Georgia Tech College of Computing

CS4641 Spring 2025

Multi-Class Logistic Regression
Naive Bayes

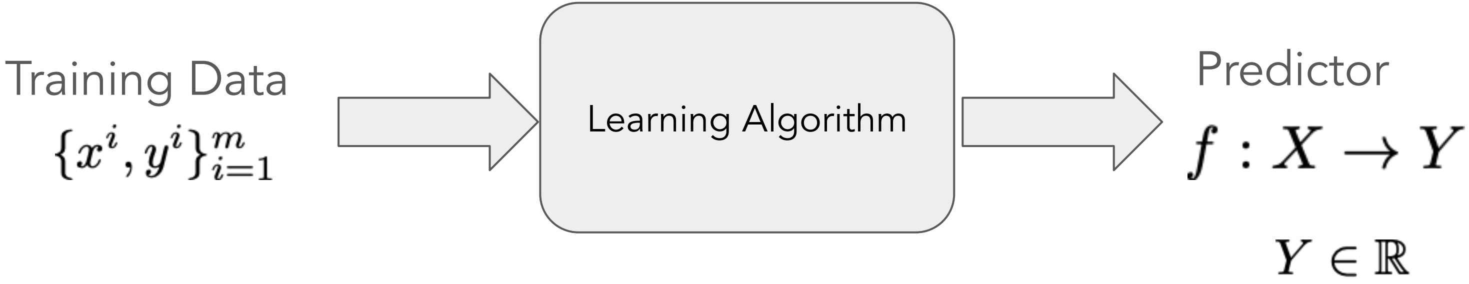
Bo Dai
School of CSE, Georgia Tech
bodai@cc.gatech.edu

ML Algorithm Pipeline

General ML Algorithm Pipeline

1. Build probabilistic models
2. Derive loss function (by MLE or MAP….)
3. Select optimizer

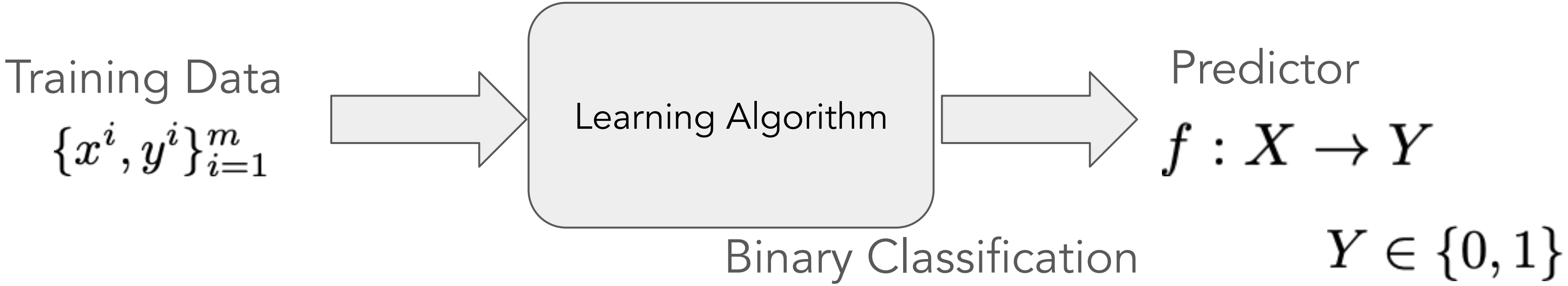
Regression Algorithms



Linear Regression Pipeline

1. Build probabilistic models:
   Gaussian Distribution + Linear Model
2. Derive loss function: MLE and MAP
3. Select optimizer
   Necessary Condition vs. (Stochastic) GD

Binary Classification Algorithms



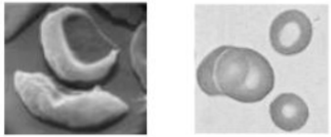
Binary Logistic Regression Pipeline

1. Build probabilistic models:
   Bernoulli Distribution + + Linear Model
2. Derive loss function: MLE and MAP
3. Select optimizer: (Stochastic) Gradient Descent

Classification Tasks

Feature, X | Label, Y

Diagnosing sickle cell anemia



Anemic cell
Healthy cell

$Y \in \{0, 1\}$

Tax Fraud Detection

Refund	Marital Status	Taxable Income
No	Married	80K

Cheat
?

