기계학습 (2022년도 2학기)

Probabilistic Models I

전북대학교 컴퓨터공학부

Maximum Likelihood

- We'll shift directions now, and spend most of the next 4 weeks talking about probabilistic models.
- This lecture
  - Maximum likelihood estimation
  - Naive Bayes

Maximum Likelihood

- Motivating example: estimating the parameter of a biased coin
  - You flip a coin 100 times. It lands heads N_H = 55 times and tails N_T = 45 times.
  - What is the probability it will come up heads if we flip again?
- Model: flips are independent Bernoulli random variables with parameter θ.
  - Assume the observations are independent and identically distributed (i.i.d.)

Maximum Likelihood

- The **likelihood function** is the probability of the observed data, as a function of θ.
- In our case, it's the probability of a particular sequence of H's and T's.
- Under the Bernoulli model with i.i.d. observations,

$$L(\theta) = p(\mathcal{D}) = \theta^{N_H}(1-\theta)^{N_T}$$ (베르누이 시행을 독립적으로 NH+NT번 수행한 것)

- This takes very small values. In this case,

$$L(0.5) = 0.5^{100} \approx 7.9 \times 10^{-31}$$

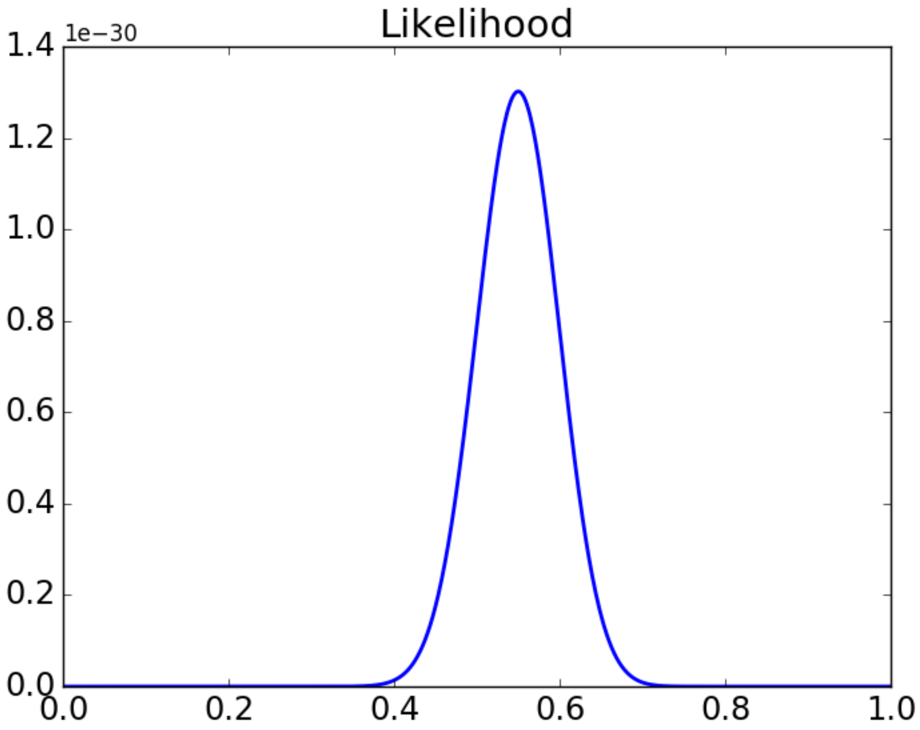
- Therefore, we usually work with log-likelihoods:

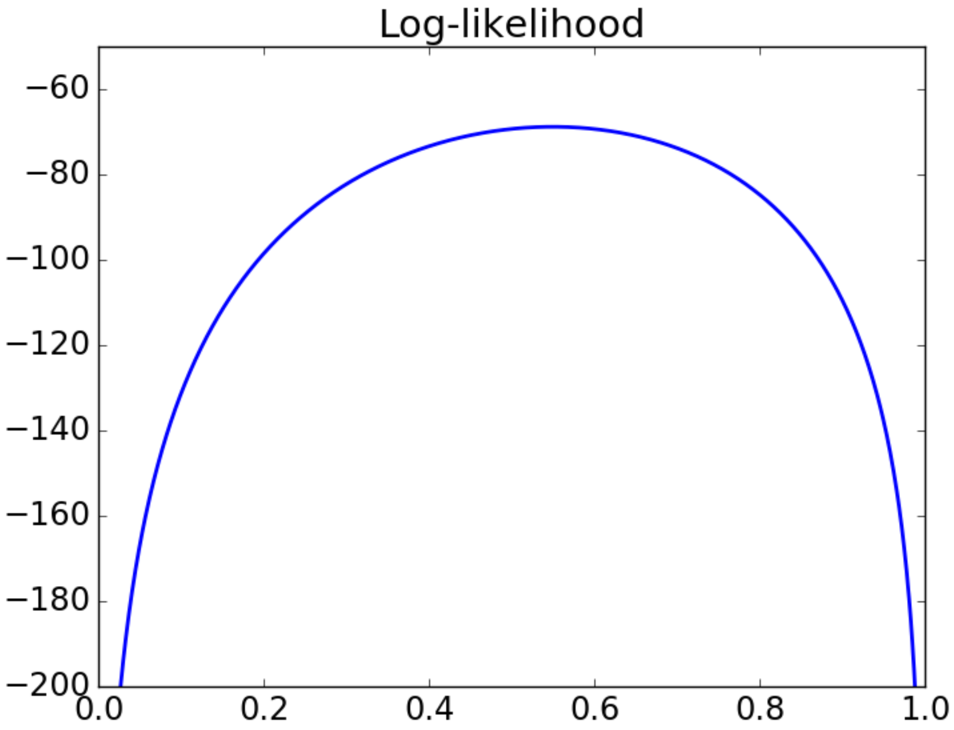
$$\ell(\theta) = \log L(\theta) = N_H \log \theta + N_T \log(1-\theta)$$

- Here, $\ell(0.5) = \log 0.5^{100} = 100 \log 0.5 = -69.31$

Maximum Likelihood

- N_H = 55, N_T = 45





Maximum Likelihood

- Good values of θ should assign high probability to the observed data. This motivates the **maximum likelihood criterion**.
- Remember how we found the optimal solution to linear regression by setting derivatives to zero? We can do that again for the coin example.

$$\begin{aligned}\frac{\mathrm{d}\ell}{\mathrm{d}\theta} &= \frac{\mathrm{d}}{\mathrm{d}\theta}\left(N_H \log \theta + N_T \log(1-\theta)\right) \\ &= \frac{N_H}{\theta} - \frac{N_T}{1-\theta}\end{aligned}$$

- Setting this to zero gives the maximum likelihood estimate:

$$\hat{\theta}_{\mathrm{ML}} = \frac{N_H}{N_H + N_T}$$

Maximum Likelihood

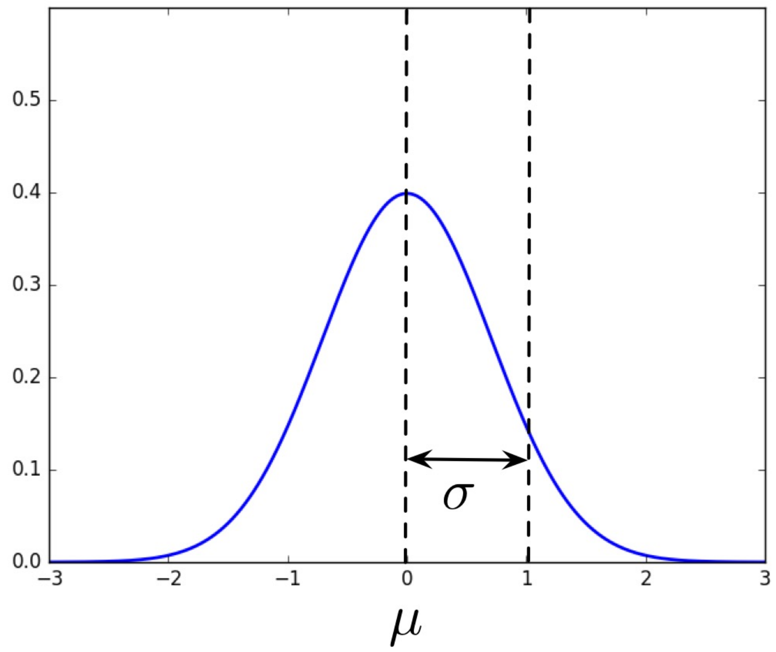
- This is equivalent to minimizing cross-entropy. Let $t_i = 1$ for heads and $t_i = 0$ for tails.

$$\begin{aligned}
\mathcal{L}_{CE} &= -\sum_i t_i \log \theta - (1 - t_i) \log(1 - \theta) \\
&= -N_H \log \theta - N_T \log(1 - \theta) \\
&= -\ell(\theta)
\end{aligned}$$

Maximum Likelihood

- Recall the Gaussian, or normal, distribution:

$$\mathcal{N}(x; \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$



- The Central Limit Theorem says that sums of lots of independent random variables are approximately Gaussian.
- In machine learning, we use Gaussians a lot because they make the calculations easy.

