CS 583: Probabilistic Graphical Models

Topic: Parameter Estimation
Chapters: 17, 19, 20

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COMPLETE DATA
CHAPTER 17

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PARAMETER ESTIMATION FOR BNS

- Assume the network structure is given

- The data $\mathcal{D}$ consists of fully observed instances of the network variables

  - $\mathcal{D} = \{x[1], x[2], \dots, x[n]\}$

- Estimate the network parameters, i.e., learn the CPDs

- Two approaches

  1. Maximum likelihood estimation

  2. Bayesian estimation

SIMPLEST CASE – ONE VARIABLE

- Imagine we have a thumbtack

- Flip it, and it comes as heads or tails

heads   tails

- Assume we flip it 100 times and it comes head 30 times

- What is θ?

THUMBTACK TOSSES

- Assume we have a set of thumbtack tosses

  - $\mathcal{D} = \{x[1], \ldots, x[n]\}$

- Also assume each toss, $x[i]$, is IID

- We define a *hypothesis space* Θ

  - Θ is the set of all parameters $\theta \in [0, 1]$

- We formulate an *objective function*

  - The objective function tells us how good a given hypothesis (in this case θ) is

LIKELIHOOD

- What is the probability, or *likelihood*, of seeing the sequence H, T, T, H, H?

  - $\theta*(1-\theta)*(1-\theta)*\theta*\theta = \theta^3(1-\theta)^2$
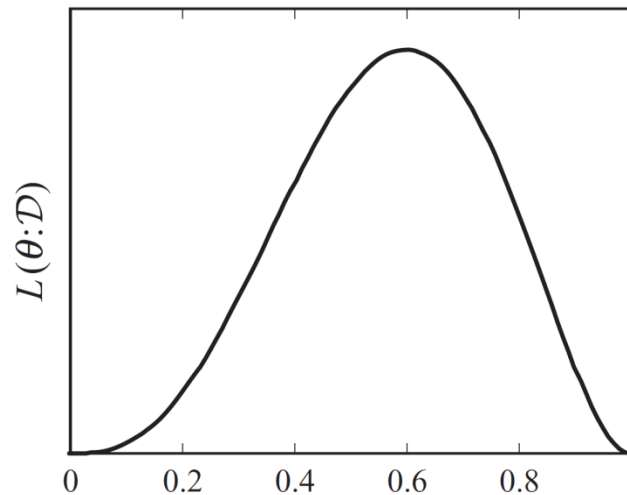
When is L(θ:$\mathcal{D}$) maximum?

LIKELIHOOD/LOG-LIKELIHOOD

- Number of heads = h, number of tails = t

- Likelihood: $L(\theta:\mathcal{D}) = \theta^h(1-\theta)^t$

- Log-likelihood: $l(\theta:\mathcal{D}) = h\ln\theta + t\ln(1-\theta)$

- Find θ that maximizes the log-likelihood

- Take derivate of $l(\theta:\mathcal{D})$ with respect to θ and set it to zero

MAXIMUM LIKELIHOOD FOR A MULTINOMIAL

- Domain of X is {A, B, C}

- We see A a times, B b times, and C c times.

- P(X=A) is p, P(X=B) is q, and P(C) = $1 - p - q$

- What are p and q?

- Proof?

CONSTRAINED OPTIMIZATION

- Assume *X* can take *k* values

- P(X=x_i) = θ_i

- Find **θ** that maximizes the entropy

  - H(X) = -$\Sigma_i\theta_i\log_2\theta_i$

- If we take the partial derive w.r.t. θ_i

  - …

CONSTRAINED OPTIMIZATION

Find $\boldsymbol{\theta}$

maximizing $f(\boldsymbol{\theta})$

subject to

$$c_1(\boldsymbol{\theta}) \quad = \quad 0$$

$$\ldots$$

$$c_m(\boldsymbol{\theta}) \quad = \quad 0$$

Form the Lagrangian:

$$F(\boldsymbol{\theta}, \boldsymbol{\lambda}) = f(\boldsymbol{\theta}) - \sum_{j=1}^{m} \lambda_j c_j(\boldsymbol{\theta})$$

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LAGRANGE MULTIPLIERS EXAMPLES

1. Maximize x*y st. x+y = 10

2. Maximize x+y st. $x^2+y^2 = 1$

3. Entropy

4. Maximum likelihood estimate for a multinomial

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ML for BNs

- Simple structure

  - $X \rightarrow Y$

- General structure

  - The key is that the parameters for each variable can be optimized independently

  - Examples

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BAYESIAN ESTIMATION

- Assume we flip a coin 10 times and we get 4 Heads, 6 Tails
  - What is P(C=H)?

