Generative Models: Fundamentals and Applications

Lecture 2: Generative Models for Discrete Data



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Outline



- Generative vs. Discriminative: Revisit
- Bayesian concept learning
- The beta-binomial model
- The Dirichlet-multinomial model
- Naive Bayes classifiers



- **Frequentist:** θ seen as fixed
 - ullet e.g., a point estimation $\hat{\theta}$
- **Bayesian:** θ seen as learned
 - □ Given data D, $P(\theta|D) = P(D|\theta)P(\theta)$



- Discriminative models are often frequentist,
 and generative models are often Bayesian
 - □ but the two dimensions are orthogonal and can be mixed

	Frequentist	Bayesian
Discriminative	Logistic Regression, SVM, Neural Nets	Bayesian Logistic Regression, Bayesian Neural Nets
Generative	GMM (with MLE), HMM (with MLE)	Naive Bayes, Bayesian GMM, Variational Bayes models



- Goal of discriminative model
 - Learn the conditional distribution $P(Y|X;\theta)$



- Goal of generative model
 - □ Learn the joint distribution $P(X, Y; \theta)$
- Generative classifier

$$P(Y = c | x, \theta) = \frac{P(Y = c, x | \theta)}{P(x | \theta)}$$

$$= \frac{P(Y = c | \theta)P(x | Y = c, \theta)}{\sum_{c' \in C} P(x, Y = c' | \theta)}$$

$$= \frac{P(Y = c | \theta)P(x | Y = c, \theta)}{\sum_{c' \in C} P(Y = c' | \theta)P(x | Y = c', \theta)}$$
class-conditional distribution
$$= \frac{P(Y = c | \theta)P(x | Y = c, \theta)}{\sum_{c' \in C} P(Y = c' | \theta)P(x | Y = c', \theta)}$$

□ Key: class-conditional distribution $P(x|Y=c,\theta)$

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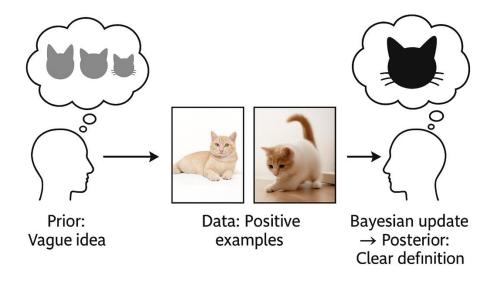


- Concept learning
 - Provide only the positive examples
 - Learn the meaning of the example

This is a cat









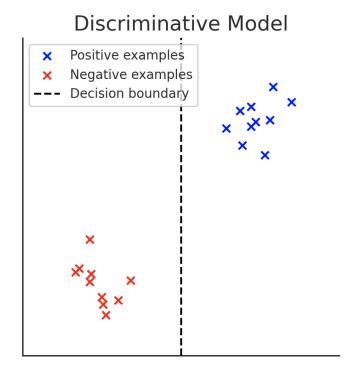
- Concept learning
 - Be equivalent to binary classification
 - The goal is to learn the indicator function f, determining which elements are in the set C.

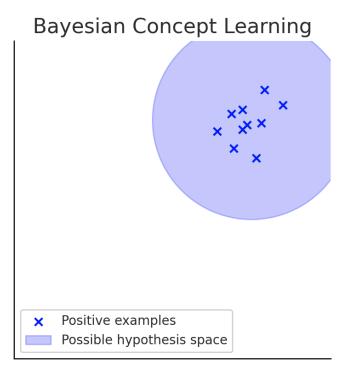
$$f(x) = \begin{cases} 1, x \in C \\ 0, x \notin C \end{cases}$$

■ **Difference:** binary classification provides both the positive and negative examples, while concept learning provides only the positive examples



Bayesian concept learning vs. binary classification





Example: number game



- Given some unknown arithmetical concepts *C*, such as "prime number" or "a number between 1 and 10"
- Given positive examples $\mathcal{D} = \{x_1, x_2, ..., x_N\} \subseteq C$
- Question: the new sample $\tilde{x} \in C$?
 - Learn a basic rule to determine whether the data follows the unknown arithmetical concepts *C*

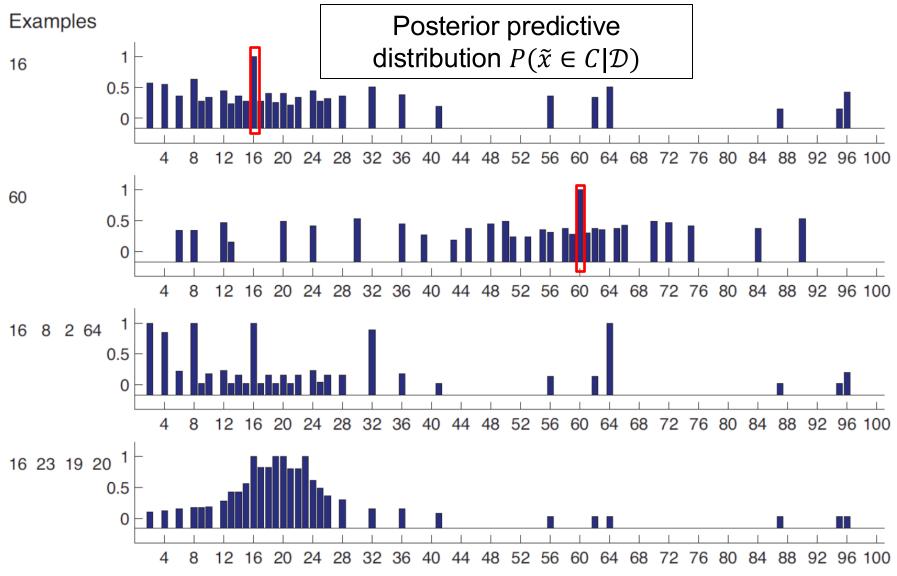
Example: number game



- Suppose \mathcal{D} and the test set are from [1,100]
- Concept set C is not clear
- Four experiments
 - Experiment 1: $\mathcal{D} = \{16\}$
 - □ Experiment 2: $\mathcal{D} = \{60\}$
 - Experiment 3: $\mathcal{D} = \{16,8,2,64\}$
 - Experiment 4: $\mathcal{D} = \{16,23,19,20\}$

Example: number game







- Posterior predictive distribution $p(\tilde{x} \in C|\mathcal{D})$
 - □ Describe the probability that $\tilde{x} \in C$ given the data \mathcal{D} for any $\tilde{x} \in \{1,2,...,100\}$
- Question: How to explain the behavior and emulate it in a machine?



Hypothesis space \mathcal{H} :

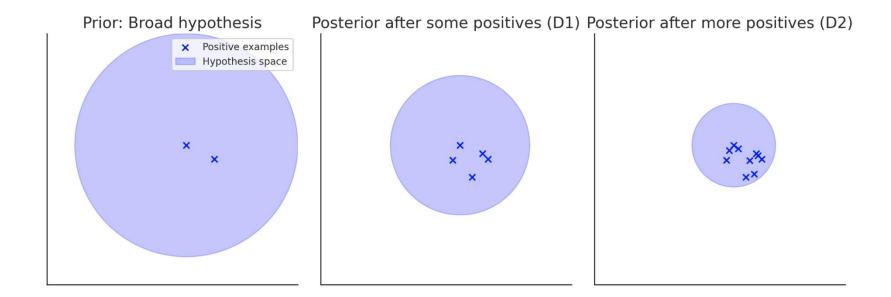
- Include all possible models or rules for the concept set
- □ Eg: odd numbers, even numbers, powers of two, all numbers ending in j (for $0 \le j \le 9$)

Version space

- \Box The subset of \mathcal{H} that is consistent with the data \mathcal{D}
- As we see more examples, the version space shrinks and we become increasingly certain about
 - Eg. $\mathcal{D} = \{16\} \rightarrow \mathcal{D} = \{16,8,2,64\}$



The shrinking of version space





- Given $\mathcal{D} = \{16,8,2,64\}$, which hypothesis is more possible?
 - $h_{two} = "powers of two"$
 - $h_{even} = "even number"$
- Extension of a concept
 - The set of numbers that belong to the concept
 - the extension of h_{two} is {2,4,8,16,32,64}
 - the extension of h_{even} is $\{2,4,6,...,98,100\}$



- Strong sampling assumption
 - Assume N examples are sampled **uniformly** at **random** from the extension of a concept.
- Likelihood $p\{\mathcal{D}|h\}$
 - the probability of independently sampling N items (with replacement) from h that happen to constitute \mathcal{D}

$$p(\mathcal{D}|h) = \left[\frac{1}{\operatorname{size}(h)}\right]^N = \left[\frac{1}{|h|}\right]^N$$



- Compute the probability $P\{\mathcal{D}|h\}$?
 - Let $\mathcal{D} = \{16\}$
 - $p(\mathcal{D}|h_{two}) = 1/6$
 - $p(\mathcal{D}|h_{even}) = 1/50$
 - \Box Let $\mathcal{D} = \{16,8,2,64\}$
 - $p(\mathcal{D}|h_{two}) = (1/6)^4 = 7.7 \times 10^{-4}$
 - $p(\mathcal{D}|h_{even}) = (1/50)^4 = 1.6 \times 10^{-7}$
 - likelihood ratio: $\frac{p(\mathcal{D}|h_{two})}{p(\mathcal{D}|h_{even})} = 4812.5$



- Size principle (Occam's razor)
 - □ The model favors the simplest (smallest) hypothesis consistent with the data

$$p(\mathcal{D}|h) = \left[\frac{1}{\operatorname{size}(h)}\right]^N = \left[\frac{1}{|h|}\right]^N$$

□ Among all hypotheses consistent with \mathcal{D} , the fewer data a hypothesis h covers, the higher its likelihood.