Maximum Likelihood

- Suppose we want to model the distribution of temperatures in Toronto in March, and we've recorded the following observations:

  -2.5 -9.9 -12.1 -8.9 -6.0 -4.8 2.4

- Assume they're drawn from a Gaussian distribution with known standard deviation $\sigma = 5$, and we want to find the mean μ.
- Log-likelihood function:

$$
\begin{aligned}
\ell(\mu) &= \log \prod_{i=1}^{N} \left[\frac{1}{\sqrt{2\pi} \cdot \sigma} \exp\left(-\frac{(x^{(i)} - \mu)^2}{2\sigma^2} \right) \right] \\
&= \sum_{i=1}^{N} \log \left[\frac{1}{\sqrt{2\pi} \cdot \sigma} \exp\left(-\frac{(x^{(i)} - \mu)^2}{2\sigma^2} \right) \right] \\
&= \sum_{i=1}^{N} \underbrace{-\frac{1}{2} \log 2\pi - \log \sigma}_{\text{constant}} - \frac{(x^{(i)} - \mu)^2}{2\sigma^2}
\end{aligned}
$$

Maximum Likelihood

- Maximize the log-likelihood by setting the derivative to zero:

$$\ell(\mu) = \sum_{i=1}^{N} \underbrace{-\frac{1}{2}\log 2\pi - \log \sigma}_{\text{constant}} - \frac{(x^{(i)} - \mu)^2}{2\sigma^2}$$

$$\begin{aligned} 0 = \frac{\mathrm{d}\ell}{\mathrm{d}\mu} &= -\frac{1}{2\sigma^2}\sum_{i=1}^{N}\frac{\mathrm{d}}{\mathrm{d}\mu}(x^{(i)} - \mu)^2 \\ &= \frac{1}{\sigma^2}\sum_{i=1}^{N} x^{(i)} - \mu \end{aligned}$$

- Solving we get $\mu = \frac{1}{N}\sum_{i=1}^{N} x^{(i)}$
- This is just the mean of the observed values, or the **empirical mean**.

Maximum Likelihood

- In general, we don't know the true standard deviation σ, but we can solve for it as well.
- Set the partial derivatives to zero, just like in linear regression.

$$0 = \frac{\partial \ell}{\partial \mu} = -\frac{1}{\sigma^2} \sum_{i=1}^{N} x^{(i)} - \mu$$

$$0 = \frac{\partial \ell}{\partial \sigma} = \frac{\partial}{\partial \sigma} \left[\sum_{i=1}^{N} -\frac{1}{2} \log 2\pi - \log \sigma - \frac{1}{2\sigma^2} (x^{(i)} - \mu)^2 \right]$$

$$= \sum_{i=1}^{N} -\frac{1}{2} \frac{\partial}{\partial \sigma} \log 2\pi - \frac{\partial}{\partial \sigma} \log \sigma - \frac{\partial}{\partial \sigma} \frac{1}{2\sigma} (x^{(i)} - \mu)^2$$

$$= \sum_{i=1}^{N} 0 - \frac{1}{\sigma} + \frac{1}{\sigma^3} (x^{(i)} - \mu)^2$$

$$= -\frac{N}{\sigma} + \frac{1}{\sigma^3} \sum_{i=1}^{N} (x^{(i)} - \mu)^2$$

$$\hat{\mu}_{\mathrm{ML}} = \frac{1}{N} \sum_{i=1}^{N} x^{(i)}$$

$$\hat{\sigma}_{\mathrm{ML}} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (x^{(i)} - \mu)^2}$$

Maximum Likelihood

- Sometimes there is no closed-form solution. E.g., consider the gamma distribution, whose PDF is

$$\Gamma(z) = \int_0^\infty t^{z-1} e^{-t}\, dt \qquad\qquad p(x) = \frac{b^a}{\Gamma(a)} x^{a-1} e^{-bx},$$

  where Γ is the gamma function, a generalization of the factorial function to continuous values.

- There is no closed-form solution, but we can still optimize the log-likelihood using gradient ascent.