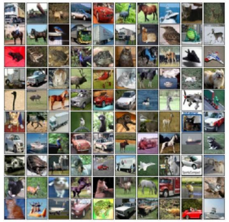
$Y \in \{0, 1\}$

Web Classification

Sports
Science
News

$Y \in \{0, 1, 2, \ldots, k\}$

Image Classification



Airplane
Automobile
Bird
...

$Y \in \{0, 1, 2, \ldots, k\}$

Multiclass Logistic Regression Algorithms

Training Data
$\{x^i, y^i\}_{i=1}^m$

Learning Algorithm

Classifier
$f : X \rightarrow Y$

Multiclass Logistic Regression Algorithms

Training Data

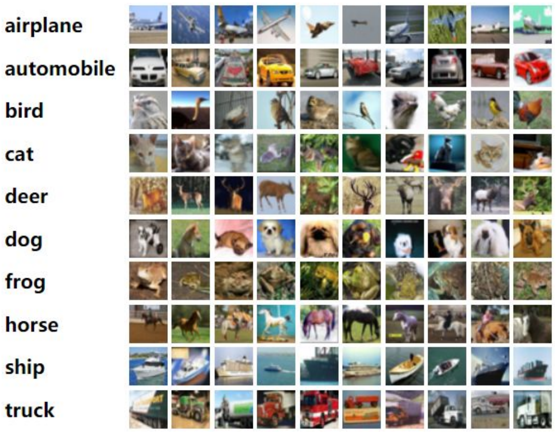
$\{x^i, y^i\}_{i=1}^m$

Learning Algorithm

Classifier

$f : X \to Y$

Multiclass Classification $\quad Y \in \{0, 1, \ldots, k\}$



Multiclass Logistic Regression Algorithms

Training Data $\{x^i, y^i\}_{i=1}^m$ → Learning Algorithm → Classifier $f : X \rightarrow Y$

Multiclass Classification $Y \in \{0, 1, \ldots, k\}$

Multiclass Logistic Regression Pipeline

1. Build probabilistic models
2. Derive loss function (by MLE or MAP)
3. Select optimizer

Probabilistic Model in Binary Classification:
Bernoulli Likelihood

$$\begin{cases} p & \text{if } y = 1 \\ 1 - p & \text{if } y = 0 \end{cases} \qquad p \in [0, 1]$$

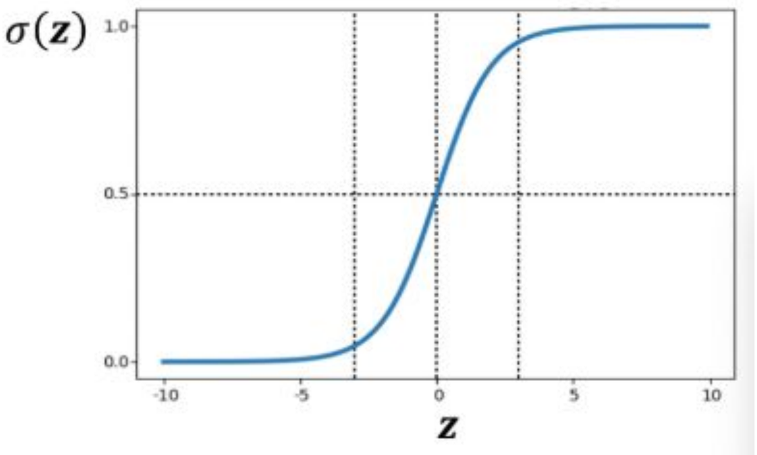
$$p(y) = p^y (1 - p)^{(1-y)}$$

Probabilistic Model in Binary Classification:
Bernoulli Likelihood

$$p(y) = p^y(1-p)^{(1-y)}$$

$$p(y|x;\theta) = p(y=1|\theta^\top x)^y\{1 - p(y=1|\theta^\top x)\}^{(1-y)}$$

$$\sigma(\mathbf{z}) = \frac{1}{1+e^{-\mathbf{z}}} = \frac{e^{\mathbf{z}}}{1+e^{\mathbf{z}}}$$



$$p(y=1|\theta^\top x) = \sigma(\theta^\top x) \in [0,1]$$

Probabilistic Model in Multiclass Classification:
Categorical Likelihood

$$p(y = i) = p_i, \quad \sum_{i=1}^{k} p_i = 1, \quad p_i \geq 0$$

$$p(y) = \prod_{i=1}^{k} p_i^{y_i}$$

$$p = (p_1, p_2, \ldots, p_k)$$

$$y = (y_1, y_2, \ldots, y_k), \quad y_i \in 0, 1, \quad \sum_{i=1}^{k} y_i = 1$$