Prior



- Given $\mathcal{D} = \{16,8,2,64\}$, which hypothesis seems "conceptually unnatural"?
 - $h_{two} = "powers of two"$
 - $h_{two} = \{2,4,8,16,32,64\}$
 - $p(\mathcal{D}|h_{two}) = (1/6)^4$
 - $h'_{two} = "powers of two except 32"$
 - $h'_{two} = \{2,4,8,16,64\}$
 - $p(\mathcal{D}|h'_{two}) = (1/5)^4$
 - □ The likelihood of h'_{two} is higher than that of h_{two}

Prior



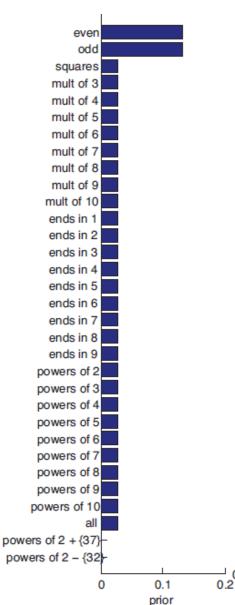
- Prior
 - Assign low prior probability to unnatural concepts
- Eg: given 𝔰={1200,1500,900,1400}, classify 400 and 1183?
 - □ The numbers are from some arithmetic rule
 - 400 is likely but 1183 is unlikely
 - □ The numbers are examples of healthy cholesterol levels
 - 400 is unlikely but 1183 is likely

Example: what prior to use



Hypothesis space

- Even numbers
- Odd numbers
- Squares
- □ Multiples of j ($3 \le j \le 10$)
- $\blacksquare \quad \text{Ends in j } (1 \le j \le 9)$
- □ Powers of j $(2 \le j \le 10)$
- All
- □ Powers of 2, plus 37
- □ Powers of 2, except 32





posterior = normalization (likelihood times prior)

$$p(h|\mathcal{D}) = \frac{p(\mathcal{D}|h)p(h)}{\sum_{h' \in \mathcal{H}} p(\mathcal{D}, h')} = \frac{p(h)\mathbb{I}(\mathcal{D} \in h)/|h|^N}{\sum_{h' \in \mathcal{H}} p(h')\mathbb{I}(\mathcal{D} \in h')/|h'|^N}$$

- Prior vs. Posterior
 - Prior: Without training data, quantify the possibility of each hypothesis
 - Posterior: Given training data, quantify the possibility of each hypothesis

- Given $\mathcal{D}=\{16\}$
 - \bullet *h*="powers of 2"
 - Prior

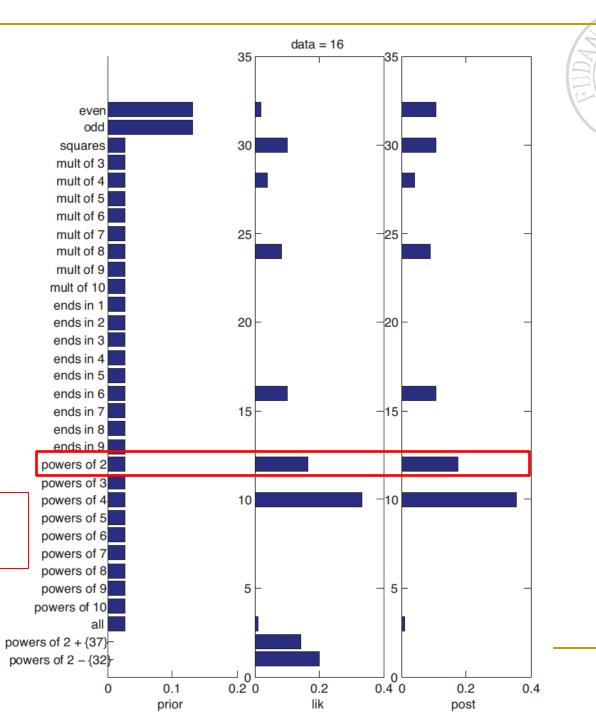
$$p(h) = 0.025$$

Likelihood

$$p(\mathcal{D}|h) = 1/6$$

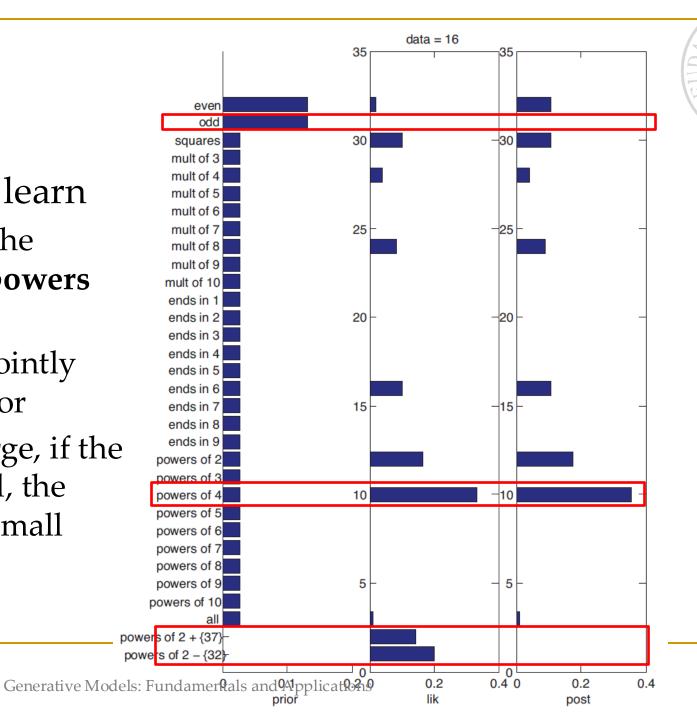
Posterior

$$p(h|\mathcal{D}) = \frac{0.0042}{sum}$$

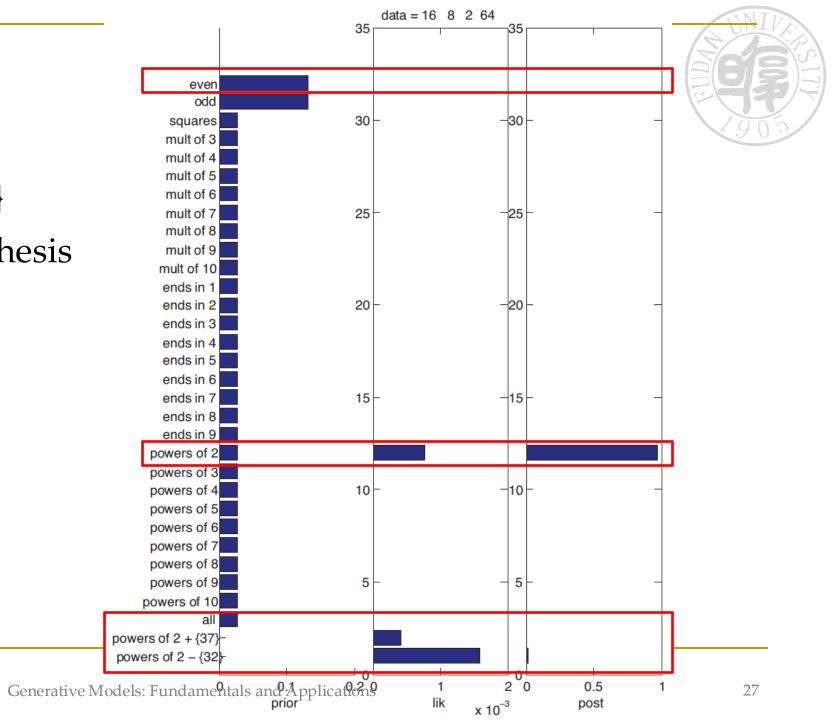


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- From the results, we learn
 - The hypothesis with the highest posterior is "powers of 4"
 - Prior and likelihood jointly determine the posterior
 - Even if the prior is large, if the likelihood is too small, the posterior can still be small
 - And vice versa



