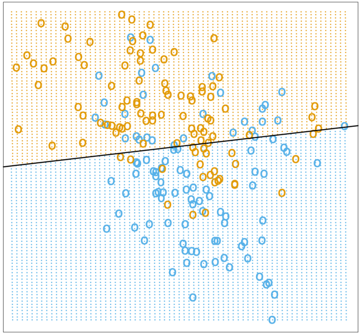
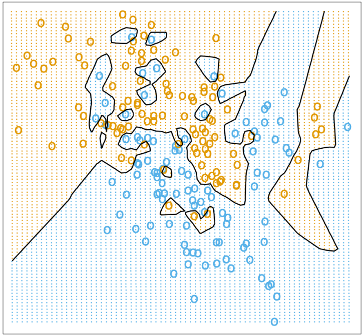
- Discrete label/output space $\Rightarrow$ essentially f is non-differentiable.
- Ambiguity on boundaries, and the trade-off between precision and robustness





K-Nearest Neighbor Classifier: Maybe The Simplest Classifier

- Given a set of labeled data $\{\boldsymbol{x}_n, y_n\}$, where $y_n \in \{0, 1\}$
- 1-NN: For a sample $\boldsymbol{x}$

$$y_{\boldsymbol{x}} := \arg\min_{y_n} d(\boldsymbol{x}_n, \boldsymbol{x})$$

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$$\hat{p}(y|\boldsymbol{x}) = \frac{1}{|\mathcal{N}_h(\boldsymbol{x})|} \sum_{n \in \mathcal{N}_h(\boldsymbol{x})} \{d(\boldsymbol{x}_n, \boldsymbol{x}) \leq h\} y_n$$

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- Is it a special case of Nadaraya-Watson estimator?

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Naïve Bayes Classifier: More Extensions

Multinomial Naïve Bayes: For $\boldsymbol{x} \in \mathbb{N}^D$:

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Bernoulli Naïve Bayes: For $\boldsymbol{x} \in \{0,1\}^D$:

$$p(\boldsymbol{x}|y=k) = \prod_{d=1}^{D} p_{k,d}^{x_d} (1 - p_{k,d})^{(1-x_d)} \tag{7}$$

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Motivations:

- The data belonging to different classes have clustering structures.

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- Relax the assumption of feature independence

Principle: (Take two-class case as an example)

- Assume $p(\boldsymbol{x}|y=0)$ and $p(\boldsymbol{x}|y=1)$ are normal distributions:

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- **Bayes optimal solution:**

$$y_{\boldsymbol{x}} = 1 \quad \Leftrightarrow \quad \exists T,\ \log \frac{p(\boldsymbol{x}|y=1)}{p(\boldsymbol{x}|y=0)} > T \tag{10}$$

Typically, we set $T=0$.

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$$\log \frac{p(\boldsymbol{x}|y=1)}{p(\boldsymbol{x}|y=0)} = 2(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)^T \boldsymbol{\Sigma}^{-1} \boldsymbol{x} - (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{\mu}_1 + \boldsymbol{\mu}_0) > 0 (= T) \tag{11}$$

Derive it.

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- **Decision criterion:**

$$y_{\boldsymbol{x}} = 1 \quad \Leftrightarrow \quad \langle \boldsymbol{w}, \boldsymbol{x} \rangle > c, \ \text{where}$$
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- Let's think about the geometrical interpretation of LDA.

Generalized LDA/QDA: Fisher's Linear Discriminant

Motivations:

- Relax the assumption of shared covariance matrix
- Relax the assumption of Gaussian conditional distribution

Principle:

- For the two classes, estimate their means and covariances $\{\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i\}_{i=0,1}$.
- Project the data to 1D along a direction $\boldsymbol{w}$ (Derive the projected means and covariances)

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- **Fisher's separation** between two distributions: the ratio of the variance between the projected classes to the variance within the projected classes

$$S = \frac{\sigma^2_{\text{between}}}{\sigma^2_{\text{within}}} = \frac{(\boldsymbol{w}^T(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0))^2}{\boldsymbol{w}^T(\boldsymbol{\Sigma}_0 + \boldsymbol{\Sigma}_1)\boldsymbol{w}} \tag{13}$$