1-of-k code

Probabilistic Model in Multiclass Classification: Categorical Likelihood

$$p(y) = \prod_{i=1}^{k} p_i^{y_i}$$

$$p = (p_1, p_2, \ldots, p_k)$$

$$p(y|\{\theta_i^\top x\}_{i=1}^k) = \prod_{i=1}^{k} p(y_i = 1|\theta_i^\top x)^{y_i}$$

Softmax Parametrization

$$p(y_i = 1|\theta_i^\top x) \in (0,1), \quad \sum_{i=1}^{k} p(y_i = 1|\theta_i^\top x) = 1$$

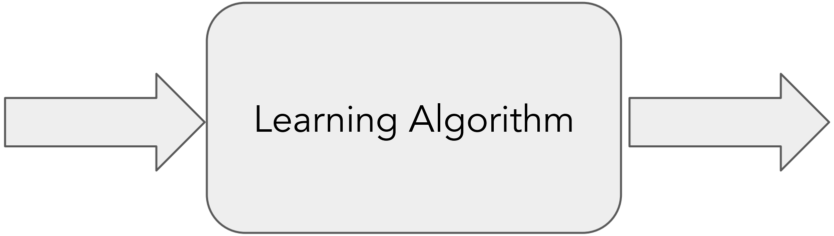
Positivity $$p(y_i = 1|\theta_i^\top x) \propto \exp(\theta_i^\top x)$$

Normalization $$p(y_i = 1|\theta_i^\top x) = \frac{\exp(\theta_i^\top x)}{\sum_{i=1}^{k} \exp(\theta_i^\top x)}$$

Multiclass Logistic Regression Algorithms

Training Data

$\{x^i, y^i\}_{i=1}^m$



Classifier

$f : X \to Y$

Multiclass Classification $Y \in \{0, 1, \ldots, k\}$

Multiclass Logistic Regression Pipeline

1. Build probabilistic models
2. Derive loss function (by MLE or MAP)
3. Select optimizer

MLE

- Given all input data $\{x^i, y^i\}_{i=1}^m$

$$p(y^i|\theta^\top x^i) = \prod_{j=1}^{k} p(y_j^i = 1|\theta^\top x^i)^{y_j^i}$$

- Log-likelihood

$$\ell(\theta) = \sum_{i=1}^{m} \sum_{j=1}^{k} y_j^i \log p(y_j^i = 1|\theta^\top x^i)$$

MLE

- Given all input data $\{x^i, y^i\}_{i=1}^m$

$$p(y^i|\theta^\top x^i) = \prod_{j=1}^{k} p(y_j^i = 1|\theta^\top x^i)^{y_j^i}$$

- Log-likelihood

$$\ell(\theta) = \sum_{i=1}^{m}\sum_{j=1}^{k} y_j^i \log p(y_j^i = 1|\theta^\top x^i)$$

$$= \sum_{i=1}^{m}\sum_{j=1}^{k} y_j^i \log \frac{\exp(\theta_j^\top x^i)}{\sum_{c=1}^{k}\exp(\theta_c^\top x^i)}$$

$$= \sum_{i=1}^{m}\sum_{j=1}^{k} y_j^i(\theta_j^\top x^i) - \sum_{i=1}^{m}\log\sum_{c=1}^{k}\exp(\theta_c^\top x^i)$$

MLE

- Given all input data $\{x^i, y^i\}_{i=1}^m$

$$p(y^i|\theta^\top x^i) = \prod_{j=1}^{k} p(y_j^i = 1|\theta^\top x^i)^{y_j^i}$$

- Log-likelihood

$$\ell(\theta) = \sum_{i=1}^{m}\sum_{j=1}^{k} y_j^i \log p(y_j^i = 1|\theta^\top x^i) \quad \text{cross-entropy}$$

$$= \sum_{i=1}^{m}\sum_{j=1}^{k} y_j^i \log \frac{\exp(\theta_j^\top x^i)}{\sum_{c=1}^{k} \exp(\theta_c^\top x^i)}$$

$$= \sum_{i=1}^{m}\sum_{j=1}^{k} y_j^i (\theta_j^\top x^i) - \sum_{i=1}^{m} \log \sum_{c=1}^{k} \exp(\theta_c^\top x^i)$$