- Given $\mathcal{D} = \{16, 8, 2, 64\}$
 - Five possible hypothesis



- Given $\mathcal{D} = \{16, 8, 2, 64\}$
 - h="powers of 2"
 - Prior

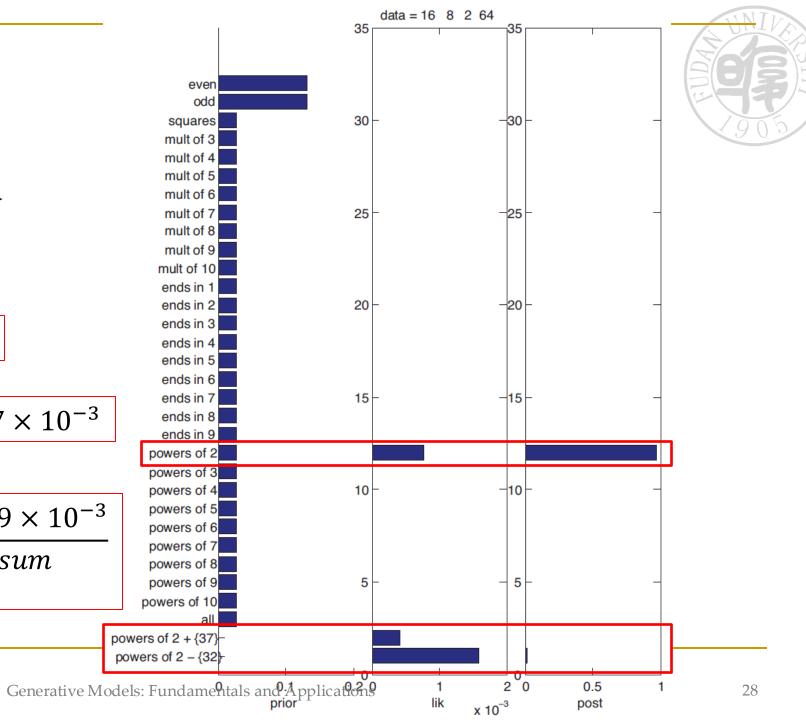
$$p(h) = 0.025$$

Likelihood

$$p(\mathcal{D}|h) = 0.77 \times 10^{-3}$$

Posterior

$$p(h|\mathcal{D}) = \frac{0.019 \times 10^{-3}}{sum}$$
$$\approx 1$$





Result:

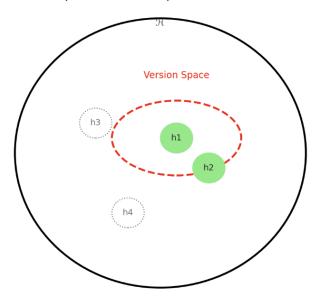
- Assigning small priors to unnatural hypotheses helps avoid overfitting the data
- □ When $|\mathcal{D}|$ is sufficiently large, $p(h | \mathcal{D})$ will peak at a single hypothesis (reach its maximum)
- Taken as the optimal hypothesis
- □ Take-away:
 - Prior prevents overfitting, and more data changes likelihood which sharpens the posterior to the true hypothesis.



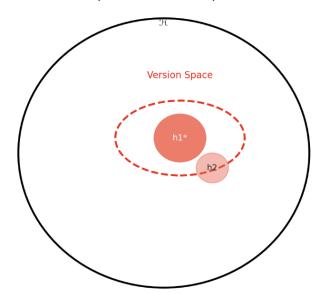
Step 1: Hypothesis space

h1 h2 h2

Step 2: Version space after data



Step 3: Posterior update



Summary of Concepts



- Hypothesis space: the set of all possible hypotheses (concepts)
- Hypothesis: a specific member or concept of the hypothesis space
- Version space: the subset of hypotheses consistent with observed data
- **Extension**: the set of samples that satisfy a given hypothesis
- Prior: initial belief or bias over hypotheses before seeing data
- Likelihood: probability of observing the data given a hypothesis (sampling from its extension)
- Posterior: updated belief about a hypothesis after observing data
- Optimal hypothesis: the hypothesis with the highest posterior probability

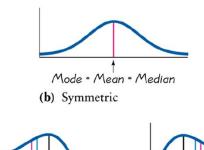


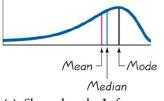
■ MAP (Maximum *a Posteriori*) estimate

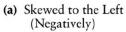
$$\max_{h \in \mathcal{H}} p(h|\mathcal{D})$$

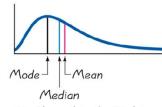
It simply finds the posterior mode

$$\hat{h}^{MAP} = \operatorname{argmax}_h p(h|\mathcal{D})$$





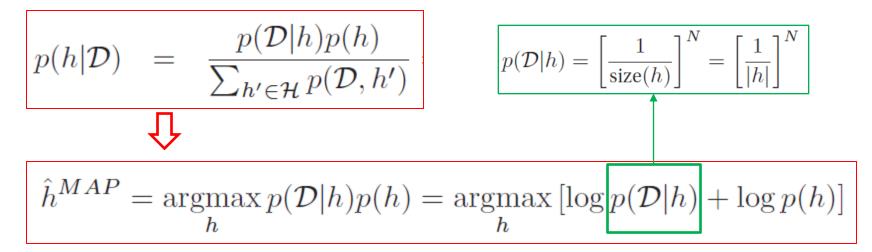




(c) Skewed to the Right (Positively)



MAP estimate



Note:

- The log-likelihood grows linearly with the number of elements *N*.
- When N is sufficiently large, MAP is dominated by the log-likelihood and becomes almost independent of the log-prior.



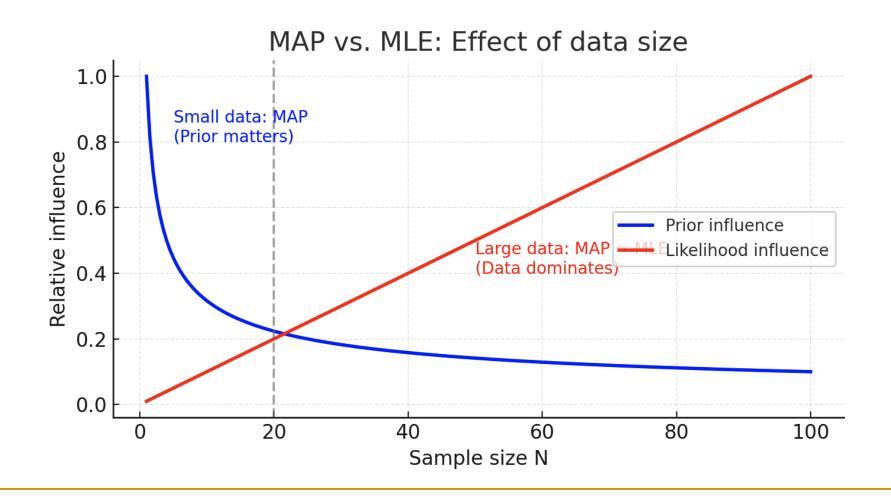
- MLE (Max-likelihood Estimation)
 - \Box Choose $\hat{\theta}$ that maximize the likelihood of the observed data

$$\hat{ heta}_{MLE} = rg \max_{ heta} p(\mathcal{D} \mid heta)$$

□ For MAP, if we have enough data, we see that the data overwhelms the prior. In this case, the MAP estimate converges towards the MLE

$$\hat{ heta}_{MAP} = rg \max_{ heta} p(\mathcal{D} \mid heta) p(heta)$$







- If the true hypothesis is in the hypothesis space
 - □ The MAP estimate will converge upon this hypothesis.