Maximum Likelihood

- So far, maximum likelihood has told us to use empirical counts or statistics:
  - Bernoulli: $\theta = \frac{N_H}{N_H + N_T}$
  - Gaussian: $\mu = \frac{1}{N} \sum x^{(i)}$, $\sigma^2 = \frac{1}{N} \sum (x^{(i)} - \mu)^2$
- This doesn't always happen; the class of probability distributions that have this property is exponential families.

$$f_X(x|\theta) = h(x) \exp(\eta(\theta)^\top T(x) - A(\theta))$$

  - θ: distribution parameters
  - $\eta(\theta)$: natural parameter
  - $T(x)$: sufficient statistic

Maximum Likelihood

- We've been doing maximum likelihood estimation all along!
  - Squared error loss (e.g. linear regression)

$$p(t|y) = \mathcal{N}(t; y, \sigma^2)$$
$$-\log p(t|y) = \frac{1}{2\sigma^2}(y - t)^2 + \text{const}$$

  - Cross-entropy loss (e.g. logistic regression)

$$p(t = 1|y) = \text{Bernoulli}(t; y)$$
$$-\log p(t|y) = -t \log y - (1 - t)\log(1 - y)$$

Generative vs Discriminative

Two approaches to classification:

- **Discriminative approach**: estimate parameters of decision boundary/class separator directly from labeled examples.
  - Tries to solve: How do I separate the classes?
  - learn $p(\mathrm{y}|\mathbf{x})$ directly (logistic regression models)
  - learn mappings from inputs to classes (least-squares, decision trees)
- **Generative approach**: model the distribution of inputs characteristic of the class (Bayes classifier).
  - Tries to solve: What does each class "look" like?
  - Build a model of $p(\mathbf{x}|\mathrm{y})$
  - Apply Bayes Rule

Bayes Classifier

- Aim to classify text into spam/not-spam (yes c=1; no c=0)
- Use bag-of-words features, get binary vector **x** for each email
  - bag-of-words features: 사용할 수 있는 단어들을 미리 정해져 있고, 이 단어들이 입력 텍스트에 포함되어 있는가를 binary로 표시
  - 텍스트를 vector 형태로 변환하기 위해 필요함
- Example: “You are one of the very few who have been selected as a winners for the free $1000 Gift Card."
- Vocabulary:
  - "a": 1
  - ...
  - “car": 0
  - “card": 1
  - ...
  - “win": 0
  - “winner": 1
  - “winter": 0
  - ...
  - “you": 1

Bayes Classifier

- Given features $\mathbf{x} = [\mathrm{x}_1, \mathrm{x}_2, \cdots, \mathrm{x}_\mathrm{d}]^T$ we want to compute class probabilities using Bayes Rule:

$$\underbrace{p(c|\mathbf{x})}_{\text{Pr. class given words}} = \frac{p(\mathbf{x}, c)}{p(\mathbf{x})} = \frac{\overbrace{p(\mathbf{x}|c)}^{\text{Pr. words given class}} \quad p(c)}{p(\mathbf{x})}$$

- More formally

$$\text{posterior} = \frac{\text{Class likelihood} \times \text{prior}}{\text{Evidence}}$$

- How can we compute p(x) for the two class case? (Do we need to?)

$$p(\mathbf{x}) = p(\mathbf{x}|c=0)p(c=0) + p(\mathbf{x}|c=1)p(c=1)$$

- To compute $p(\mathrm{c}|\mathbf{x})$ we need: $p(\mathbf{x}|c)$ and $p(c)$

Naive Bayes

- Assume we have two classes: spam and non-spam. We have a dictionary of D words, and binary features $\mathbf{x} = [\mathrm{x}_1, \mathrm{x}_2, \cdots, \mathrm{x}_\mathrm{D}]$ saying whether each word appears in the e-mail.
- If we define a joint distribution $\mathrm{p}(c, \mathrm{x}_1, \mathrm{x}_2, \cdots, \mathrm{x}_\mathrm{D})$, this gives enough information to determine $\mathrm{p}(c)$ and $\mathrm{p}(\mathbf{x}|c)$.

$$
\begin{aligned}
p(C_k, x_1, \ldots, x_n) &= p(x_1, \ldots, x_n, C_k) \\
&= p(x_1 \mid x_2, \ldots, x_n, C_k)\, p(x_2, \ldots, x_n, C_k) \\
&= p(x_1 \mid x_2, \ldots, x_n, C_k)\, p(x_2 \mid x_3, \ldots, x_n, C_k)\, p(x_3, \ldots, x_n, C_k) \\
&= \cdots \\
&= p(x_1 \mid x_2, \ldots, x_n, C_k)\, p(x_2 \mid x_3, \ldots, x_n, C_k) \cdots p(x_{n-1} \mid x_n, C_k)\, p(x_n \mid C_k)\, p(C_k)
\end{aligned}
$$

- Problem: specifying a joint distribution over D+1 binary variables requires 2^{D+1} entries. This is computationally prohibitive and would require an absurd amount of data to fit.