MAP

- Likelihood

$$p(y=j|x,\theta) = \frac{\exp(\theta_j^\top x)}{\sum_{c=1}^{k}\exp(\theta_c^\top x)}$$

- Prior

$$p(\theta) \propto \exp(-\lambda\|\theta\|_2^2)$$

$$\max_\theta \log p(\theta|\{x^i, y^i\}_{i=1}^m) = \log L(\theta) + \log p(\theta)$$

$$= \sum_{i=1}^{m}\sum_{j=1}^{k} y_j^i \theta_j^\top x^i - \sum_{i=1}^{m}\log\sum_{c=1}^{k}\exp(\theta_c^\top x^i) - \lambda||\theta||_2^2$$

Logistic Regression is a Linear Classifier

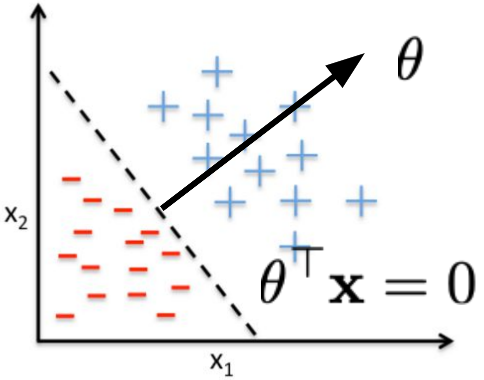
- Decision boundaries for Logistic Regression?
  - At the decision boundary, label 1/0 are equiprobable.

$$P(y=1|\mathbf{x},\theta) = \frac{1}{1+e^{-\theta^\top \mathbf{x}}}, \qquad P(y=0|\mathbf{x},\theta) = \frac{1}{1+e^{\theta^\top \mathbf{x}}}$$

to be equal: $e^{-\theta^\top \mathbf{x}} = e^{\theta^\top \mathbf{x}}$, whose only solution is $\theta^\top \mathbf{x} = 0.$

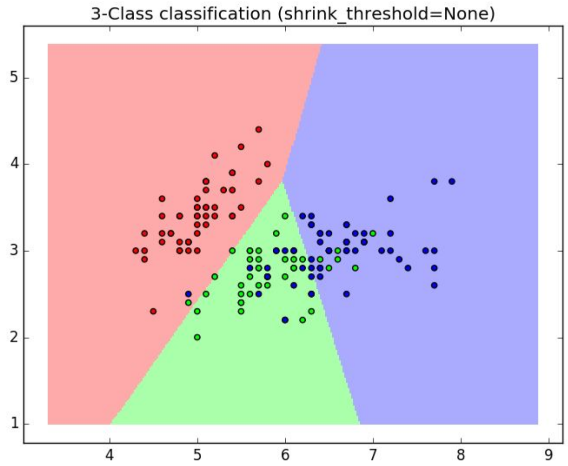
✓ ⇒ Decision boundary is linear.

✓ ⇒ Logistic regression is a probabilistic linear classifier.



Multiclass Logistic Regression is a Linear Classifier

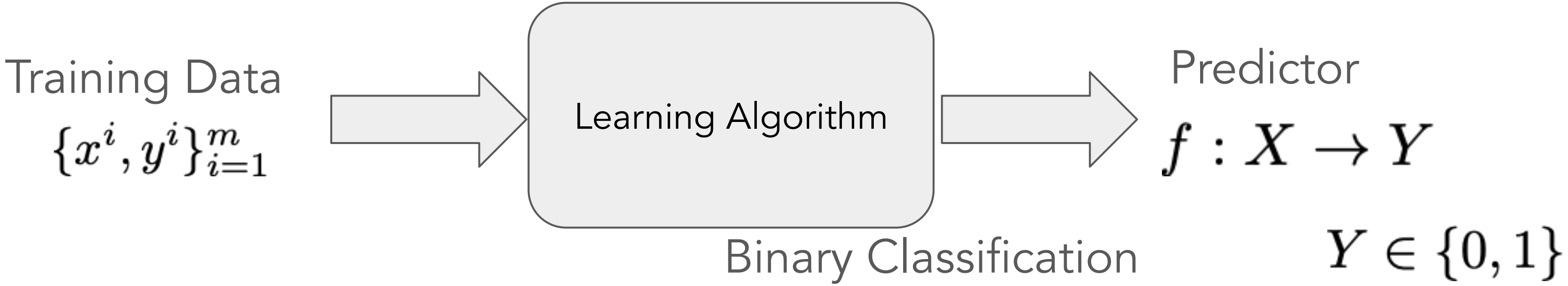
- Decision boundaries for Multiclass Logistic Regression?