- If our hypothesis class is not rich enough to represent the "truth"
 - Converge on the hypothesis that is as close as possible to the truth



Posterior predictive distribution

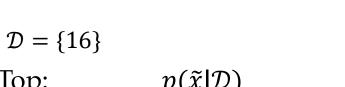
$$p(\tilde{x}|\mathcal{D}) = \sum_{h \in \mathcal{H}} p(h|\mathcal{D}) p(\tilde{x}|h, \mathcal{D}) = \sum_{h \in \mathcal{H}} p(h|\mathcal{D}) p(\tilde{x}|h)$$

□ Consider $p(h|\mathcal{D})$ as a kind of weight

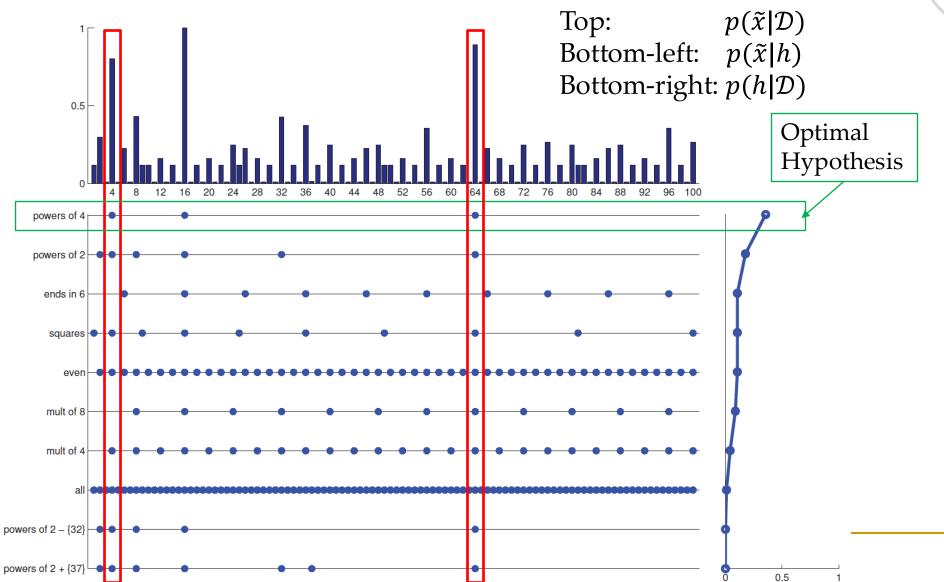
$$\sum_{h\in\mathcal{H}}\,p(h|\mathcal{D})=1$$

- a weighted average of the predictions of each individual hypothesis
 - Bayes model averaging (BMA) method

Example



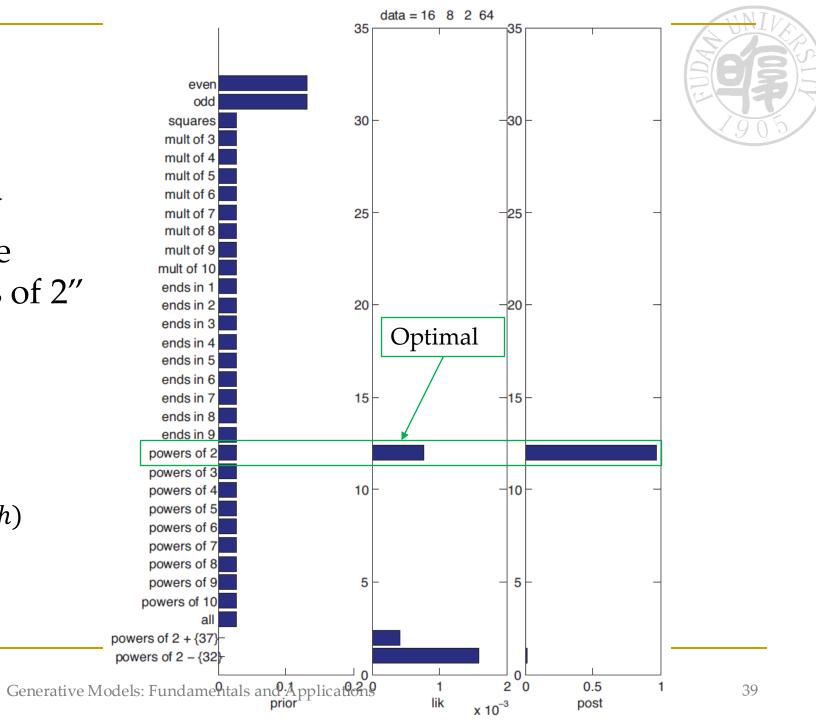
p(h | 16)



Example

- Given $\mathcal{D} = \{16, 8, 2, 64\}$
 - The posterior for the hypothesis "powers of 2" is close to 1

$$p(\tilde{x}|\mathcal{D}) = \sum_{h \in \mathcal{H}} p(h|\mathcal{D}) p(\tilde{x}|h)$$
$$= \sum_{h \in \mathcal{H}} \delta_{\hat{h}^{MAP}}(h) p(\tilde{x}|h)$$
$$\approx p(\tilde{x}|\hat{h}^{MAP})$$





- Plug-in approximation
 - □ If we have "figured things out", posterior becomes a delta function centered at the MAP estimate

$$p(\tilde{x}|\mathcal{D}) = \sum_{h \in \mathcal{H}} p(h|\mathcal{D})p(\tilde{x}|h)$$
$$\approx p(\tilde{x}|\hat{h}^{MAP})$$



- BMA vs. plug-in (MAP)
 - Sample space by MAP: from narrow to wide
 - For a single hypothesis
 - As training data increases, the sample space generated by the MAPselected hypothesis expands
 - Example
 - $D = \{16\}$: the optimal hypothesis is "powers of 4", generated samples $\{4, 16, 64\}$
 - $D = \{16^{7}, 8^{7}, 2^{7}, 64\}$: the optimal hypothesis is "powers of 2", generated samples $\{2^{7}, 4^{7}, 8^{7}, 16^{7}, 32^{7}, 64\}$



- BMA vs. plug-in (MAP)
 - Sample space by BMA: from wide to narrow
 - For the entire hypothesis space
 - As training data increases, some hypotheses are assigned weight 0, so the effective sample space shrinks
 - Example
 - $D = \{16\}$: many hypotheses are consistent with the data
 - $D = \{16^{7}, 8^{7}, 2^{7}, 64\}$: fewer hypotheses remain consistent with the data, inconsistent ones have weight 0

A more complex prior



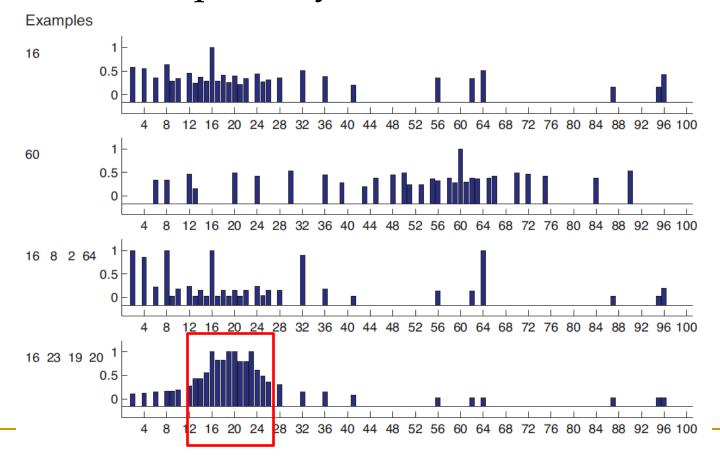
- Mixture of several priors
 - □ E.g., in number game
 - p_{rules} : arithmetical concepts
 - $p_{interval}$: intervals between n and m

$$p(h) = \pi_0 p_{\text{rules}}(h) + (1 - \pi_0) p_{\text{interval}}(h)$$

A more complex prior



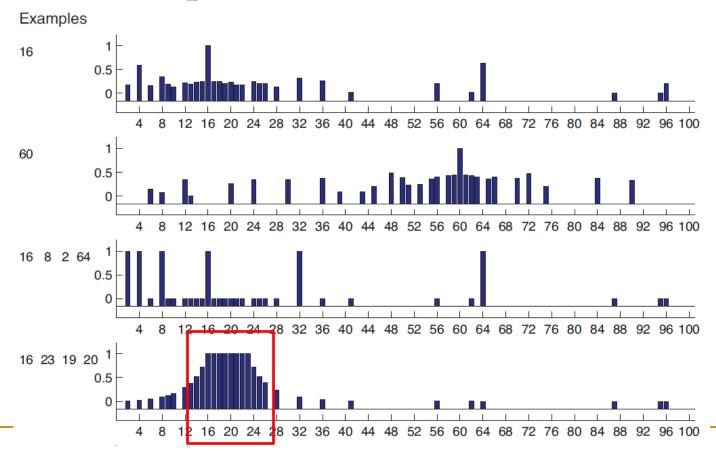
Arithmetical concepts only



A more complex prior



Arithmetical concepts + intervals between n and m



Outline



- Generative vs. Discriminative: Revisit
- Bayesian concept learning
- The beta-binomial model
- The Dirichlet-multinomial model
- Naive Bayes classifiers

The beta-binomial model



- Continuous case
 - Unknown parameters are continuous
 - Hypothesis space is (some subset) of \mathbb{R}^{K}
 - K is the number of parameters
 - Replace sums with integrals
 - Posterior

$$p(h|\mathcal{D}) = \frac{p(\mathcal{D}|h)p(h)}{\sum_{h'\in\mathcal{H}} p(\mathcal{D}, h')}$$

$$p(\tilde{x}|\mathcal{D}) = \sum_{h \in \mathcal{H}} p(h|\mathcal{D}) p(\tilde{x}|h, \mathcal{D}) = \sum_{h \in \mathcal{H}} p(h|\mathcal{D}) p(\tilde{x}|h)$$

