CS434b/654b: Pattern Recognition
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Lecture 5

Maximum Likelihood Parameter Estimation

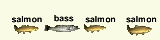
Introducton

- Bayesian Decision Theory in previous lectures tells us how to design an optimal classifier if we knew:
  - $P(c_i)$ (priors)
  - $P(x \mid c_i)$ (class-conditional densities)
- Unfortunately, we rarely have this complete information!
- Suppose we know the shape of distribution, but not the parameters
  - Two types of parameter estimation
    - Maximum Likelihood Estimation
    - Bayesian Estimation (will not do this one in detail)

Today

- Introduction to parameter estimation
  - Maximum Likelihood Estimation
  - Bayesian Estimation
    - will not do this one in detail
    - I have more slides on this when what we'll actually go through for those who are interested

ML Parameter Estimation

- Shape of probability distribution is known
  - Happens sometimes
- Labeled training data 

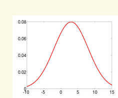
- Need to estimate parameters of probability distribution from the training data

a lot is known "easier"

little is known "harder"

Example

respected fish expert says salmon's length has distribution $N(\mu_1, \sigma_1^2)$ and sea bass's length has distribution $N(\mu_2, \sigma_2^2)$



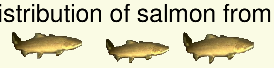
- Need to estimate parameters $\mu_1, \sigma_1^2, \mu_2, \sigma_2^2$
- Then design classifiers according to the bayesian decision theory

Independence Across Classes

- We have training data for each class

- When estimating parameters for one class, will only use the data collected for that class
  - reasonable assumption that data from class c_i gives no information about distribution of class c_j

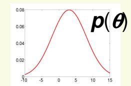
estimate parameters for distribution of salmon from



estimate parameters for distribution of bass from

ML vs. Bayesian Parameter Estimation

- **Maximum Likelihood**
  - Parameters θ are unknown but fixed (i.e. not random variables)
- **Bayesian Estimation**
  - Parameters θ are random variables having some known a priori distribution (prior)
  - Can lead to better results but is more difficult



- After parameters are estimated with either ML or Bayesian Estimation we use methods from Bayesian decision theory for classification

Independence Across Classes

- For each class c_i we have a proposed density $p_i(x/c_i)$ with unknown parameters θ^i which we need to estimate
- Since we assumed independence of data across the classes, estimation is an identical procedure for all classes
- To simplify notation, we drop sub-indexes and say that we need to estimate parameters θ for density $p(x)$
  - the fact that we need to do so for each class on the training data that came from that class is implied

Maximum Likelihood Parameter Estimation

- We have density $p(x)$ which is completely specified by parameters $\theta=[\theta_1,\dots,\theta_k]$
  - If $p(x)$ is $N(\mu,\sigma^2)$ then $\theta=[\mu,\sigma^2]$
- To highlight that $p(x)$ depends on parameters θ we will write $p(x/\theta)$
  - Note overloaded notation, $p(x/\theta)$ is **not** a conditional density
- Let $D=\{x_1, x_2,\dots, x_n\}$ be the n independent training samples in our data
  - If $p(x)$ is $N(\mu,\sigma^2)$ then $x_1, x_2,\dots, x_n$ are iid samples from $N(\mu,\sigma^2)$

Maximum Likelihood Parameter Estimation

- Consider the following function, which is called likelihood of θ with respect to the set of samples D

$$p(D|\theta) = \prod_{k=1}^{k=n} p(x_k|\theta) = F(\theta)$$

- Note if D is fixed $p(D|\theta)$ is **not** a density
- Maximum likelihood estimate (abbreviated MLE) of θ is the value of θ that maximizes the likelihood function $p(D|\theta)$

$$\hat{\theta} = \arg\max_{\theta}(p(D|\theta))$$

ML Parameter Estimation vs. ML Classifier

- Recall ML classifier

  decide class c_i which maximizes $p(x|c_i)$ (fixed data: x)

- Compare with ML parameter estimation

  choose θ that maximizes $p(D|\theta)$ (fixed data: D)