✓ ⇒ Decision boundary is linear.

✓ ⇒ Multiclass Logistic regression is a probabilistic linear classifier.

Multiclass Logistic Regression Algorithms



Multiclass Logistic Regression Pipeline

1. Build probabilistic models
2. Derive loss function (by MLE or MAP)
3. Select optimizer

Select Optimizer

$$\ell(\theta) = \sum_{i=1}^{m} \sum_{j=1}^{k} y_j^i (\theta_j^\top x^i) - \sum_{i=1}^{m} \log \sum_{c=1}^{k} \exp(\theta_c^\top x^i)$$

- Necessary Condition
- (Stochastic) Gradient Descent

Necessary Condition?

$$p(y = j|x, \theta) = \frac{\exp(\theta_j^\top x)}{\sum_{c=1}^{k} \exp(\theta_c^\top x)}$$

$$\frac{\partial \log L(\theta)}{\partial \theta} = \sum_{i=1}^{m} \sum_{j=1}^{k} (y_j^i - p(y_j^i = 1|x^i, \theta))x^i = 0$$

Nonlinear Equation!
Does NOT admit a closed-form solution

Gradient Calculation of MLE

$$\max_{\theta} \log L(\theta) = \sum_{i=1}^{m}\sum_{j=1}^{k} y_j^i \theta_j^\top x^i - \sum_{i=1}^{m} \log \sum_{c=1}^{k} \exp(\theta_c^\top x^i)$$

$$\frac{\partial \log L(\theta)}{\partial \theta} = \sum_{i=1}^{m}\sum_{j=1}^{k} (y_j^i - p(y_j^i = 1 | x^i, \theta)) x^i$$

$$p(y_j^i = 1 | x^i, \theta) = \frac{\exp(\theta_j^\top x^i)}{\sum_{c=1}^{k} \exp(\theta_c^\top x^i)}$$

Gradient Calculation of MAP

$$\max_{\theta} \log L(\theta) = \sum_{i=1}^{m} \sum_{j=1}^{k} y_j^i \theta_j^\top x^i - \sum_{i=1}^{m} \log \sum_{c=1}^{k} \exp(\theta_c^\top x^i) - \lambda ||\theta||_2^2$$

$$\frac{\partial \log L(\theta)}{\partial \theta} = \sum_{i=1}^{m} \sum_{j=1}^{k} (y_j^i - p(y_j^i = 1 | x^i, \theta)) x^i - 2\lambda\theta$$

(Stochastic) Gradient Descent

- Initialize parameter θ^0

- Do

$$\theta^{t+1} \leftarrow \theta^t + \eta \sum_{i=1}^{m} \sum_{j=1}^{k} (y_j^i - p(y_j^i = 1 | x^i, \theta)) x^i \boxed{-2\lambda\theta}$$

Multiclass Logistic Regression Algorithms

Training Data

$\{x^i, y^i\}_{i=1}^m$

Learning Algorithm

Classifier

$f : X \to Y$

Multiclass Classification $Y \in \{0, 1, \ldots, k\}$

Multiclass Logistic Regression Pipeline

1. Build probabilistic models:
   Categorical Distribution + Linear Model
2. Derive loss function: MLE and MAP
3. Select optimizer: (Stochastic) Gradient Descent

