Classification

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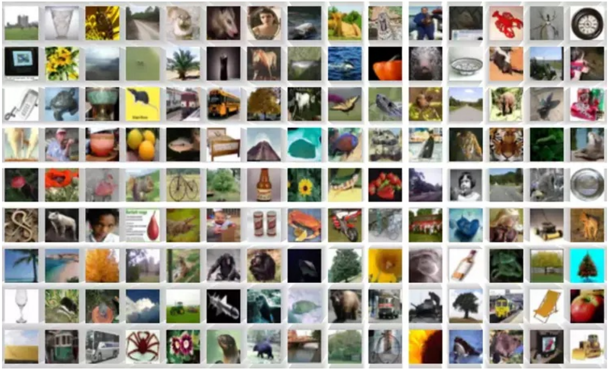
Classification problem

- Classification: assign a label (or category, class) to an observation based on its features
- $\mathcal{X}$: input space (e.g. $\mathbb{R}^d$); $\mathcal{Y}$: output space (e.g. $\{1, 2, \ldots, K\}$)
- $x \in \mathcal{X}$: feature vector, input, data point...
- $y \in \mathcal{Y}$: label, category, class...
- Classifier: a mapping $f : \mathcal{X} \to \mathcal{Y}$
- Goal: construct a classifier f that accurately predicts the label y given the features x

MNIST dataset

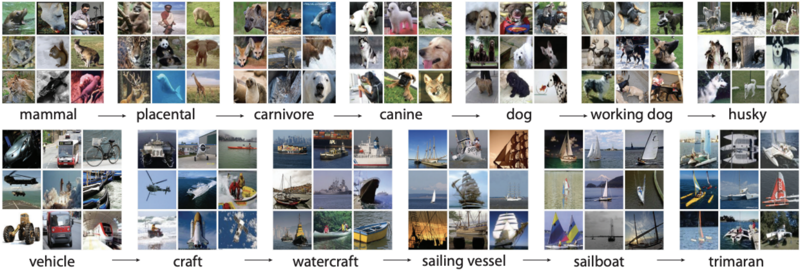
- Input: 28x28 gray scale (1 channel) images, i.e., $\mathcal{X} = \mathbb{R}^{28\times 28}$ or $\mathbb{R}^{784}$
- Output: digits 0 through 9 (i.e., $\mathcal{Y} = \{0, 1, \ldots, 9\}$)

CIFAR datasets



- Input: 32×32 RGB color (3 channels) images, i.e., $\mathcal{X} = \mathbb{R}^{32\times32\times3}$ or $\mathbb{R}^{3072}$
- Output: 10 classes (airplanes, cars, birds, cats, deer, dogs, frogs, horses, ships, and trucks) or 100 classes

ImageNet dataset



- Input: varies, often high-resolution (often $224 \times 224 \times 3$)
- Output: 1000 different categories

Mathematical set-up

- Modeling assumption: the data (input-output pairs) come from an underlying data distribution ρ over $\mathcal{X} \times \mathcal{Y}$
- Training data: $(x_1, y_1), \ldots, (x_n, y_n) \overset{\text{i.i.d.}}{\sim} \rho$
- Error metric: for any given classifier f, its risk, defined as the average (expected) classification error on a new data is

$$R(f) := \mathbb{P}_{(X,Y)\sim\rho}(f(X) \neq Y)$$

- Supervised learning: build a classifier f based on training data, that makes the average classification error as small as possible

Questions

- Does there exists a "best" classifier?

  — this lecture

- Can we construct this "best" classifier with the information of ρ?

  — this lecture

- What can we do when we only have a finite number of training data?