Naive Bayes

- We'd like to impose structure on the distribution such that:
  - it can be compactly represented
  - learning and inference are both tractable
- Probabilistic graphical models are a powerful and wide-ranging class of techniques for doing this. We'll just scratch the surface here.

Naive Bayes

$$p(a,b|c) = p(a|b,c)p(b|c) = p(a|c)p(b|c)$$

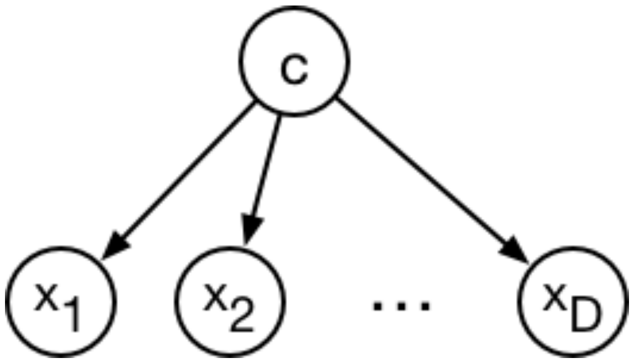
- Naive Bayes makes the assumption that the word features x_i are conditionally independent given the class *c*.
  - This means x_i and x_j are independent under the conditional distribution $\mathrm{p}(\mathbf{x}|c)$.
  - Note: this doesn't mean they're independent. (E.g., "gift" and "card" are correlated insofar as they both depend on *c*.)
  - Mathematically,

$$p(c, x_1, \ldots, x_D) = p(c)p(x_1|c) \cdots p(x_D|c).$$

- Compact representation of the joint distribution
  - Prior probability of class: $\mathrm{p}(c = 1) = \theta_c$
  - Conditional probability of word feature given class: $\mathrm{p}(\mathrm{x}_j = 1|c) = \theta_{jc}$
  - $2D + 1$ parameters total

Bayes Nets

- We can represent this model using an directed graphical model, or Bayesian network:



- This graph structure means the joint distribution factorizes as a product of conditional distributions for each variable given its parent(s).
- Intuitively, you can think of the edges as reflecting a causal structure. But mathematically, this doesn't hold without additional assumptions.

Naive Bayes: Learning

- Want to maximize $\sum_{i=1}^{N} \log p(x_j^{(i)} \mid c^{(i)})$
- This is a minor variant of our coin flip example. Let
  $\theta_{ab} = p(x_j = a \mid c = b)$. Note $\theta_{1b} = 1 - \theta_{0b}$.
- Log-likelihood:

$$\sum_{i=1}^{N} \log p(x_j^{(i)} \mid c^{(i)}) = \sum_{i=1}^{N} c^{(i)} x_j^{(i)} \log \theta_{11} + \sum_{i=1}^{N} c^{(i)} (1 - x_j^{(i)}) \log(1 - \theta_{11})$$
$$+ \sum_{i=1}^{N} (1 - c^{(i)}) x_j^{(i)} \log \theta_{10} + \sum_{i=1}^{N} (1 - c^{(i)})(1 - x_j^{(i)}) \log(1 - \theta_{10})$$

- Obtain maximum likelihood estimates by setting derivatives to zero:

$$\theta_{11} = \frac{N_{11}}{N_{11} + N_{01}} \qquad \theta_{10} = \frac{N_{10}}{N_{10} + N_{00}}$$

where N_{ab} is the counts for $\mathrm{x}_j = a$ and $c = b$.

Naive Bayes: Inference

- We predict the category by performing inference in the model.
- Apply Bayes' Rule:

$$p(c \mid \mathbf{x}) = \frac{p(c)p(\mathbf{x} \mid c)}{\sum_{c'} p(c')p(\mathbf{x} \mid c')}$$

$$= \frac{p(c) \prod_{j=1}^{D} p(x_j \mid c)}{\sum_{c'} p(c') \prod_{j=1}^{D} p(x_j \mid c')}$$

- We need not compute the denominator if we're simply trying to determine the mostly likely *c*.
- Shorthand notation:

$$p(c \mid \mathbf{x}) \propto p(c) \prod_{j=1}^{D} p(x_j \mid c)$$

Naive Bayes

- Naive Bayes is an amazingly cheap learning algorithm!
- Training time: estimate parameters using maximum likelihood
  - Compute co-occurrence counts of each feature with the labels.
  - Requires only one pass through the data!
- Test time: apply Bayes' Rule
  - Cheap because of the model structure. (For more general models, Bayesian inference can be very expensive and/or complicated.)
- We covered the Bernoulli case for simplicity. But our analysis easily extends to other probability distributions.
- Unfortunately, it's usually less accurate in practice compared to discriminative models due to its “naive" independence assumption.