Naive Bayes Classification

Training Data

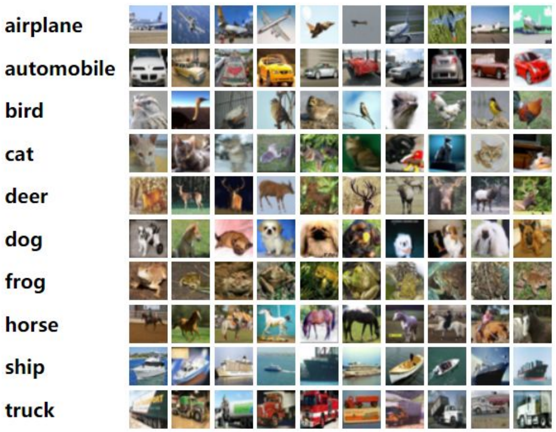
$$\{x^i, y^i\}_{i=1}^m$$

Learning Algorithm

Classifier

$$f : X \to Y$$

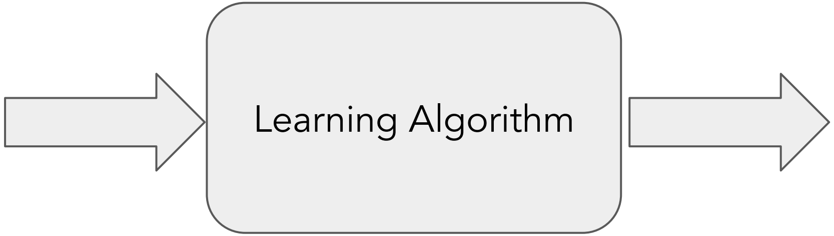
Multiclass Classification $\quad Y \in \{0, 1, \ldots, k\}$



Naive Bayes Classification

Training Data

$\{x^i, y^i\}_{i=1}^m$



Classifier

$f : X \to Y$

Multiclass Classification $Y \in \{0, 1, \ldots, k\}$

Gaussian Naive Bayes Pipeline

1. Build probabilistic models
2. Derive loss function (by MLE or MAP)
3. Select optimizer

Bayes' Rule

Softmax in Multiclass Classification

$$p(y_i = 1|\theta_i^\top x) = \frac{\exp(\theta_i^\top x)}{\sum_{i=1}^{k} \exp(\theta_i^\top x)}$$

likelihood

Prior

$$P(y|x) = \frac{P(x|y)P(y)}{P(x)} = \frac{P(x,y)}{\sum_z P(x,y)}$$

posterior

normalization constant

Bayes' Rule

likelihood

Prior

$$P(y|x) = \frac{P(x|y)P(y)}{P(x)} = \frac{P(x,y)}{\sum_z P(x,y)}$$

posterior

normalization constant

Prior: $P(y)$ $\quad \pi = (\pi_1, \pi_2, \ldots, \pi_k), \quad \sum_{i=1}^{k} \pi_i = 1, \pi_i \geq 0$

Likelihood (class conditional distribution : $p(x|y) = \mathcal{N}(x|\mu_y, \Sigma_y)$

Posterior: $P(y|x) = \dfrac{P(y)\mathcal{N}(x|\mu_y, \Sigma_y)}{\sum_y P(y)\mathcal{N}(x|\mu_y, \Sigma_y)}$

Decision with Bayes' Rule

- The posterior probability of a test point

$$q_i(x) := P(y = i|x) = \frac{P(x|y)P(y)}{P(x)}$$

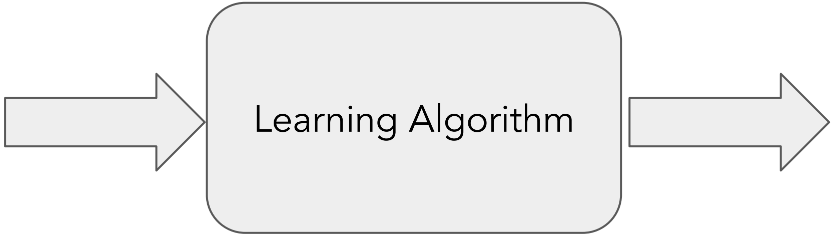
- Bayes decision rule:
  - If $q_i(x) > q_j(x)$, then $y = i$, otherwise $y = j$

- Alternatively:
  - If ratio $l(x) = \frac{P(x|y=i)}{P(x|y=j)} > \frac{P(y=j)}{P(y=i)}$, then $y = i$, otherwise $y = j$
  - Or look at the log-likelihood ratio $h(x) = \ln \frac{q_i(x)}{q_j(x)}$

Naive Bayes

Training Data

$\{x^i, y^i\}_{i=1}^m$



Classifier

$f : X \to Y$

Multiclass Classification $Y \in \{0, 1, \ldots, k\}$

General ML Algorithm Pipeline

1. Build probabilistic models
2. Derive loss function (by MLE or MAP)
3. Select optimizer

MLE of Naive Bayes

$$\theta = [\mu, \Sigma, \pi], \quad Z = \sqrt{(2\pi)^D \det(\Sigma)}$$

$$p(x^i|y^i_j = 1, \theta) = \frac{1}{Z} \exp\left(-\frac{1}{2}(x^i - \mu_j)^\top \Sigma_j^{-1}(x^i - \mu_j)\right)$$

$$P(y) \qquad \pi = (\pi_1, \pi_2, \ldots, \pi_k), \quad \sum_{i=1}^{k} \pi_i = 1, \pi_i \geq 0$$