- ML classifier and ML parameter estimation use the same principles applied to different problems

Maximum Likelihood Estimation (MLE)

$$p(D|\theta) = \prod_{k=1}^{k=n} p(x_k|\theta)$$

- If D is allowed to vary and θ is fixed, by independence $p(D|\theta)$ is the joint density for $D=\{x_1, x_2, \dots, x_n\}$
- If θ is allowed to vary and D is fixed, $p(D|\theta)$ is not density, it is likelihood $F(\theta)$!
- Recall our approximation of integral trick

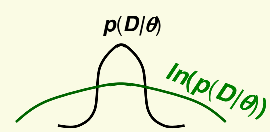
$$Pr[D \in B[x_1, \dots, x_n]|\theta] \approx \varepsilon \prod_{k=1}^{k=n} p(x_k|\theta)$$

- Thus ML chooses θ that is most likely to have given the observed data D

Maximum Likelihood Estimation (MLE)

- Instead of maximizing $p(D|\theta)$, it is usually easier to maximize $\ln(p(D|\theta))$
- Since log is monotonic

$$\hat{\theta} = \arg\max_{\theta}(p(D|\theta)) =$$
$$= \arg\max_{\theta}(\ln p(D|\theta))$$



- To simplify notation, $\ln(p(D|\theta)) = l(\theta)$

$$\hat{\theta} = \arg\max_{\theta} l(\theta) = \arg\max_{\theta}\left(\ln \prod_{k=1}^{k=n} p(x_k|\theta)\right) = \arg\max_{\theta}\left(\sum_{k=1}^{n} \ln p(x_k|\theta)\right)$$

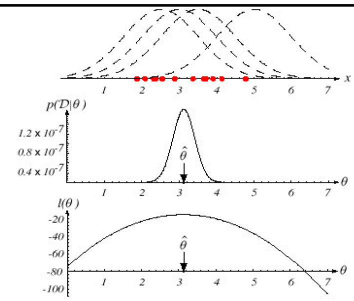


FIGURE 3.1. The top graph shows several training points in one dimension, known or assumed to be drawn from a Gaussian of a particular variance, but unknown mean. Four of the infinite number of candidate source distributions are shown in dashed lines. The middle figure shows the likelihood $p(\mathcal{D}|\theta)$ as a function of the mean. If we had a very large number of training points, this likelihood would be very narrow. The value that maximizes the likelihood is marked $\hat{\theta}$; it also maximizes the logarithm of the likelihood—that is, the log-likelihood $l(\theta)$, shown at the bottom. Note that even though they look similar, the likelihood $p(\mathcal{D}|\theta)$ is shown as a function of θ whereas the conditional density $p(x|\theta)$ is shown as a function of x. Furthermore, as a function of θ, the likelihood $p(\mathcal{D}|\theta)$ is not a probability density function and its area has no significance. From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern Classification*.

2

MLE Example: Gaussian with unknown μ

- Fortunately for us, most of the ML estimates of any densities we would care about have been computed
- Let's go through an example anyway
- Let $p(x|\mu)$ be $N(\mu,\sigma^2)$ that is σ^2 is known, but μ is unknown and needs to be estimated, so $\theta = \mu$

$$\hat{\mu} = \arg\max_{\mu} l(\mu) = \arg\max_{\mu}\left(\sum_{k=1}^{n} \ln p(x_k|\mu)\right) =$$

$$= \arg\max_{\mu}\left(\sum_{k=1}^{n} \ln\left(\frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{(x_k-\mu)^2}{2\sigma^2}\right)\right)\right) =$$

$$= \arg\max_{\mu}\sum_{k=1}^{n}\left(-\ln\sqrt{2\pi}\sigma - \frac{(x_k-\mu)^2}{2\sigma^2}\right)$$

MLE: Maximization Methods

- Maximizing $l(\theta)$ can be solved using standard methods from Calculus
- Let $\theta = (\theta_1, \theta_2, \ldots, \theta_p)^t$ and let ∇_θ be the gradient operator

$$\nabla_\theta = \left[\frac{\partial}{\partial\theta_1}, \frac{\partial}{\partial\theta_2}, \ldots, \frac{\partial}{\partial\theta_p}\right]^t$$