The beta-binomial model



- Example: coin toss
 - Toss coins N times
 - \square N_1 times head up, and $N_0 = N N_1$ times tail up
 - □ Suppose $x_i \sim \text{Ber}(\theta)$, i = 1, ..., N
 - $x_i = 1$: head up
 - $x_i = 0$: tail up
 - $\theta \in [0,1]$: rate parameter (probability of heads)

Likelihood



■ Suppose the data $x_1, x_2, ..., x_N$ are i.i.d.

$$p(\mathcal{D}|\theta) = \theta^{N_1} (1 - \theta)^{N_0}$$

• Sufficient statistic: it captures all the information in the data about the parameter θ $N_1 = \sum_{i=1}^{N} \mathbb{I}(x_i = 1)$

$$N_0 = \sum_{i=1}^N \mathbb{I}(x_i = 0)$$

The beta-binomial model



- Suppose N_1 is a random variable
 - $\square N_1 \sim Bin(N, \theta)$

$$\operatorname{Bin}(N_1|N,\theta) = \binom{N}{N_1} \theta^{N_1} (1-\theta)^{N-N_1}$$

□ The likelihood for the binomial sampling model is the same as the likelihood for the Bernoulli model

Prior



- The prior has the same form as the likelihood
 - Likelihood

$$p(\mathcal{D}|\theta) = \theta^{N_1} (1 - \theta)^{N_0}$$

Prior, assume in the form of $p(\theta) \propto \theta^{\gamma_1} (1-\theta)^{\gamma_2}$

$$p(\theta) \propto \theta^{\gamma_1} (1 - \theta)^{\gamma_2}$$

Hence, posterior

$$p(\theta|\mathcal{D}) \propto p(\mathcal{D}|\theta)p(\theta) = \theta^{N_1}(1-\theta)^{N_0}\theta^{\gamma_1}(1-\theta)^{\gamma_2} = \theta^{N_1+\gamma_1}(1-\theta)^{N_0+\gamma_2}$$

- Conjugate prior
 - the prior and the posterior have the same form

Beta
$$(\theta|a,b) \propto \theta^{a-1} (1-\theta)^{b-1}$$



Multiply the likelihood by the beta prior

$$p(\theta|\mathcal{D}) \propto \text{Bin}(N_1|N_1 + N_0, \theta) \text{Beta}(\theta|a, b)$$

$$\propto \operatorname{Beta}(\theta|N_1+a,N_0+b)$$

Example



- (a) With a relatively weak prior, the posterior is very close to the likelihood, as the data overwhelms the prior.
- (b) With a stronger prior, the posterior becomes a compromise between the prior and the likelihood.

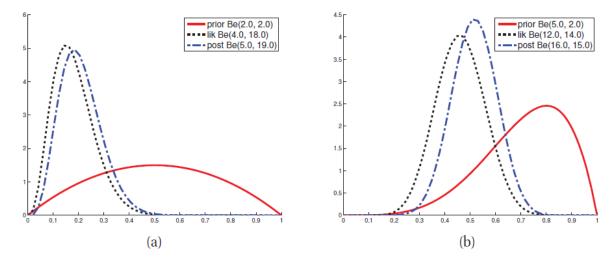
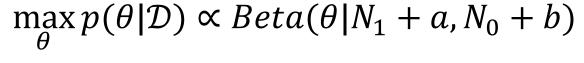


Figure 3.6 (a) Updating a Beta(2, 2) prior with a Binomial likelihood with sufficient statistics $N_1 = 3$, $N_0 = 17$ to yield a Beta(5,19) posterior. (b) Updating a Beta(5, 2) prior with a Binomial likelihood with sufficient statistics $N_1 = 11$, $N_0 = 13$ to yield a Beta(16, 15) posterior. Figure generated by binomialBetaPosteriorDemo.



MAP estimate

$$Beta(a,b): mode = \frac{a-1}{a+b-2}$$





$$\hat{\theta}_{MAP} = \frac{a + N_1 - 1}{a + N_1 + b + N_0 - 2} = \frac{a + N_1 - 1}{a + b + N - 2}.$$

- MLE
 - □ If the prior is uniformly distributed (a=b=1)

$$\hat{\theta}_{MLE} = \frac{N_1}{N}$$



Posterior mean

$$Beta(a,b)$$
: mean = $\frac{a}{a+b}$

$$\bar{\theta} = \frac{a + N_1}{a + N_1 + b + N_0} = \frac{a + N_1}{a + b + N}$$

□ Let $\alpha_0 = a + b$, and let the prior mean $m_1 = a/\alpha_0$

$$\mathbb{E}\left[\theta|\mathcal{D}\right] = \frac{\alpha_0 m_1 + N_1}{N + \alpha_0} = \frac{\alpha_0}{N + \alpha_0} m_1 + \frac{N}{N + \alpha_0} \frac{N_1}{N} = \lambda m_1 + (1 - \lambda)\hat{\theta}_{MLE}$$

where
$$\lambda = \frac{\alpha_0}{N + \alpha_0}$$

 Result: the posterior mean is convex combination of the prior mean and the MLE



• Equivalent sample size of the prior $\alpha_0 = a + b$

Beta
$$(\theta|a,b) \propto \theta^{a-1} (1-\theta)^{b-1}$$

• Equivalent sample size of the posterior $N + \alpha_0$

$$p(\theta|\mathcal{D}) \propto \text{Beta}(\theta|N_1 + a, N_0 + b)$$

- Ratio of the prior to posterior equivalent sample size λ
 - \Box The smaller λ , the closer the posterior mean is to the MLE
 - \Box The smaller λ , the closer the posterior mode is to the MLE



Posterior variance

$$Beta(a,b)$$
: var = $\frac{ab}{(a+b)^2(a+b+1)}$

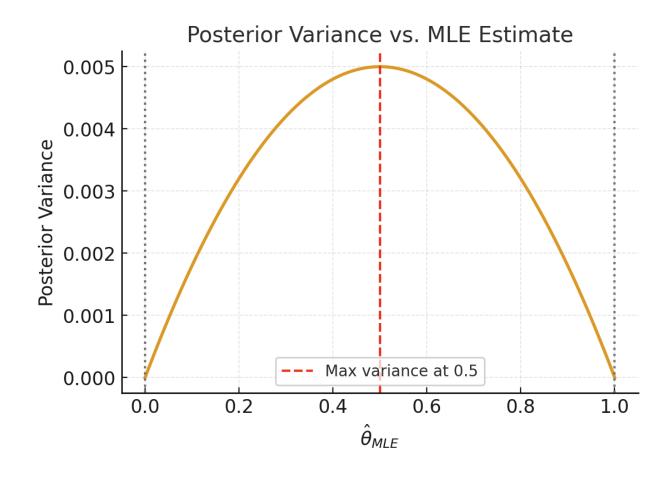
$$\operatorname{var}\left[\theta|\mathcal{D}\right] = \frac{(a+N_1)(b+N_0)}{(a+N_1+b+N_0)^2(a+N_1+b+N_0+1)}$$

 \square If $N \gg a, b$

$$\operatorname{Var}[\theta|\mathcal{D}] \approx \frac{N_1 N_0}{N^2 N} = \frac{\hat{\theta}_{MLE} (1 - \hat{\theta}_{MLE})}{N}$$

- The variance is maximized when $\hat{\theta}_{MLE} = 0.5$
- The variance is minimized when $\hat{\theta}_{MLE}=0$, 1







Generate one data

BMA

$$p(\tilde{x} = 1 \mid \mathcal{D}) = \int_0^1 p(\tilde{x} = 1 \mid \theta) p(\theta \mid \mathcal{D}) d\theta$$

$$= \int_0^1 \theta \operatorname{Beta}(\theta \mid N_1 + a, N_0 + b) d\theta$$

$$= \mathbb{E}[\theta \mid \mathcal{D}]$$
Posterior mean
$$= \frac{N_1 + a}{N + a + b}$$



- Overfitting and the black swan paradox
 - Zero count problem or the sparse data problem
 - Suppose the sample size is very small,

$$\Box$$
 E.g., $N = 3$, $N_1 = 0$

Suppose we use plug-in the MLE

Result: heads are impossible.