  — next few weeks

Bayes optimal classifier: binary case

- Consider the binary case: $\mathcal{Y} = \{0, 1\}$
- Define the Bayes classifier: for any $x \in \mathcal{X}$,

$$f^\star(x) := \begin{cases} 1, & \text{if } \mathbb{P}(Y = 1 \mid X = x) \geq \mathbb{P}(Y = 0 \mid X = x), \\ 0, & \text{otherwise.} \end{cases}$$

Theorem 2.1 (Bayes optimal classifier: binary case)

The Bayes classifier $f^\star$ minimizes the misclassification error, i.e.,

$$f^\star \in \underset{f:\mathcal{X}\to\mathcal{Y}}{\arg\min}\, \mathbb{P}_{(X,Y)\sim\rho}(f(X) \neq Y).$$

A few remarks

Bayes optimal classifier

$$f^\star(x) \coloneqq \begin{cases} 1, & \text{if } \mathbb{P}(Y = 1 \mid X = x) \geq \mathbb{P}(Y = 0 \mid X = x), \\ 0, & \text{otherwise.} \end{cases}$$

- Depends on the true underlying data distribution ρ
- The optimal classifier might not be unique
- When $\mathcal{X}$ is discrete, it is equivalent to

$$f^\star(x) \coloneqq \begin{cases} 1, & \text{if } \mathbb{P}(X = x, Y = 1) \geq \mathbb{P}(X = x, Y = 0), \\ 0, & \text{otherwise.} \end{cases}$$

Bayes risk: binary case

- Bayes risk:
$$R^\star := \mathbb{P}_{(X,Y)\sim\rho}(f^\star(X) \neq Y)$$
- The Bayes risk serves as a lower bound for the classification error that any practical classifier can achieve:
$$R^\star = \min_{f:\mathcal{X}\to\mathcal{Y}} \mathbb{P}_{(X,Y)\sim\rho}(f(X) \neq Y).$$
- It represents the inherent uncertainty in the classification problem due to overlapping distributions of the classes.
- Excess risk: $R(f) - R^\star$

Bayes optimal classifier: multiclass setting

- Consider the multiclass case: $\mathcal{Y} = \{1, \ldots, K\}$
- Define the Bayes classifier: for any $x \in \mathcal{X}$,

$$f^\star(x) \coloneqq \operatorname*{arg\,max}_{y \in \mathcal{Y}} \mathbb{P}(Y = y \mid X = x)$$

Theorem 2.2 (Bayes optimal classifier: multiclass case)

The Bayes classifier $f^\star$ minimizes the misclassification error, i.e.,

$$f^\star \in \operatorname*{arg\,min}_{f : \mathcal{X} \to \mathcal{Y}} \mathbb{P}_{(X,Y)\sim\rho}(f(X) \neq Y).$$

More general loss function?

- Consider more general loss function $\ell : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$
- Define the risk for a classifier $f : \mathcal{X} \to \mathcal{Y}$ as

$$R_\ell(f) := \mathbb{E}_{(X,Y)\sim\rho}[\ell(f(X), Y)]$$

- Example: with 0-1 loss $\ell(y, y') = \mathbb{1}\{y \neq y'\}$, we recover the average classification error

$$R(f) = \mathbb{P}_{(X,Y)\sim\rho}(f(X) \neq Y)$$

- Goal: find f that minimizes the risk $R_\ell(f)$ (the Bayes classifier might not be optimal...)

Question: Can you think of settings where other types of loss functions are more appropriate than the 0-1 loss?

Example: traffic signs

- $\mathcal{Y} = \{\text{stop sign}, 50 \text{ mph}, 40 \text{ mph}\}$.
- Predicting 50 mph when it is actually a stop sign is worse than predicting 40 mph when it is actually 50mph.
- 0-1 loss is not suitable here...

Supervised learning

- In practice, we don't know ρ. It is in general impossible to compute the Bayes classifier $f^\star$
- Goal: build a classifier $f : \mathcal{X} \to \mathcal{Y}$ based on training data $(x_1, y_1), \ldots, (x_n, y_n) \overset{\text{i.i.d.}}{\sim} \rho$
- Hope: achieve small excess risk $R(f) - R^\star$
- High-level framework:
  - Make some modeling assumptions on ρ
  - Design a good classifier f under this setup
  - For example, a good classifier may satisfy

    $$R(f) - R^\star \leq h(n)$$

    where $h(n)$ is a function of the sample size n describing the rate of convergence, e.g., $h(n) = O(1/n)$.