- Set of necessary conditions for an optimum is:

$$\nabla_\theta l = 0$$

- Also have to check that θ that satisfies the above condition is maximum, not minimum or saddle point. Also check the boundary of range of θ

MLE Example: Gaussian with unknown μ

$$\arg\max_{\mu}(l(\mu)) = \arg\max_{\mu}\sum_{k=1}^{n}\left(-\ln\sqrt{2\pi}\sigma - \frac{(x_k-\mu)^2}{2\sigma^2}\right)$$

$$\frac{d}{d\mu}(l(\mu)) = \sum_{k=1}^{n}\frac{1}{\sigma^2}(x_k-\mu) = 0 \Rightarrow \sum_{k=1}^{n} x_k - n\mu = 0 \Rightarrow$$

$$\Rightarrow \hat{\mu} = \frac{1}{n}\sum_{k=1}^{n} x_k$$

- Thus the ML estimate of the mean is just the average value of the training data, very intuitive!
  - average of the training data would be our guess for the mean even if we didn't know about ML estimates

MLE for Gaussian with unknown μ, σ^2

- Similarly it can be shown that if $p(x/\mu,\sigma^2)$ is $N(\mu, \sigma^2)$, that is x both mean and variance are unknown, then again very intuitive result

$$\hat{\mu} = \frac{1}{n}\sum_{k=1}^{n} x_k \qquad \hat{\sigma}^2 = \frac{1}{n}\sum_{k=1}^{n}(x_k - \hat{\mu})^2$$

- Similarly it can be shown that if $p(x/\mu,\Sigma)$ is $N(\mu, \Sigma)$, that is x is a multivariate gaussian with both mean and covariance matrix unknown, then

$$\hat{\mu} = \frac{1}{n}\sum_{k=1}^{n} x_k \qquad \hat{\Sigma} = \frac{1}{n}\sum_{k=1}^{n}(x_k - \hat{\mu})(x_k - \hat{\mu})^t$$

How to Measure Performance of MLE?s

- It is usually much easier to compute an almost equivalent measure of performance, the ***mean squared error***: $E\left[(\theta - \hat{\theta})^2\right]$
- Do a little algebra, and use Var(X)=E(X^2)-(E(X))^2

$$E\left[(\theta - \hat{\theta})^2\right] = \underbrace{Var(\hat{\theta})}_{\text{variance}} + \underbrace{\left(E(\hat{\theta}) - \theta\right)^2}_{\text{bias}}$$

estimator should have low variance ***expectation should be close to the true θ***

How to Measure Performance of MLE?

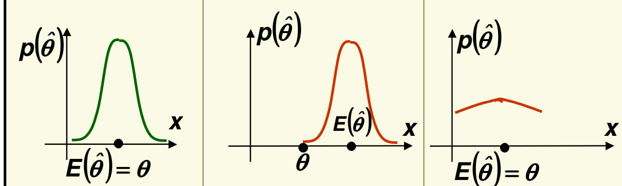
- How good is a ML estimate $\hat{\theta}$?
  - or actually any other estimate of a parameter?
- The natural measure of error would be $|\theta - \hat{\theta}|$
- But $|\theta - \hat{\theta}|$ is random, we cannot compute it before we carry out experiments
  - We want to say something meaningful about our estimate as a function of θ
- A way to solve this difficulty is to ***average*** the error, i.e. compute the ***mean absolute error***

$$E\left[|\theta - \hat{\theta}|\right] = \int |\theta - \hat{\theta}| \, p(x_1, x_2, \ldots, x_n) dx_1 dx_2 \ldots dx_n$$

How to Measure Performance of MLE?