MLE of Naive Bayes

$$\theta = [\mu, \Sigma, \pi], \quad Z = \sqrt{(2\pi)^D \det(\Sigma)}$$

$$p(x^i | y^i_j = 1, \theta) = \frac{1}{Z} \exp\left(-\frac{1}{2} (x^i - \mu_j)^\top \Sigma_j^{-1} (x^i - \mu_j) \right)$$

$$P(y) \qquad \pi = (\pi_1, \pi_2, \ldots, \pi_k), \quad \sum_{i=1}^{k} \pi_i = 1, \pi_i \geq 0$$

$$\log L(\theta) = \log p(x, y | \theta)$$

MLE of Naive Bayes

$$\theta = [\mu, \Sigma, \pi], \quad Z = \sqrt{(2\pi)^D \det(\Sigma)}$$

$$p(x^i | y^i_j = 1, \theta) = \frac{1}{Z} \exp\left(-\frac{1}{2}(x^i - \mu_j)^\top \Sigma_j^{-1} (x^i - \mu_j) \right)$$

$$\log L(\theta) = \log p(x, y|\theta) = \log p(y|\theta) + \log p(x|y, \theta)$$

$$\log L(\theta) = \sum_{i=1}^{N} \sum_{j=1}^{k} y^i_j \log \pi_j - \sum_{i=1}^{N} \log Z - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{k} y^i_j (x^i - \mu_j)^\top \Sigma_j^{-1} (x^i - \mu_j)$$

Want $\arg\max_{\theta} \log L(\theta)$ subject to $\sum_{j=1}^{k} \pi_j = 1$

MAP of Naive Bayes

$$p(\theta) \propto \exp(-\lambda\|\theta\|_2^2)$$

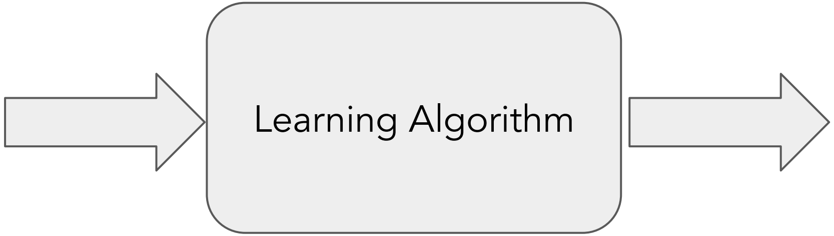
$$\log L(\theta) = \log p(x, y|\theta) = \log p(y|\theta) + \log p(x|y, \theta)$$

$$\max_{\theta} \log p(\theta|\{x^i, y^i\}_{i=1}^m) = \log L(\theta) + \log p(\theta)$$

Naive Bayes

Training Data

$\{x^i, y^i\}_{i=1}^m$



Classifier

$f : X \to Y$

Multiclass Classification $\quad Y \in \{0, 1, \ldots, k\}$

General ML Algorithm Pipeline

1. Build probabilistic models
2. Derive loss function (by MLE or MAP)
3. Select optimizer

Select Optimizer

$$\sum_{i=1}^{N}\sum_{j=1}^{k} y_j^i \log \pi_j - \log Z - \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{k} y_j^i (x^i - \mu_j)^\top \Sigma_j^{-1} (x^i - \mu_j)$$

- Necessary Condition
- (Stochastic) Gradient Descent

Gradient Calculation of MLE

Take derivative w.r.t μ_k

$$\frac{\partial \log L}{\partial \mu_k} = -\sum_{i=1}^{N} y_k^i \Sigma_k^{-1}(x^i - \mu_k) = 0$$

$$\boxed{\mu_k = \frac{\sum_{i=1}^{N} y_k^i x^i}{\sum_{i=1}^{N} y_k^i}}$$

Necessary Condition for MLE

Take derivative w.r.t Σ_k^{-1} (not Σ_k)

Note:

$$\frac{\partial \log L}{\partial \Sigma_k^{-1}} = -\sum_{i=1}^{N} y_k^i \left[-\frac{\partial \log Z_k}{\partial \Sigma_k^{-1}} - \frac{1}{2}(x^i - \mu_k)(x^i - \mu_k)^\top \right] = 0$$

$$\boxed{\Sigma_k = \frac{\sum_{i=1}^{N} y_k^i (x^i - \mu_k)(x^i - \mu_k)^\top}{\sum_{i=1}^{N} y_k^i}}$$

