## Basics of Parameter Estimation in Probabilistic Models

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#### Probabilistic Machine Learning (CS772A)

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#### **Parameter Estimation**

• Given: data  $\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N\}$  generated i.i.d. from a probabilistic model

$$\mathbf{x}_n \sim p(\mathbf{x}|\theta) \qquad \forall n = 1, \dots, N$$

- $\bullet$  Goal: estimate parameter  $\theta$  from the observed data  ${\cal D}$
- First, recall the Bayes rule: The posterior probability  $p(\theta|\mathbf{X})$  is

$$p(\theta|\mathbf{X}) = \frac{p(\mathbf{X}|\theta)p(\theta)}{p(\mathbf{X})} = \frac{p(\mathbf{X}|\theta)p(\theta)}{\int_{\theta} p(\mathbf{X}|\theta)p(\theta)d\theta} = \frac{\text{likelihood} \times \text{prior}}{\text{marginal probability}}$$

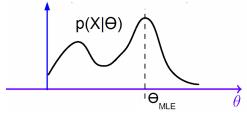
- $p(\mathbf{X}|\theta)$ : probability of data  $\mathbf{X}$  (or "likelihood") for a specific  $\theta$
- $p(\theta)$ : prior distribution (our prior belief about  $\theta$  without seeing any data)
- p(X): marginal probability (or "evidence") likelihood averaged over all θ's (also normalizes the numerator to make p(θ|X) a probability distribution)

## Maximum Likelihood Estimation (MLE)

- Perhaps the simplest (but widely used) parameter estimation method
- Finds the parameter  $\theta$  that maximizes the likelihood  $p(\mathbf{X}|\theta)$

$$\mathcal{L}(\theta) = p(\mathbf{X}|\theta) = p(\mathbf{x}_1, \dots, \mathbf{x}_N \mid \theta) = \prod_{n=1}^N p(\mathbf{x}_n \mid \theta)$$

• Note: Likelihood is a function of  $\boldsymbol{\theta}$ 



## Maximum Likelihood Estimation (MLE)

 MLE typically maximizes the log-likelihood instead of the likelihood (doesn't affect the estimation because log is monotonic)

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Log-likelihood:

$$\log \mathcal{L}(\theta) = \log p(\mathbf{X} \mid \theta) = \log \prod_{n=1}^{N} p(\mathbf{x}_n \mid \theta) = \sum_{n=1}^{N} \log p(\mathbf{x}_n \mid \theta)$$

Maximum Likelihood parameter estimation

$$\hat{\theta}_{MLE} = \arg\max_{\theta} \log \mathcal{L}(\theta) = \arg\max_{\theta} \sum_{n=1}^{N} \log p(\boldsymbol{x}_n \mid \theta)$$

## **MLE: Consistency**

• If the assumed model  $p(\mathbf{x}|\theta)$  has the same form as the true underlying model, then the MLE is consistent as the number of observations  $N \to \infty$ 

$$\hat{\theta}_{MLE} \rightarrow \theta_*$$

where  $\theta_*$  is the parameter of the true underlying model  $p(\mathbf{x}|\theta_*)$  that generated the data

• A rough informal proof: In the limit  $N o \infty$ 

• Thus  $\hat{\theta}_{MLE}$ , the maximizer of  $\mathcal{L}(\theta)$ , minimizes the KL divergence between  $p(\mathbf{x}|\theta_*)$  and  $p(\mathbf{x}|\theta_*)$ . Since both have the same form,  $\theta = \theta_*$ 

### MLE via a simple example

- Consider a sequence of N coin tosses (call head = 0, tail = 1)
- Each outcome  $x_n$  is a binary random variable  $\in \{0, 1\}$
- Assume  $\theta$  to be probability of a head (parameter we wish to estimate)
- Each likelihood term  $p(x_n \mid \theta)$  is Bernoulli:  $p(x_n \mid \theta) = \theta^{x_n} (1 \theta)^{1 x_n}$
- Log-likelihood:  $\sum_{n=1}^{N} \log p(\mathbf{x}_n \mid \theta) = \sum_{n=1}^{N} \mathbf{x}_n \log \theta + (1 \mathbf{x}_n) \log(1 \theta)$
- Taking derivative of the log-likelihood w.r.t.  $\theta$ , and setting it to zero gives

$$\hat{\theta}_{MLE} = \frac{\sum_{n=1}^{N} \mathbf{x}_n}{N}$$

- $\hat{\theta}_{MLE}$  in this example is simply the fraction of heads!
- MLE doesn't have a way to express our prior belief about θ. Can be problematic especially when the number of observations is very small (e.g., suppose we only observed heads in a small number of coin-tosses).