- Assume we flip a thumbtack 10 times and we get 4 Heads, 6 Tails
  - What is P(T=H)?

- What if we repeat the flips 10M times and we get 4M Heads and 6M Tails?

- Bayesian estimation will let us encode our *prior knowledge*

INDEPENDENCE?

- Earlier, we assumed the tosses are independent

- This is true if we know θ

- If we don't know θ, then each toss tells us something about θ, thus the next toss
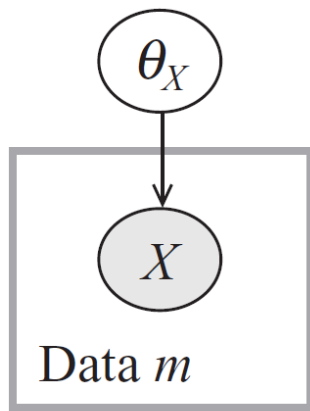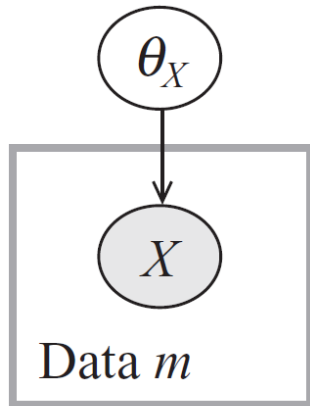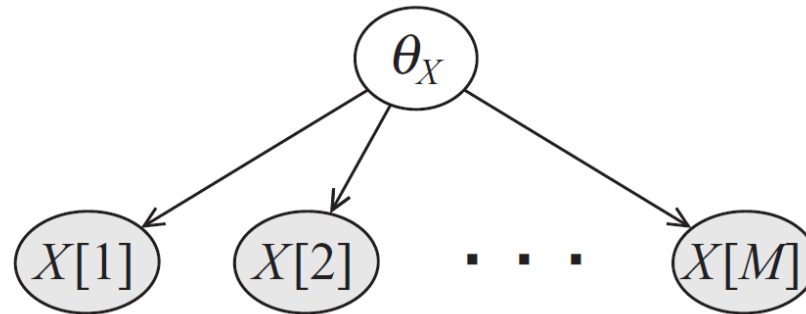

(a)
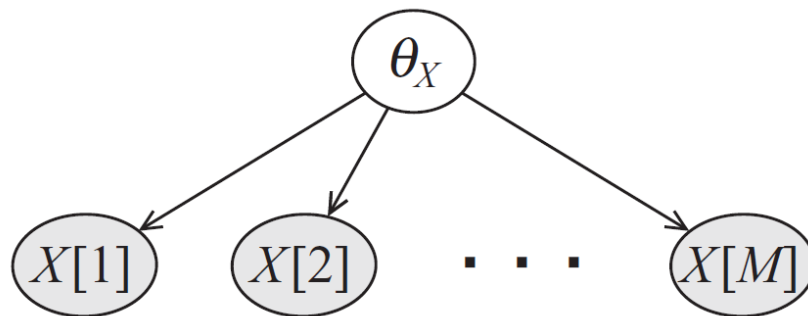
(b)