- Overfitting and the black swan paradox
 - Bayes theorem: Laplace's rule of succession
 - Suppose the prior is uniform on [0,1]

$$p(\tilde{x} = 1|\mathcal{D}) = \frac{a + N_1}{a + b + N} = \frac{N_1 + 1}{N + 2} = \frac{N_1 + 1}{N_1 + 1 + N_0 + 1}$$

Add-one smoothing: Beta(1, 1)



- Generate multiple data: beta-binomial distribution
 - ightharpoonup Predict the number of heads, x, in M future trials

$$p(x|\mathcal{D}, M) = \int_0^1 \text{Bin}(x|M, \theta) \text{ Beta}(\theta|N_1 + a, N_0 + b) \ d\theta$$

$$= {M \choose x} \frac{1}{B(N_1 + a, N_0 + b)} \int_0^1 \theta^x \ (1 - \theta)^{M - x} \theta^{N_1 + a - 1} \ (1 - \theta)^{N_0 + b - 1} \ d\theta$$

$$= {M \choose x} \frac{B(x + N_1 + a, M - x + N_0 + b)}{B(N_1 + a, N_0 + b)}$$

$$\triangleq Bb(x|N_1 + a, N_0 + b, M)$$



- beta-binomial distribution
 - Mean

$$\mathbb{E}[x|\mathcal{D}] = M \frac{N_1 + a}{N + a + b}$$

Variance

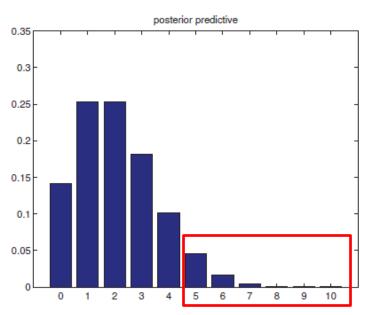
$$Var[x|\mathcal{D}] = \frac{M(N_1 + a)(N_0 + b)}{(N + a + b)^2} \frac{N + a + b + M}{N + a + b + 1}$$

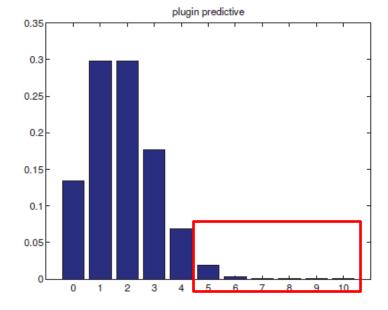
Experiment



 Bayesian prediction has longer tails, spreading its probability mass more widely, and is therefore less prone to overfitting and black swan type paradoxes

$$N_1 = 3, N_0 = 17$$
 Beta(2,2) prior





Outline



- Generative vs. Discriminative: Revisit
- Bayesian concept learning
- The beta-binomial model
- The Dirichlet-multinomial model
- Naive Bayes classifiers



Example:

- □ Infer the probability that a dice with K sides comes up as face k
- □ Given $\mathcal{D} = \{x_1, x_2, ..., x_N | x_i \in \{1, 2, ..., K\}\}$
- Likelihood

where

$$p(\mathcal{D}|\boldsymbol{\theta}) = \prod_{k=1}^{K} \theta_k^{N_k}$$

$$N_k = \sum_{i=1}^N \mathbb{I}(x_i = k)$$



Prior: conjugate prior

$$\operatorname{Dir}(\boldsymbol{\theta}|\boldsymbol{\alpha}) = \frac{1}{B(\boldsymbol{\alpha})} \prod_{k=1}^{K} \theta_k^{\alpha_k - 1} \mathbb{I}(\boldsymbol{\theta} \in S_K)$$

Posterior

$$p(\theta|\mathcal{D}) \propto p(\mathcal{D}|\theta)p(\theta)$$

$$= \prod_{k=1}^{K} \theta_k^{N_k} \frac{1}{B(\alpha)} \prod_{k=1}^{K} \theta_k^{\alpha_k - 1} \mathbb{I}(\theta \in S_K)$$

$$\propto \prod_{k=1}^{K} \theta_k^{N_k + \alpha_k - 1}$$

$$\propto \text{Dir}(\theta|N_1 + \alpha_1, N_2 + \alpha_2, \dots, N_K + \alpha_K)$$



MAP estimate

$$\hat{\theta}_k = \frac{N_k + \alpha_k - 1}{N + \alpha_0 - K}$$

where

$$\alpha_0 \triangleq \sum_{k=1}^K \alpha_k$$

MLE: uniform prior

$$\hat{\theta}_k = N_k/N$$



Posterior predictive

$$p(X = j|\mathcal{D}) = \int p(X = j|\theta)p(\theta|\mathcal{D})d\theta$$

$$= \int p(X = j|\theta_j) \left[\int p(\theta_{-j}, \theta_j|\mathcal{D})d\theta_{-j} \right] d\theta_j$$

$$= \int \theta_j p(\theta_j|\mathcal{D})d\theta_j = \mathbb{E}\left[\theta_j|\mathcal{D}\right] = \frac{\alpha_j + N_j}{\sum_k (\alpha_k + N_k)} = \frac{\alpha_j + N_j}{\alpha_0 + N}$$

where θ_{-j} are all the components of $\boldsymbol{\theta}$ except θ_{j}

Beta-Binomial vs. Dirichlet-Multinomial



	Beta-Binomial Model	Dirichlet-Multinomial Model
Task scenario	Binary classification (coin toss: head/tail)	Multi-class classification (dice roll: 1,2,,K)
Parameters	$\theta \in [0,1]$:probability of "head"	$\theta = (\theta_1,, \theta_K)$, class probabilities, $\sum_k \theta_k = 1$
Prior	Beta distribution: Beta $(\theta a,b)$	Dirichlet distribution: $Dir(\theta \alpha_1,, \alpha_K)$
Likelihood	Binomial: Bin($N_1 N,\theta$)	Multinomial: Mult($N_1,, N_K N, \theta$)
Conjugacy	Beta is the conjugate prior of Binomial	Dirichlet is the conjugate prior of Multinomial
Posterior	$\theta \mid D \sim \text{Beta}(a + N_1, b + N_0)$	$\theta \mid D \sim \text{Dir}(\alpha_1 + N_1, \dots, \alpha_K + N_K)$
Posterior predictive	$p(\tilde{x} = 1 \mid D) = \frac{a + N_1}{a + b + N}$	$p(\tilde{x} = j \mid D) = \frac{\alpha_j + N_j}{\alpha_0 + N}$
Intuition	"Pseudo-counts": $a - 1$ heads, $b - 1$ tails	"Pseudo-counts": $\alpha_k - 1$ for each class, total $\alpha_0 - K$

Outline



- Generative vs. Discriminative: Revisit
- Bayesian concept learning
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- Naive Bayes classifiers

Naive Bayes classifiers



Classify vectors of discrete-valued features to C classes

$$\mathbf{x} = (x_1, x_2, ..., x_D)^T \in \{1, 2, ..., K\}^D$$

- K is the number of values for each feature
- D is the number of features
- □ Compute the probability $P(Y = c | \mathbf{x}, \theta)$



- Generative model, revisit
 - □ Key: learn class-conditional density $P(\mathbf{x}|Y=c,\theta)$

$$P(Y = c | \mathbf{x}, \theta) = \frac{P(\mathbf{x}, Y = c | \theta)}{P(\mathbf{x} | \theta)}$$

$$= \frac{P(\mathbf{x}, Y = c | \theta)}{\sum_{c' \in C} P(\mathbf{x}, Y = c' | \theta)}$$

$$= \frac{P(Y = c | \theta) P(\mathbf{x} | Y = c, \theta)}{\sum_{c' \in C} P(Y = c' | \theta) P(\mathbf{x} | Y = c', \theta)}$$
class-conditional distribution



 Assumption: the features are conditionally independent given the class label

$$p(\mathbf{x}|y=c,\boldsymbol{\theta}) = \prod_{j=1}^{D} p(x_j|y=c,\boldsymbol{\theta}_{jc})$$

- Even if the naive Bayes assumption is not true, it often results in classifiers that work well
 - The model is quite simple (it only has O(CD) parameters, for C classes and D features)



- In the case of binary features $x_j \in \{0,1\}$
 - Multivariate Bernoulli naive Bayes
 - Use the Bernoulli distribution

$$p(\mathbf{x}|y=c,\boldsymbol{\theta}) = \prod_{j=1}^{D} \operatorname{Ber}(x_j|\mu_{jc})$$

• μ_{jc} is the probability that feature j occurs in class c



- In the case of categorical features $x_j \in \{1, ..., K\}$
 - multinomial Naive Bayes
 - Use the multinomial distribution

$$p(\mathbf{x}|y = c, \boldsymbol{\theta}) = \prod_{j=1}^{D} \operatorname{Cat}(x_j | \boldsymbol{\mu}_{jc})$$

• μ_{ic} is a histogram over the K possible values for x_i in class c.