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## Maximum-a-Posteriori Estimation (MAP)

- Allows incorporating our prior belief (without having seen any data) about  $\theta$  via a prior distribution  $p(\theta)$
- $p(\theta)$  specifies what the parameter looks like a priori

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• Finds the parameter  $\theta$  that maximizes the posterior probability of  $\theta$  (i.e., probability in the light of the observed data)

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$$\theta_{MAP} = \arg \max_{\theta} p(\theta | \mathbf{X})$$

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## Maximum-a-Posteriori (MAP) Estimation

• Maximum-a-Posteriori parameter estimation: Find the  $\theta$  that maximizes the (log of) posterior probability of  $\theta$ 

$$\hat{\theta}_{MAP} = \arg \max_{\theta} p(\theta | \mathbf{X}) = \arg \max_{\theta} \frac{p(\mathbf{X}|\theta)p(\theta)}{p(\mathbf{X})}$$

$$= \arg \max_{\theta} p(\mathbf{X}|\theta)p(\theta)$$

$$= \arg \max_{\theta} \log p(\mathbf{X}|\theta)p(\theta)$$

$$= \arg \max_{\theta} \{\log p(\mathbf{X}|\theta) + \log p(\theta)\}$$

$$\hat{\theta}_{MAP} = \arg \max_{\theta} \{ \sum_{n=1}^{N} \log p(\boldsymbol{x}_n | \theta) + \log p(\theta) \}$$

- Same as MLE except the extra log-prior-distribution term!
- Note: When  $p(\theta)$  is a uniform prior, MAP reduces to MLE

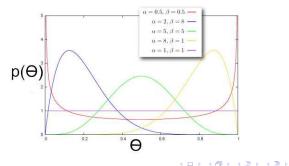
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## MAP via a simple example

- Let's again consider the coin-toss problem (estimating the bias of the coin)
- Each likelihood term is Bernoulli:  $p(\mathbf{x}_n|\theta) = \theta^{\mathbf{x}_n}(1-\theta)^{1-\mathbf{x}_n}$
- Since  $heta \in (0,1)$ , we assume a Beta prior:  $heta \sim \mathsf{Beta}(lpha,eta)$

$$p(\theta) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} \theta^{\alpha - 1} (1 - \theta)^{\beta - 1}$$

•  $\alpha,\beta$  are called hyperparameters of the prior



## MAP via a simple example

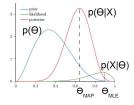
- The log posterior probability =  $\sum_{n=1}^{N} \log p(\mathbf{x}_n | \theta) + \log p(\theta)$
- Ignoring the constants w.r.t.  $\theta$ , the log posterior probability:  $\sum_{n=1}^{N} \{ \mathbf{x}_n \log \theta + (1 - \mathbf{x}_n) \log(1 - \theta) \} + (\alpha - 1) \log \theta + (\beta - 1) \log(1 - \theta) \}$
- $\bullet\,$  Taking derivative w.r.t.  $\theta$  and setting to zero gives

$$\hat{\theta}_{MAP} = \frac{\sum_{n=1}^{N} \mathbf{x}_n + \alpha - 1}{N + \alpha + \beta - 2}$$

- Note: For  $\alpha = 1, \beta = 1$ , i.e.,  $p(\theta) = \text{Beta}(1, 1)$  (which is equivalent to a uniform prior), we get the same solution as  $\hat{\theta}_{MLE}$
- Note: Hyperparameters of the prior (in this case  $\alpha$ ,  $\beta$ ) can often be thought of as "pseudo-observations". E.g., in the coin-toss example,  $\alpha 1$ ,  $\beta 1$  are the expected numbers of heads and tails, respectively, before seeing any data

## **Point Estimation vs Full Posterior**

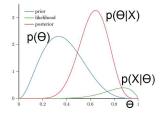
- $\bullet\,$  Note that MLE and MAP only provide us with a best "point estimate" of  $\theta\,$ 
  - MLE gives  $\theta$  that maximizes  $p(\mathbf{X}|\theta)$  (likelihood, or probability of data given  $\theta$ )
  - MAP gives  $\theta$  that maximizes  $p(\theta|\mathbf{X})$  (posterior probability of the parameter  $\theta$ )
- MLE does not incorporate any prior knowledge about parameters
- MAP does incorporate prior knowledge but still only gives a point estimate



- Point estimate doesn't capture the uncertainty about the parameter  $\theta$
- The full posterior  $p(\theta|\mathbf{X})$  gives a more complete picture (e.g., gives an estimate of uncertaintly in the learned parameters, gives more robust predictions/undertainty in predictions, and many other benefits that we will see later during the semester)