Linear Methods for Classification

Linear classifiers

- Linear classifiers
  - Hyperplane $\mathcal{H}_{\boldsymbol{\beta},\beta_0} = \{\boldsymbol{x} \in \mathbb{R}^d : \langle \boldsymbol{\beta}, \boldsymbol{x} \rangle + \beta_0 = 0\}$
  - Half planes cut by $\mathcal{H}_{\boldsymbol{\beta},\beta_0}$:

$$\mathcal{H}^+_{\boldsymbol{\beta},\beta_0} = \{\boldsymbol{x} \in \mathbb{R}^d : \langle \boldsymbol{\beta}, \boldsymbol{x} \rangle + \beta_0 \geq 0\},$$
$$\mathcal{H}^-_{\boldsymbol{\beta},\beta_0} = \{\boldsymbol{x} \in \mathbb{R}^d : \langle \boldsymbol{\beta}, \boldsymbol{x} \rangle + \beta_0 < 0\}.$$

  - Example: in the binary case, the linear classifier has the form

$$f(\boldsymbol{x}) = \mathbb{1}\{\boldsymbol{x} \in \mathcal{H}^+_{\boldsymbol{\beta},\beta_0}\}$$

- Three approaches to learn a linear classifier from the data:
  - Linear discriminant analysis (LDA)
  - Logistic regression
  - Support vector machines (SVMs)

Linear discriminant analysis (LDA)

- Model set-up: $\mathcal{X} = \mathbb{R}^d$, $\mathcal{Y} = \{1, \ldots, K\}$. For $k = 1, \ldots, K$,

$$\mathbb{P}(Y = k) = \omega_k, \qquad X \mid Y = k \sim \mathcal{N}(\boldsymbol{\mu}_k, \boldsymbol{\Sigma})$$

  where $\omega_k \geq 0$, $\sum_{k=1}^{K} \omega_k = 1$, $\mu_k \in \mathbb{R}^d$, $\boldsymbol{\Sigma} \in \mathbb{S}_+^d$

- The Bayes classifier under this setup: for any $\boldsymbol{x}$, compute

$$\delta_k(\boldsymbol{x}) \coloneqq \underbrace{\boldsymbol{x}^\top \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_k - \frac{1}{2} \boldsymbol{\mu}_k^\top \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_k + \log \omega_k}_{\propto \mathbb{P}(Y=k \mid \boldsymbol{x}) + \text{constant}} .$$

  Let $f^\star(\boldsymbol{x}) = \arg\max_{1 \leq k \leq K} \delta_k(\boldsymbol{x})$.

- Issue: model parameters are unknown...

Plug-in approach

- Suppose we have i.i.d. data $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_n, y_n)$
- For each $1 \le k \le K$, let $n_k = \sum_{i=1}^{n} \mathbb{1}\{y_i = k\}$ and

$$\widehat{\boldsymbol{\mu}}_k = \frac{1}{n_k} \sum_{i: y_i = k} \boldsymbol{x}_i, \qquad \widehat{\omega}_k = \frac{n_k}{n}$$

- Estimate the covariance matrix

$$\widehat{\boldsymbol{\Sigma}} = \frac{1}{N - K} \sum_{k=1}^{K} \sum_{i: y_i = k} (\boldsymbol{x}_i - \widehat{\boldsymbol{\mu}}_k)(\boldsymbol{x}_i - \widehat{\boldsymbol{\mu}}_k)^\top$$

- Replace $\boldsymbol{\mu}_k$, ω_k, $\boldsymbol{\Sigma}$ with $\widehat{\boldsymbol{\mu}}_k$, $\widehat{\omega}_k$, $\widehat{\boldsymbol{\Sigma}}$

$$\widehat{\delta}_k(\boldsymbol{x}) := \underbrace{\boldsymbol{x}^\top \widehat{\boldsymbol{\Sigma}}^{-1} \widehat{\boldsymbol{\mu}}_k - \frac{1}{2} \widehat{\boldsymbol{\mu}}_k^\top \widehat{\boldsymbol{\Sigma}}^{-1} \widehat{\boldsymbol{\mu}}_k + \log \widehat{\omega}_k}_{\text{linear in } \boldsymbol{x}}.$$