$$E\left[(\theta - \hat{\theta})^2\right] = \underbrace{Var(\hat{\theta})}_{\text{variance}} + \underbrace{\left(E(\hat{\theta}) - \theta\right)^2}_{\text{bias}}$$

ideal case ***bad case*** ***bad case***



no bias *low variance* | *large bias* *low variance* | *no bias* *high variance*

Bias and Variance for MLE of the Mean

- Let's compute the bias for ML estimate of the mean

$$E[\hat{\mu}] = E\left[\frac{1}{n}\sum_{k=1}^{n} x_k\right] = \frac{1}{n}\sum_{k=1}^{n} E[x_k] = \frac{1}{n}\sum_{k=1}^{n}\mu = \mu$$

  - Thus this estimate is unbiased!
- How about variance of ML estimate of the mean?

$$E\left[(\hat{\mu}-\mu)^2\right] = E\left[\hat{\mu}^2 - 2\mu\hat{\mu} + \mu^2\right] = \mu^2 - 2\mu E(\hat{\mu}) + E\left(\left(\frac{1}{n}\sum_{k=1}^{n} x_k\right)^2\right)$$
$$= \frac{\sigma^2}{n}$$

- Thus variance is very small for a large number of samples (the more samples, the smaller is variance)
- Thus the MLE of the mean is a very good estimator

MLE Bias for Mean and Variance

- How about ML estimate for the variance?

$$E[\hat{\sigma}^2] = E\left[\frac{1}{n}\sum_{k=1}^{n}(x_k - \hat{\mu})^2\right] = \frac{n-1}{n}\sigma^2 \neq \sigma^2$$

  - Thus this estimate is biased!
    - This is because we used $\hat{\mu}$ instead of true μ
  - Bias →0 as n→ infinity, *asymptotically* unbiased
  - Unbiased estimate $\hat{\sigma}^2 = \frac{1}{n-1}\sum_{k=1}^{n}(x_k - \hat{\mu})^2$
- Variance of MLE of variance can be shown to go to 0 as n goes to infinity

Bias and Variance for MLE of the Mean

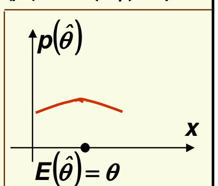
- Suppose someone claims they have a new great estimator for the mean, just take the first sample!

$$\hat{\mu} = x_1$$

- Thus this estimator is unbiased: $E(\hat{\mu}) = E(x_1) = \mu$
- However its variance is:

$$E\left[(\hat{\mu}-\mu)^2\right] = E\left[(x_1-\mu)^2\right] = \sigma^2$$

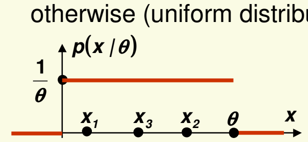
- Thus variance can be very large and does not improve as we increase the number of samples

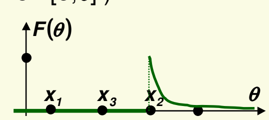


no bias
high variance

MLE for Uniform distribution U[0,θ]

- X is U[0,θ] if its density is 1/θ inside [0,θ] and 0 otherwise (uniform distribution on [0,θ])





- The likelihood is $F(\theta) = \prod_{k=1}^{k=n} p(x_k\,|\,\theta) = \begin{cases} \frac{1}{\theta^n} & \text{if } \theta \geq \max\{x_1,\ldots,x_n\} \\ 0 & \text{if } \theta < \max\{x_1,\ldots,x_n\} \end{cases}$
- Thus $\hat{\theta} = \arg\max_{\theta}\left(\prod_{k=1}^{k=n} p(x_k\,|\,\theta)\right) = \max\{x_1,\ldots,x_n\}$
- This is not very pleasing since for sure θ should be larger than any observed x!