Necessary Condition for MLE

Take derivative w.r.t Σ_k^{-1} (not Σ_k)

Note:

$$\frac{\partial \det(A)}{\partial A} = \det(A) A^{-\top}$$

$$\det(A^{-1}) = \det(A)^{-1}$$

$$\frac{\partial x^\top A x}{\partial A} = x x^\top$$

$$\Sigma^\top = \Sigma$$

$$\frac{\partial \log L}{\partial \Sigma_k^{-1}} = -\sum_{i=1}^{N} y_k^i \left[-\frac{\partial \log Z_k}{\partial \Sigma_k^{-1}} - \frac{1}{2}(x^i - \mu_k)(x^i - \mu_k)^\top \right] = 0$$

Necessary Condition for MLE

$$Z_k = \sqrt{(2\pi)^D \det(\Sigma_k)}$$

$$\frac{\partial \log Z_k}{\partial \Sigma_k^{-1}} = \frac{1}{Z_k}\frac{\partial Z_k}{\partial \Sigma_k^{-1}} = (2\pi)^{-D/2}\det(\Sigma_k)^{-1/2}(2\pi)^{D/2}\frac{\partial \det(\Sigma_k^{-1})^{-1/2}}{\partial \Sigma_k^{-1}}$$

$$= \det(\Sigma_k^{-1})^{1/2}\left(-\frac{1}{2}\right)\det(\Sigma_k^{-1})^{-3/2}\det(\Sigma_k^{-1})\Sigma_k^\top = -\frac{1}{2}\Sigma_k$$

$$\frac{\partial \log L}{\partial \Sigma_k^{-1}} = -\sum_{i=1}^{N} y_k^i \left[\frac{1}{2}\Sigma_k - \frac{1}{2}(x^i - \mu_k)(x^i - \mu_k)^\top\right] = 0$$

$$\boxed{\Sigma_k = \frac{\sum_{i=1}^N y_k^i (x^i - \mu_k)(x^i - \mu_k)^\top}{\sum_{i=1}^N y_k^i}}$$

Necessary Condition for MLE

Use Lagrange multiplier to derive π_k

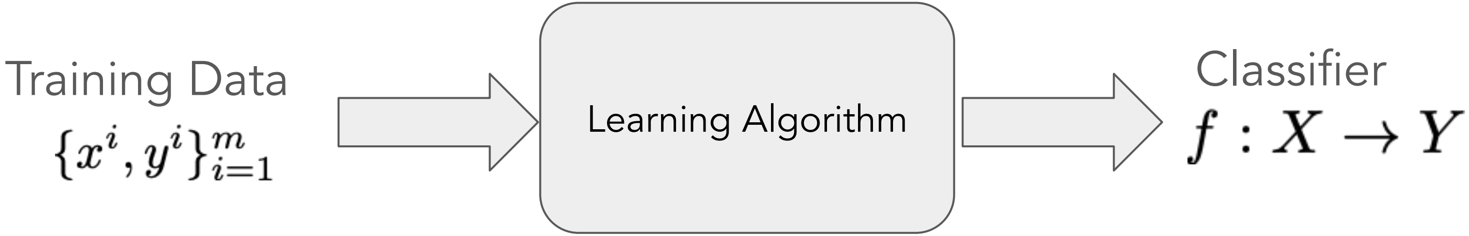
$$\frac{\partial L(\theta)}{\partial \pi_k} + \lambda \frac{\partial \sum_k \pi_k}{\partial \pi_k} = 0 \Rightarrow \lambda = -\sum_{i=1}^{N} y_k^i \frac{1}{\pi_k}$$

$$\pi_k = -\frac{\sum_{i=1}^{N} y_k^i}{\lambda}$$

Apply constraint: $\sum_k \pi_k = 1 \Rightarrow \lambda = -N$

$$\boxed{\pi_k = \frac{\sum_{i=1}^{N} y_k^i}{N}}$$

Naive Bayes



Multiclass Classification $\quad Y \in \{0, 1, \ldots, k\}$

Gaussian Naive Bayes Pipeline

1. Build probabilistic models: Gaussian Likelihood
2. Derive loss function: MLE or MAP
3. Select optimizer: Necessary Condition

Q&A

HW 2 is out

Due: Feb 17th

Team Formation Due: Feb 10th