BAYESIAN ESTIMATION

- Rather than a single θ, we will instead have a probability distribution, P(θ), over θ
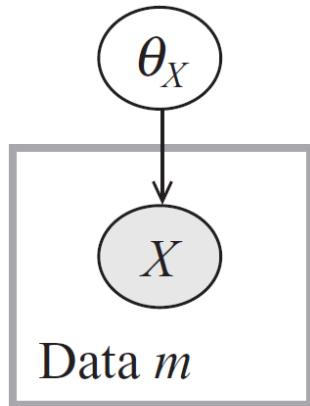
BAYESIAN ESTIMATION
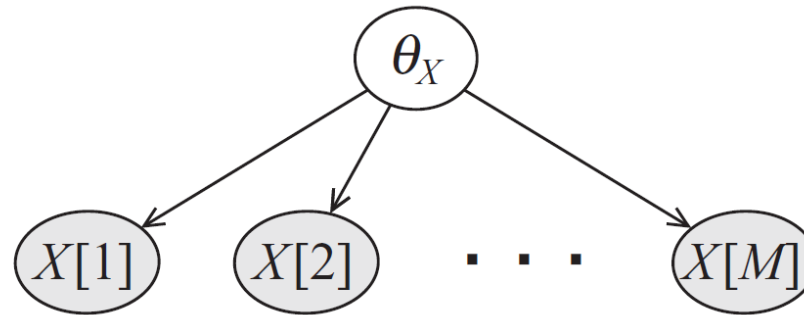

(a)   (b)

- We treat the parameter θ as a random variable

- We ascribe a prior probability to θ, P(θ), encoding our prior knowledge

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PARAMETERS

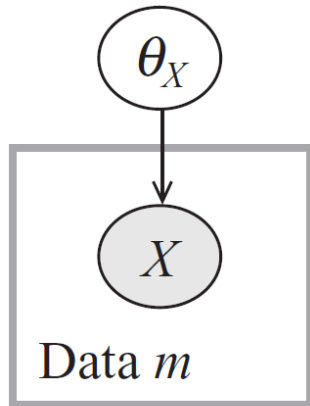(a)   (b)

- $P(X[i] = x^1 \mid \theta_x) = \theta; P(X[i] = x^0 \mid \theta_x) = (1 - \theta)$

- $P(\theta_x)?$

  - A continuous distribution over the interval [0,1]
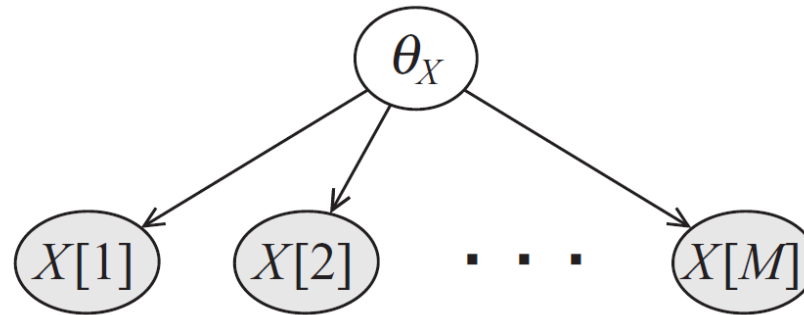
POSTERIOR AND PREDICTION

- We are interested in
  - The probability of the next instance, given data
    - P(x[M+1] | D)
  - The posterior distribution of θ given data
    - P(θ | D)

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FACTORIZATION

(a)

(b)

$$P(x[1], x[2], ..., x[M], \theta_X) \quad = \quad P(\theta_X)\prod_{m=1}^{M} P(x[m] \mid \theta_X)$$

$$= \quad P(\theta_X)\theta^{M[1]}(1-\theta)^{M[0]}$$

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POSTERIOR AND P(X[M+1] | D)

Posterior distribution

$$P(\theta_X \mid D) = \frac{P(x[1],...,x[M] \mid \theta_X)P(\theta_X)}{P(x[1],...,x[M])}$$

$$P(x[M+1] \mid D) \quad = \quad \int_0^1 P(x[M+1] \mid \theta_X, x[1],...x[M])P(\theta_X \mid x[1],...,x[M])d\theta$$

$$= \quad \int_0^1 \underbrace{P(x[M+1] \mid \theta_X)}\underbrace{P(\theta_X \mid x[1],...,x[M])}d\theta$$

θ or 1-θ
(if binary)