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- Fisher's linear discriminant finds the optimal projection $\boldsymbol{w}$ to maximize the separation:

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(Derive it. Hint: Consider $\frac{\partial \log S}{\partial \boldsymbol{w}} = \mathbf{0}$)

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- Recall the decision criterion is

$$\langle \boldsymbol{w}, \boldsymbol{x} \rangle > c, \quad \text{where} \quad c = \langle \boldsymbol{w}, \frac{1}{2}(\boldsymbol{\mu}_0 + \boldsymbol{\mu}_1) \rangle = \frac{1}{2}\boldsymbol{\mu}_1 \boldsymbol{\Sigma}_1^{-1} \boldsymbol{\mu}_1 - \frac{1}{2}\boldsymbol{\mu}_0 \boldsymbol{\Sigma}_0^{-1} \boldsymbol{\mu}_0. \tag{15}$$

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- **The covariance of all the classes**:

$$\boldsymbol{\Sigma}_{\text{between}} = \frac{1}{C}\sum_{i=1}^{C}(\boldsymbol{\mu}_i - \boldsymbol{\mu})(\boldsymbol{\mu}_i - \boldsymbol{\mu})^T, \quad \text{where} \quad \boldsymbol{\mu} = \frac{1}{C}\sum_{i=1}^{C}\boldsymbol{\mu}_i$$

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$$\boldsymbol{\Sigma}_{\text{between}} = \frac{1}{C}\sum\nolimits_{i=1}^{C}(\boldsymbol{\mu}_i - \boldsymbol{\mu})(\boldsymbol{\mu}_i - \boldsymbol{\mu})^T, \quad \text{where} \quad \boldsymbol{\mu} = \frac{1}{C}\sum\nolimits_{i=1}^{C}\boldsymbol{\mu}_i \tag{16}$$

- Fisher's separation becomes

$$S = \frac{\boldsymbol{w}^T\boldsymbol{\Sigma}_{\text{between}}\boldsymbol{w}}{\boldsymbol{w}^T\boldsymbol{\Sigma}\boldsymbol{w}}.$$

Multi-class LDA

- From find a hyperplane to find a subspace which appears to contain all of the class variability.

Practical Implementation:

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- When $\boldsymbol{w}$ is an eigenvector of $\boldsymbol{\Sigma}^{-1}\boldsymbol{\Sigma}_{\text{between}}$, the separation is equal to the corresponding eigenvalue.

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One against the rest

- Train C LDA classifiers, each of which maximizes the separation of one class and the remaining classes.

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Pairwise classification

- Train $C(C-1)/2$ LDA classifiers, each of which maximize the separation of arbitrary two classes.

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$$X\beta = \eta = g(\mu) = \ln\left(\frac{\mu}{1-\mu}\right) \Rightarrow \quad \mu = \frac{\exp(X\beta)}{1+\exp(X\beta)} = \underbrace{\frac{1}{1+\exp(-X\beta)}}_{\text{Sigmoid}} \tag{18}$$

Learning Logistic Regression (LR) via The MLE of The GLM

- Given a set of labeled data $\{\boldsymbol{x}_n, y_n\}_{n=1}^N$, the MLE of LR is

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- As a result, (19) becomes the (binary) cross entropy loss:

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- No closed-form solution, GD or SGD is required.

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From Logistic Regression to Softmax Regression

Given labeled data for C classes:

- From Bernoulli distribution to Categorical Distribution: $p(\boldsymbol{y}) = \prod_{i=1}^{C} p_i^{y_i}$, where $\boldsymbol{y}$ is one-hot label vector.

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(Question: Is softmax shift-invariant?)

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- MLE:

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In many tasks, their performance is similar, especially for simple 2-classification problems for low-dimensional data.

In Summary

- Classification problem and its challenges
- Linear discriminant analysis (LDA)
- Logistic regression

Next...

- Support-Vector Machine (SVM)