- In the case of real-valued features:
 - Gaussian Naive Bayes
 - Use the Gaussian distribution

$$p(\mathbf{x}|y=c,\boldsymbol{\theta}) = \prod_{j=1}^{D} \mathcal{N}(x_j|\mu_{jc},\sigma_{jc}^2)$$

- μ_{jc} is the mean of feature j in objects of class c
- σ_{ic}^2 is the variance of feature *j* in objects of class c

Model fitting



- How to "train" a naive Bayes classifier
 - MLE
 - MAP estimate
 - Bayesian estimation
 - Compute the full posterior $p(\theta|\mathcal{D})$

MLE for NBC



■ The probability for a single data (\mathbf{x}_i, y_i)

$$p(\mathbf{x}_i, y_i | \boldsymbol{\theta}) = p(y_i | \boldsymbol{\pi}) \prod_j p(x_{ij} | y_i, \theta_j)$$
$$= \prod_c \pi_c^{\mathbb{I}(y_i = c)} \prod_j \prod_c p(x_{ij} | \theta_{jc})^{\mathbb{I}(y_i = c)}$$

 \blacksquare π : the parameters for class prior

MLE for NBC



■ The probability for data set \mathcal{D}

$$p(\mathcal{D}|\boldsymbol{\theta}) = \prod_{i=1}^{N} \left(\prod_{c} \pi_{c}^{\mathbb{I}(y_{i}=c)} \prod_{j} \prod_{c} p(x_{ij}|\theta_{jc})^{\mathbb{I}(y_{i}=c)} \right)$$

■ The log-likelihood for data set \mathcal{D}

$$\log p(\mathcal{D}|\boldsymbol{\theta}) = \sum_{c=1}^{C} N_c \log \pi_c + \sum_{j=1}^{D} \sum_{c=1}^{C} \sum_{i:y_i=c} \log p(x_{ij}|\boldsymbol{\theta}_{jc})$$

MLE for NBC



- The log-likelihood for data set \mathcal{D}
 - the class prior (uniform distribution)

$$\hat{\pi}_c = \frac{N_c}{N}$$

Suppose all features are binary

$$\hat{\theta}_{jc} = \frac{N_{jc}}{N_c}$$



Trouble for MLE: overfitting

Solution: Bayesian estimation

$$p(\boldsymbol{\theta}|\mathcal{D}) = \frac{P(\boldsymbol{\theta})P(\mathcal{D}|\boldsymbol{\theta})}{\int_{\boldsymbol{\theta}'} P(\boldsymbol{\theta}')P(\mathcal{D}|\boldsymbol{\theta}') d\boldsymbol{\theta}'}$$



Prior

$$p(\boldsymbol{\theta}) = p(\boldsymbol{\pi}) \prod_{j=1}^{D} \prod_{c=1}^{C} p(\theta_{jc})$$

 \blacksquare π : Dir(α) prior

 θ_{jc} : Beta(β_0 , β_1) prior

- Special case: $\alpha = 1$, $\beta = 1$
 - Add-one or Laplace smoothing



Posterior

$$p(\theta|\mathcal{D}) \propto p(\theta)p(\mathcal{D}|\theta)$$

$$= \left\{ p(\pi) \prod_{j=1}^{D} \prod_{c=1}^{C} p(\theta_{jc}) \right\} \prod_{i=1}^{N} \left\{ \left[\prod_{c=1}^{C} \pi_c^{\mathbb{I}(y_i=c)} \right] \left[\prod_{c=1}^{C} \prod_{j=1}^{D} \operatorname{Ber}(x_{ij}|\theta_{jc})^{\mathbb{I}(y_i=c)} \right] \right\}$$

$$= \left\{ p(\pi) \prod_{i=1}^{N} \prod_{c=1}^{C} \pi_c^{\mathbb{I}(y_i=c)} \right\} \prod_{j=1}^{D} \prod_{c=1}^{C} \left\{ p(\theta_{jc}) \prod_{i=1}^{N} \operatorname{Ber}(x_{ij}|\theta_{jc})^{\mathbb{I}(y_i=c)} \right\}$$

$$= \left\{ \operatorname{Dir}(\alpha) \prod_{c=1}^{C} \pi_c^{N_c} \right\} \prod_{j=1}^{D} \prod_{c=1}^{C} \left\{ \operatorname{Beta}(\beta_0, \beta_1) (1 - \theta_{jc})^{N_c - N_{jc}} \theta_{jc}^{N_{jc}} \right\}$$

$$\propto \operatorname{Dir}(N_1 + \alpha_1, N_2 + \alpha_2, \cdots, N_C + \alpha_C) \prod_{j=1}^{D} \prod_{c=1}^{C} \operatorname{Beta}(N_c - N_{jc} + \beta_0, N_{jc} + \beta_1)$$



Posterior

$$p(\boldsymbol{\theta}|\mathcal{D}) = p(\boldsymbol{\pi}|\mathcal{D}) \prod_{j=1}^{D} \prod_{c=1}^{C} p(\theta_{jc}|\mathcal{D})$$

$$p(\boldsymbol{\pi}|\mathcal{D}) = \text{Dir}(N_1 + \alpha_1 \dots, N_C + \alpha_C)$$

$$p(\theta_{jc}|\mathcal{D}) = \text{Beta}((N_c - N_{jc}) + \beta_0, N_{jc} + \beta_1)$$

Posterior mean

$$\overline{\theta}_{jc} = \frac{N_{jc} + \beta_1}{N_c + \beta_0 + \beta_1}$$

$$\overline{\pi}_c = \frac{N_c + \alpha_c}{N + \alpha_0}$$



MAP estimate

$$\hat{\pi}_c = \frac{N_c + \alpha_c - 1}{N + \alpha_0 - C}, \quad \hat{\theta}_{jc} = \frac{N_{jc} + \beta_1 - 1}{N_c + \beta_1 + \beta_1 - 2}$$

- The MAP estimate can be directly computed by combining prior counts with empirical counts.
- Very simple to implement, with low computational complexity, and easy to extend.



Predict the label y for new data x

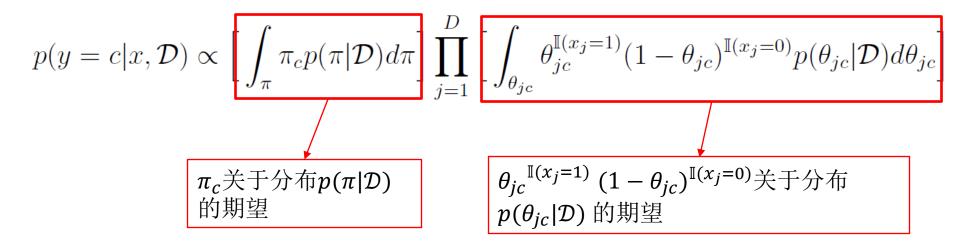
$$p(y = c|x, \mathcal{D}) \propto p(y = c|\mathcal{D})p(x|y = c, \mathcal{D})$$
$$= p(y = c|\mathcal{D}) \prod_{j=1}^{D} p(x_j|y = c, \mathcal{D})$$

Bayesian procedure

$$p(y = c|x, \mathcal{D}) \propto \left[\int_{\pi} p(y = c|\pi) p(\pi|\mathcal{D}) d\pi \right] \prod_{j=1}^{D} \left[\int_{\theta_{jc}} p(x_j|y = c, \theta_{jc}) p(\theta_{jc}|\mathcal{D}) d\theta_{jc} \right]$$
$$= \left[\int_{\pi} \operatorname{Cat}(y = c|\pi) p(\pi|\mathcal{D}) d\pi \right] \prod_{j=1}^{D} \left[\int_{\theta_{jc}} \operatorname{Ber}(x_j|y = c, \theta_{jc}) p(\theta_{jc}|\mathcal{D}) d\theta_{jc} \right]$$



Rewrite the prediction probability





Plug in the posterior mean parameters

$$p(y = c | \mathbf{x}, \mathcal{D}) \propto \overline{\pi}_c \prod_{j=1}^{D} (\overline{\theta}_{jc})^{\mathbb{I}(x_j = 1)} (1 - \overline{\theta}_{jc})^{\mathbb{I}(x_j = 0)}$$

$$\bar{\pi}_c = \frac{N_c + \alpha_c}{N + \alpha_0}, \ \bar{\theta}_{jc} = \frac{N_{jc} + \beta_1}{N_c + \beta_0 + \beta_1}$$