Posterior

Think of taking a weighted average

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P(x[M+1] | D)

$$P(x[M+1] \mid x[1],...,x[M]) \quad = \quad \int_0^1 P(x[M+1] \mid \theta_X) P(\theta_X \mid x[1],...,x[M]) d\theta$$

$$= \quad \int_0^1 P(x[M+1] \mid \theta_X) \frac{P(\theta_X) P(x[1],...,x[M] \mid \theta_X)}{P(x[1],...,x[M])}$$

P(*x*[1], …, *x*[M]) is a constant

$$P(x[M+1] \mid x[1],...,x[M]) \propto \int_0^1 P(x[M+1] \mid \theta_X) P(\theta_X) P(x[1],...,x[M] \mid \theta_X) d\theta$$

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UNIFORM PRIOR

- We have a uniform prior over θ_x. That is, $p(\theta_x)=1$

- $P(X[M+1]=x^1 \mid x[1],\ldots,x[M])$?

UNIFORM PRIOR

- We have a uniform prior over θ_X. That is, $p(\theta_X)=1$

- $P(X[M+1]=x^1 \mid x[1],\ldots,x[M])$? That is, $P(X[M+1]=x^1 \mid D)$?

- For the binary case, $P(X[M+1]=x^1 \mid D) = (t + 1) / (t + f + 2)$, where t is the number of True cases and f is the number of False cases in D

- This is also called *Laplace smoothing*

- What about the posterior, $P(\theta \mid D)$, if the prior $P(\theta)$ is uniform?

Beta Distribution

- $\theta \sim \text{Beta}(\alpha,\beta)$ if $P(\theta) = \gamma\theta^{\alpha-1}(1-\theta)^{\beta-1}$ where γ is a normalizing constant

- Mean: $\alpha/(\alpha+\beta)$

- Mode: $(\alpha-1)/(\alpha+\beta-2)$

- Note that the mode is closer to the mean when α and β are large

- Read more at

  - https://en.wikipedia.org/wiki/Beta_distribution

BETA DISTRIBUTION
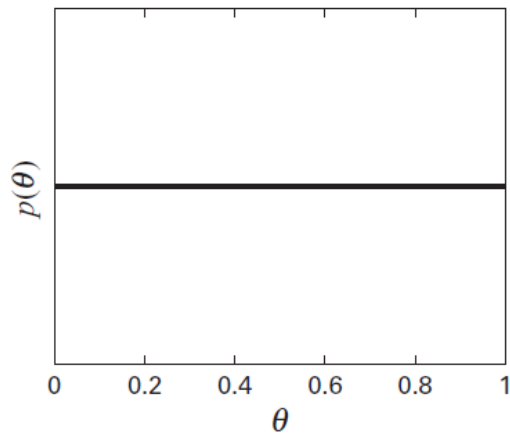
$Beta(1,1)$
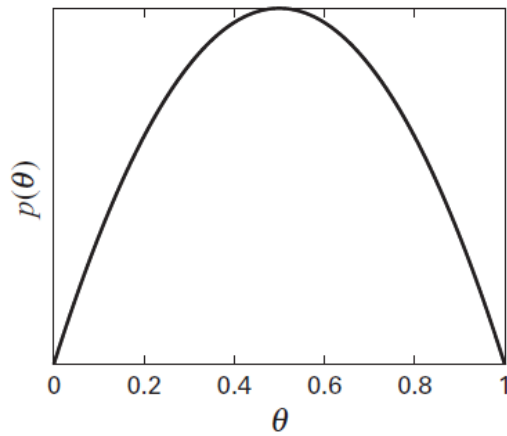
$Beta(2,2)$