Generalization

- Consider a more general set-up: for $k = 1, \ldots, K$, assume

$$\mathbb{P}(Y = k) = \omega_k, \qquad X \mid Y = k \sim \mathcal{N}(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_{\color{red}k})$$

  where $\omega_k \geq 0$, $\sum_{k=1}^{K} \omega_k = 1$, $\mu_k \in \mathbb{R}^d$, $\boldsymbol{\Sigma}_k \in \mathbb{S}_+^d$
- This setup will lead to the so-called quadratic discriminant analysis (QDA)
- After class: derive QDA
  - What is the Bayes classifier under this setup?
  - How to derive a practical (data-driven) classifier?

Logistic regression

- Model set-up: $\mathcal{X} = \mathbb{R}^d$, $\mathcal{Y} = \{0, 1, \ldots, K\}$. Let

$$\mathbb{P}(Y = k \mid \boldsymbol{x}) = \frac{\exp(\boldsymbol{\beta}_k^\top \boldsymbol{x} + \beta_{0,k})}{1 + \sum_{k'=1}^K \exp(\boldsymbol{\beta}_{k'}^\top \boldsymbol{x} + \beta_{0,k'})}, \quad (1 \le k \le K),$$

$$\mathbb{P}(Y = 0 \mid \boldsymbol{x}) = \frac{1}{1 + \sum_{k'=1}^K \exp(\boldsymbol{\beta}_{k'}^\top \boldsymbol{x} + \beta_{0,k})},$$

where the parameters $\boldsymbol{\beta}_k \in \mathbb{R}^d$, $\beta_{0,k} \in \mathbb{R}$ for $k = 1, \ldots, K$

Logistic regression

- Model set-up: $\mathcal{X} = \mathbb{R}^d \times \{1\}$, $\mathcal{Y} = \{0, 1, \ldots, K\}$. Let

$$\mathbb{P}(Y = k \mid \boldsymbol{x}) = \frac{\exp(\boldsymbol{\beta}_k^\top \boldsymbol{x})}{1 + \sum_{k'=1}^K \exp(\boldsymbol{\beta}_{k'}^\top \boldsymbol{x})}, \qquad (k = 1, \ldots, K),$$
$$\mathbb{P}(Y = 0 \mid \boldsymbol{x}) = \frac{1}{1 + \sum_{k'=1}^K \exp(\boldsymbol{\beta}_{k'}^\top \boldsymbol{x})},$$

  where the parameters $\boldsymbol{\beta}_k \in \mathbb{R}^{d+1}$ for $k = 1, \ldots, K$
- Bayes classifier: $f(\boldsymbol{x}) = \arg\max_{0 \le k \le K} \mathbb{P}(Y = k \mid \boldsymbol{x})$
- Estimate $\boldsymbol{\beta}_k$'s: maximum likelihood estimation (MLE)

Maximum likelihood estimation

- Suppose we have i.i.d. data $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_n, y_n)$
- The negative log-likelihood function

$$\ell(\boldsymbol{\beta}) = -\frac{1}{n}\sum_{k=1}^{K}\sum_{i:y_i=k}\boldsymbol{x}_i^\top\boldsymbol{\beta}_k + \frac{1}{n}\sum_{i=1}^{n}\log\left[1 + \sum_{k'=1}^{K}\exp(\boldsymbol{x}_i^\top\boldsymbol{\beta}_{k'})\right]$$

- Maximum likelihood estimation (MLE)

$$\widehat{\boldsymbol{\beta}} := \arg\min_{\boldsymbol{\beta}} \ell(\boldsymbol{\beta})$$

- Convex optimization: solve by e.g., gradient descent

$$\boldsymbol{\beta}^{(t+1)} = \boldsymbol{\beta}^{(t)} - \eta\nabla\ell(\boldsymbol{\beta}^{(t)}) \qquad (t = 0, 1, \ldots)$$