Plug in the point estimate: MLE or MAP

$$p(y = c|x, \mathcal{D}) \propto p(y = c|\mathcal{D}) \prod_{j=1}^{D} p(x_j|y = c, \mathcal{D})$$

$$= p(y = c|\hat{\pi}) \prod_{j=1}^{D} p(x_j|y = c, \hat{\theta}_{jc})$$

$$= \hat{\pi}_c \prod_{j=1}^{D} \hat{\theta}_{jc}^{\mathbb{I}(x_j=1)} (1 - \hat{\theta}_{jc})^{\mathbb{I}(x_j=0)},$$

$$\hat{\pi}_c = \frac{N_c}{N}$$

$$\hat{\theta}_{jc} = \frac{N_{jc}}{N_c}$$



Classifier

$$y = f^*(x) = \underset{c=1,2,\cdots,C}{\operatorname{arg\,max}} p(y = c | X = x, \mathcal{D})$$
$$= \underset{c=1,2,\cdots,C}{\operatorname{arg\,max}} \tilde{\pi}_c \prod_{j=1}^D \tilde{\theta}_{jc}^{\mathbb{I}(x_j=1)} (1 - \hat{\theta}_{jc})^{\mathbb{I}(x_j=0)}$$



■ 给定训练数据如下表所示,其中, $X^{(1)} \in \{1,2,3\}$, $x^{(2)} \in \{S,M,L\}$ 为特征, $Y \in \{-1,1\}$ 为类标记。

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
$X^{(1)}$	1	1	1	1	1	2	2	2	2	2	3	3	3	3	3
$x^{(2)}$	S	М	М	S	S	S	М	М	L	L	L	М	М	L	L
Υ	-1	-1	1	1	-1	-1	-1	1	1	1	1	1	1	1	-1

试根据给定训练数据学习一个朴素贝叶斯分类器并确定 $x = (2,S)^T$ 的类标记。



MLE

□ 计算 class prior

$$N_1 = 9$$

$$N_{-1} = 6$$

$$N = 15$$

$$\hat{\pi}_{-1} = \frac{N_{-1}}{N} = \frac{6}{15}$$

$$\hat{\pi}_{1} = \frac{N_{1}}{N} = \frac{9}{15}$$

$$\hat{\theta}_{1,1,1} = \frac{N_{1,1,1}}{N_1} = \frac{2}{9}$$

$$\hat{\theta}_{2,1,1} = \frac{N_{2,1,1}}{N_1} = \frac{3}{9}$$

$$\hat{\theta}_{S,2,1} = \frac{N_{S,2,1}}{N_1} = \frac{1}{9}$$

$$\hat{\theta}_{M,2,1} = \frac{N_{M,2,1}}{N_1} = \frac{2}{9}$$

$$\widehat{\theta}_{3,1,1} = \frac{N_{3,1,1}}{N_{\text{herative Models: Fundamentals and Application}} = \frac{N_{L,2,1}}{9}$$



 \Box 计算 $\hat{\theta}_{k,j,c}$

$$\hat{\theta}_{1,1,-1} = \frac{N_{1,1,-1}}{N_{-1}} = \frac{3}{6}$$

$$\hat{\theta}_{S,2,-1} = \frac{N_{S,2,-1}}{N_{-1}} = \frac{3}{6}$$

$$\hat{\theta}_{S,2,-1} = \frac{N_{S,2,-1}}{N_{-1}} = \frac{3}{6}$$

$$\hat{\theta}_{M,2,-1} = \frac{N_{M,2,-1}}{N_{-1}} = \frac{3}{6}$$

$$\hat{\theta}_{M,2,-1} = \frac{N_{M,2,-1}}{N_{-1}} = \frac{3}{6}$$

$$\hat{\theta}_{M,2,-1} = \frac{N_{M,2,-1}}{N_{-1}} = \frac{3}{6}$$

$$\hat{\theta}_{L,2,-1} = \frac{N_{L,2,-1}}{N_{-1}} = \frac{1}{6}$$



 \square 预测 $p(Y = c | \mathbf{x}, \mathcal{D})$

$$p(Y = 1 | (2, S)^{T}, \mathcal{D}) \propto \hat{\pi}_{1} (\hat{\theta}_{2,1,1})^{\mathbb{I}(X^{(1)} = 2)} (\hat{\theta}_{S,2,1})^{\mathbb{I}(X^{(2)} = S)}$$
$$= \frac{9}{15} \times \frac{3}{9} \times \frac{1}{9} = \frac{1}{45}$$

$$p(Y = -1|(2,S)^{T}, \mathcal{D}) \propto \hat{\pi}_{-1} (\hat{\theta}_{2,1,-1})^{\mathbb{I}(X^{(1)}=2)} (\hat{\theta}_{S,2,-1})^{\mathbb{I}(X^{(2)}=S)}$$
$$= \frac{6}{15} \times \frac{2}{6} \times \frac{3}{6} = \frac{1}{15}$$

所以数据 $(2,S)^T$ 预测的标签为-1



- Bayes estimation
 - □ 计算 class prior

$$N_1 = 9$$

$$N_{-1} = 6$$

$$N = 15$$

$$\bar{\pi}_{-1} = \frac{N_{-1} + 1}{N + 2} = \frac{7}{17}$$

$$\bar{\pi}_{1} = \frac{N_{1} + 1}{N + 2} = \frac{10}{17}$$



Bayes estimation

$$\bar{\theta}_{1,1,1} = \frac{N_{1,1,1} + 1}{N_1 + 3} = \frac{3}{12} \qquad \bar{\theta}_{S,2,1} = \frac{N_{S,2,1} + 1}{N_1 + 3} = \frac{2}{12}$$

$$\bar{\theta}_{2,1,1} = \frac{N_{2,1,1} + 1}{N_1 + 3} = \frac{4}{12} \qquad \bar{\theta}_{M,2,1} = \frac{N_{M,2,1} + 1}{N_1 + 3} = \frac{5}{12}$$

$$\bar{\theta}_{3,1,1} = \frac{N_{3,1,1} + 1}{N_1 + 3} = \frac{5}{12} \qquad \bar{\theta}_{L,2,1} = \frac{N_{L,2,1} + 1}{N_1 + 3} = \frac{5}{12}$$



 \Box 计算 $\bar{\theta}_{k,j,c}$

$$\bar{\theta}_{1,1,-1} = \frac{N_{1,1,-1}+1}{N_{-1}+3} = \frac{4}{9} \qquad \bar{\theta}_{S,2,-1} = \frac{N_{S,2,-1}+1}{N_{-1}+3} = \frac{4}{9}
\bar{\theta}_{2,1,-1} = \frac{N_{2,1,-1}+1}{N_{-1}+3} = \frac{3}{9} \qquad \bar{\theta}_{M,2,-1} = \frac{N_{M,2,-1}+1}{N_{-1}+3} = \frac{3}{9}
\bar{\theta}_{3,1,-1} = \frac{N_{3,1,-1}+1}{N_{-1}+3} = \frac{2}{9} \qquad \bar{\theta}_{L,2,-1} = \frac{N_{L,2,-1}+1}{N_{-1}+3} = \frac{2}{9}$$



 \square 预测 $p(Y = c | \mathbf{x}, \mathcal{D})$

$$p(Y = 1 | (2, S)^{T}, \mathcal{D}) \propto \bar{\pi}_{1} (\bar{\theta}_{2,1,1})^{\mathbb{I}(X^{(1)} = 2)} (\bar{\theta}_{5,2,1})^{\mathbb{I}(X^{(2)} = S)}$$
$$= \frac{10}{17} \times \frac{4}{12} \times \frac{2}{12} = 0.0327$$

$$p(Y = -1|(2,S)^{T}, \mathcal{D}) \propto \bar{\pi}_{-1} (\bar{\theta}_{2,1,-1})^{\mathbb{I}(X^{(1)}=2)} (\bar{\theta}_{S,2,-1})^{\mathbb{I}(X^{(2)}=S)}$$
$$= \frac{7}{17} \times \frac{3}{9} \times \frac{4}{9} = 0.0610$$

所以数据 $(2,S)^T$ 预测的标签为-1

Summary



Bayesian concept learning

- In discrete hypothesis spaces, update hypothesis posterior using Bayes' rule
- MAP estimation: select the hypothesis with the highest posterior probability

Parametric Bayesian estimation

- Beta-Binomial model: extend parameter estimation to the binomial case
- Dirichlet-Multinomial model: further extend to the multinomial case
- Provides a unified framework from discrete to continuous distributions

Summary



Naive Bayes classifiers

- Generative modeling: estimating class-conditional distribution $p(x \mid y)$
- To simplify, conditional independence assumption

Parameter estimation in Naive Bayes

- Point estimates: MLE / MAP simple and efficient
- Bayesian Naive Bayes: keep full posterior distribution over parameters
 - □ In prediction, often approximated by posterior mean or MAP for tractability

Key message

Naive Bayes combines Bayesian parameter estimation with generative inference; Achieves simplicity $(\mathcal{O}(CD))$ and robustness (priors avoid overfitting)

Thanks!



Questions?