### **Point Estimation vs Full Posterior**

• Estimating (or "inferring") the full posterior can be hard in general



- In some cases, however, we can analytically compute the full posterior (e.g., when the prior distribution is "conjugate" to the likelihood)
- In other cases, it can be approximated via approximate Bayesian inference (more on this later during the semester)

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## Estimating the Full Posterior: A Simple Example

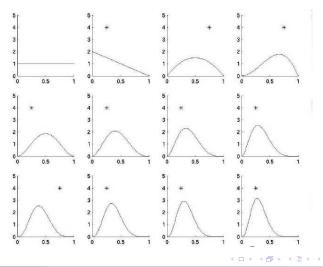
- Let's come back once more to the coin-toss example
- Recall that each likelihood term was Bernoulli:  $p(x_n|\theta) = \theta^{x_n}(1-\theta)^{1-x_n}$
- The prior  $p(\theta)$  was Beta:  $p(\theta) = \text{Beta}(\alpha, \beta) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \theta^{\alpha-1} (1-\theta)^{\beta-1}$
- The posterior is given by

$$p(\theta|\mathbf{X}) \propto \prod_{n=1}^{N} p(\mathbf{x}_{n}|\theta) p(\theta)$$
$$\propto \theta^{\alpha + \sum_{n=1}^{N} \mathbf{x}_{n} - 1} (1-\theta)^{\beta + N - \sum_{n=1}^{N} \mathbf{x}_{n} - 1}$$

- It can be verified (exercise) that the normalization constant in the above is a Beta function  $\frac{\Gamma(\alpha + \sum_{n=1}^{N} x_n)\Gamma(\beta + N \sum_{n=1}^{N} x_n)}{\Gamma(\alpha + \beta + N)}$
- Thus the posterior  $p(\theta|\mathbf{X}) = \text{Beta}(\alpha + \sum_{n=1}^{N} \mathbf{x}_n, \beta + N \sum_{n=1}^{N} \mathbf{x}_n)$
- Here, the posterior has the same form as the prior (both Beta)
- Also very easy to perform online inference (posterior can be used as a prior for the next batch of data)

#### Posterior Evolution with Observed Data

• Assume starting with a uniform prior (equivalent to Beta(1,1)) in the coin-toss example and observing a sequence of heads and tails



## **Conjugate Priors**

- If the prior distribution is conjugate to the likelihood, posterior inference is simplified significantly
- When the prior is conjugate to the likelihood, posterior also belongs to the same family of distributions as the prior
- Many pairs of distributions are conjugate to each other. E.g.,
  - Bernoulli (likelihood) + Beta (prior)  $\Rightarrow$  Beta posterior
  - Binomial (likelihood) + Beta (prior)  $\Rightarrow$  Beta posterior
  - Multinomial (likelihood) + Dirichlet (prior)  $\Rightarrow$  Dirichlet posterior
  - Poisson (likelihood) + Gamma (prior)  $\Rightarrow$  Gamma posterior
  - Gaussian (likelihood) + Gaussian (prior)  $\Rightarrow$  Gamma posterior
  - and many other such pairs ..
- Easy to identify if two distributions are conjugate to each other: their functional forms are similar. E.g., multinomial and Dirichlet

multinomial  $\propto p_1^{x_1} \dots p_K^{x_K}$ , Dirichlet  $\propto p_1^{\alpha_1} \dots p_K^{\alpha_K}$ 

## **Conjugate Priors and Exponential Family**

• Recall the exponential family of distributions

$$p(x|\theta) = h(x)e^{\eta(\theta)^{\top}T(x)-A(\theta)}$$

- $\theta$ : parameter of the family. h(x),  $\eta(\theta)$ , T(x), and  $A(\theta)$  are known functions
- p(.) depends on data x only through its sufficient statistics T(x)
- For each exp. family distribution  $p(x|\theta)$ , there is a conjugate prior of the form

$$p( heta) \propto e^{\eta( heta)^ op lpha - \gamma \mathcal{A}( heta)}$$

where  $\alpha,\gamma$  are the hyperparameters of the prior

• Updated posterior: posterior will also have the same form as the prior

$$p( heta|x) \propto p(x| heta)p( heta) \propto e^{\eta( heta)^{ op} [\mathcal{T}(x)+lpha] - [\gamma+1]\mathcal{A}( heta)}$$

• Updates by adding the sufficient statistics T(x) to prior's hyperparameters

# Next Class: Probabilistic Linear Regression

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