Bayesian Parameter Estimation

- Suppose we have some idea of the range where parameters θ should be
  - Shouldn't we formalize such prior knowledge in hopes that it will lead to better parameter estimation?
- Let θ be a random variable with prior distribution $P(\theta)$
  - This is the key difference between ML and Bayesian parameter estimation
  - This key assumption allows us to fully exploit the information provided by the data

Bayesian Estimation: Formula for $p(x|D)$

- From the definition of joint distribution:

$$p(x \mid D) = \int p(x, \theta \mid D) d\theta$$

- Using the definition of conditional probability:

$$p(x \mid D) = \int p(x \mid \theta, D) p(\theta \mid D) d\theta$$

- But $p(x|\theta,D) = p(x|\theta)$ since $p(x|\theta)$ is completely specified by θ

known unknown

$$p(x \mid D) = \int p(x \mid \theta) p(\theta \mid D) d\theta$$

- Using Bayes formula,

$$p(\theta \mid D) = \frac{p(D \mid \theta) p(\theta)}{\int p(D \mid \theta) p(\theta) d\theta} \qquad p(D \mid \theta) = \prod_{k=1}^{n} p(x_k \mid \theta)$$

Bayesian Parameter Estimation

- As in MLE, suppose $p(x|\theta)$ is completely specified if θ is given
- But now θ is a random variable with prior $p(\theta)$
  - Unlike MLE case, $p(x|\theta)$ is a conditional density
- After we observe the data D, using Bayes rule we can compute the posterior $p(\theta|D)$
- Recall that for the MAP classifier we find the class c_i that maximizes the posterior $p(c|D)$
- By analogy, a reasonable estimate of θ is the one that maximizes the posterior $p(\theta|D)$
- But θ is not our final goal, our final goal is the unknown $p(x)$
- Therefore a better thing to do is to maximize $p(x|D)$, this is as close as we can come to the unknown $p(x)$!

Bayesian Estimation vs. MLE

- So in principle $p(x|D)$ can be computed
  - In practice, it may be hard to do integration analytically, may have to resort to numerical methods

$$p(x / D) = \int p(x / \theta) \frac{\prod_{k=1}^{n} p(x_k / \theta) p(\theta)}{\int \prod_{k=1}^{n} p(x_k / \theta) p(\theta) d\theta} d\theta$$

- Contrast this with the MLE solution which requires differentiation of likelihood to get $p(x / \hat{\theta})$
  - Differentiation is easy and can always be done analytically

Bayesian Estimation vs. MLE

- $p(x/D)$ can be thought of as the weighted average of the proposed model all possible values of θ

$$p(x\mid D)=\int \underbrace{p(x\mid\theta)}_{\text{proposed model with certain }\theta}\overbrace{p(\theta\mid D)}^{\text{support }\theta\text{ receives from the data}}d\theta$$

- Contrast this with the MLE solution which always gives us a single model:

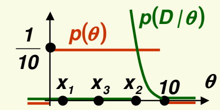
$$p(x\,/\,\hat{\theta})$$

- When we have many possible solutions, taking their sum averaged by their probabilities seems better than spitting out one solution

Bayesian Estimation: Example for U[0,θ]

- We need to compute $p(x\mid D)=\int p(x\mid\theta)p(\theta\mid D)d\theta$
  - using $p(\theta/D)=\dfrac{p(D/\theta)p(\theta)}{\int p(D/\theta)p(\theta)d\theta}$ and $p(D\mid\theta)=\prod_{k=1}^{n}p(x_k\mid\theta)$
- When computing MLE of θ, we had

$$p(D\mid\theta)=\begin{cases}\dfrac{1}{\theta^n} & \text{for } \theta\ge\max\{x_1,\dots,x_n\}\\ 0 & \text{otherwise}\end{cases}$$



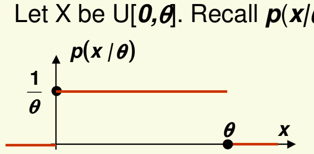
- Thus

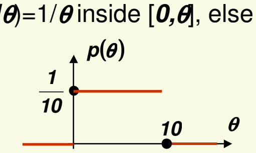
$$p(\theta/D)=\begin{cases}c\dfrac{1}{\theta^n} & \text{for } \max\{x_1,\dots,x_n\}\le\theta\le 10\\ 0 & \text{otherwise}\end{cases}$$

- where c is the normalizing constant, i.e. $c=\dfrac{1}{\int_{\max\{x_1,\dots,x_n\}}^{10}\frac{d\theta}{\theta^n}}$

Bayesian Estimation: Example for U[0,θ]

- Let X be U[$0,\theta$]. Recall $p(x/\theta)=1/\theta$ inside [$0,\theta$], else 0



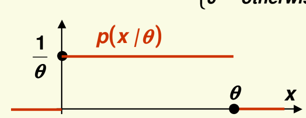


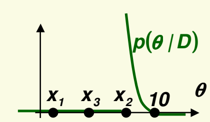
- Suppose we assume a U[0,10] prior on θ
  - good prior to use if we just now the range of θ but don't know anything else
- We need to compute $p(x\mid D)=\int p(x\mid\theta)p(\theta\mid D)d\theta$
  - with $p(\theta\mid D)=\dfrac{p(D\mid\theta)p(\theta)}{\int p(D\mid\theta)p(\theta)d\theta}$ and $p(D\mid\theta)=\prod_{k=1}^{n}p(x_k\mid\theta)$

Bayesian Estimation: Example for U[0,θ]

- We need to compute $p(x\mid D)=\int p(x\mid\theta)p(\theta\mid D)d\theta$

$$p(\theta/D)=\begin{cases}c\dfrac{1}{\theta^n} & \text{for } \max\{x_1,\dots,x_n\}\le\theta\le 10\\ 0 & \text{otherwise}\end{cases}$$





- We have 2 cases:

1. case $x<\max\{x_1,x_2,\dots,x_n\}$

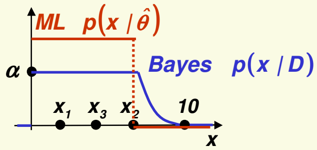
$$p(x/D)=\int_{\max\{x_1,\dots,x_n\}}^{10}c\frac{1}{\theta^{n+1}}d\theta=\boxed{\alpha}$$

constant independent of x

2. case $x>\max\{x_1,x_2,\dots,x_n\}$

$$p(x/D)=\int_x^{10}c\frac{1}{\theta^{n+1}}d\theta=\frac{c}{-n\theta^n}\Big|_x^{10}=\boxed{\frac{c}{nx^n}}-\frac{c}{n10^n}$$

Bayesian Estimation: Example for U[0,θ]



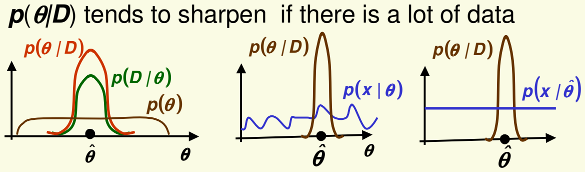
- Note that even after x >max {x_1, x_2,…, x_n}, Bayes density is not zero, which makes sense
- curious fact: Bayes density is not uniform, i.e. does not have the functional form that we have assumed!

ML vs. Bayesian Estimation: General Prior

- Maximum Likelihood Estimation
  - Easy to compute, use differential calculus
  - Easy to interpret (returns one model)
  - $p(x|\hat{\theta})$ has the assumed parametric form
- Bayesian Estimation
  - Hard compute, need multidimensional integration
  - Hard to interpret, returns weighted average of models
  - $p(x|D)$ does not necessarily have the assumed parametric form
  - Can give better results since use more information about the problem (prior information)

ML vs. Bayesian Estimation with Broad Prior

- Suppose $p(\theta)$ is flat and broad (close to uniform prior)
- $p(\theta|D)$ tends to sharpen if there is a lot of data



- Thus $p(D|\theta) \propto p(\theta|D)/p(\theta)$ will have the same sharp peak as $p(\theta|D)$
- But by definition, peak of $p(D|\theta)$ is the ML estimate $\hat{\theta}$
- The integral is dominated by the peak:

$$p(x \mid D) = \int p(x \mid \theta)p(\theta \mid D)d\theta \approx p(x \mid \hat{\theta})\int p(\theta \mid D)d\theta = p(x \mid \hat{\theta})$$

- Thus as n goes to infinity, Bayesian estimate will approach the density corresponding to the MLE!