$Beta(10,10)$
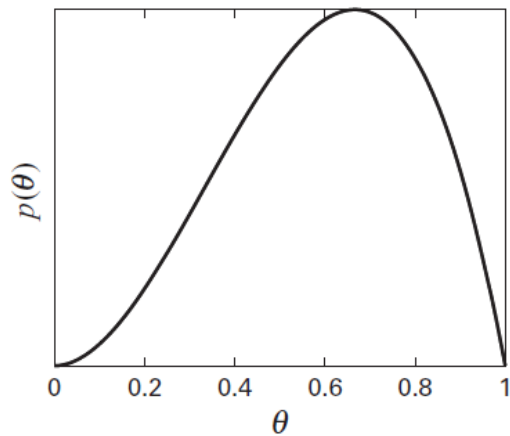
$Beta(3,2)$

$Beta(15,10)$

$Beta(0.5,0.5)$

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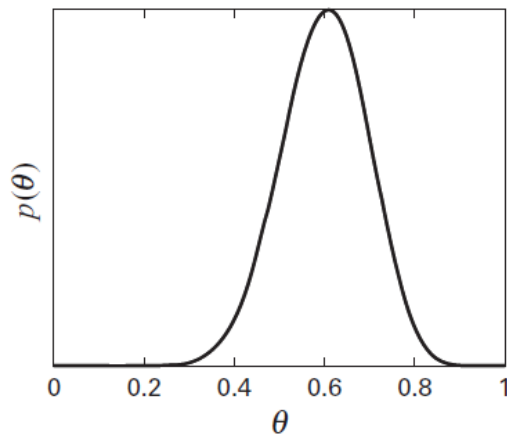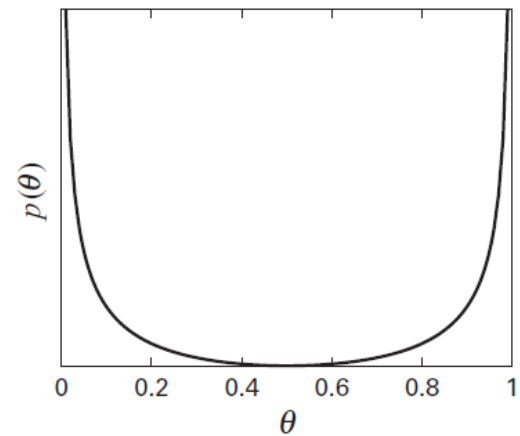
BETA DISTRIBUTION

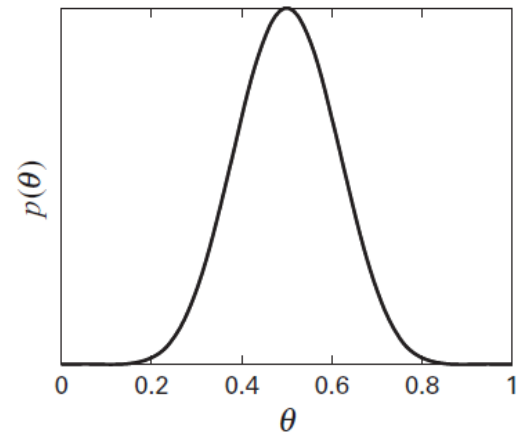- What is $P(X[M+1]=x^1 \mid D)$ if the prior is Beta(α,β)?

  - $P(X[M+1]=x^1 \mid D) = (p + \alpha) / (p + n + \alpha + \beta)$

- What is the posterior, $P(\theta \mid D)$, if the prior is Beta(α,β)?

  - $P(\theta \mid D) = \text{Beta}(p + \alpha, n + \beta)$

- α and β work like pseudo-counts for the positive and negative cases respectively

- What values to choose for α and β?

  - It depends on our belief and the strength of our belief

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DIRICHLET PRIORS

- Generalizes the Beta distribution for multinomials

$$\theta \sim Dirichlet(\alpha_1,\ldots,\alpha_K) \text{ if } P(\theta) \propto \prod_{k=1}^{K} \theta_k^{\alpha_k - 1}$$

- What is $P(X[M+1]=x^i \mid D)$ if the prior is Dirichlet?

    - $P(X[M+1]=x^i \mid D) = (n_i+\alpha_i) / (\mid D \mid + \alpha)$ where n_i is the number of times the ith case appears in D and $\alpha = \alpha_1 + \alpha_2 + \ldots + \alpha_K$

- What is the posterior, $P(\theta \mid D)$, if the prior is Dirichlet?

    - $P(\theta \mid D) = Dirichlet(n_1 + \alpha_1, n_2 + \alpha_2, \ldots, n_K + \alpha_K)$

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BAYESIAN ESTIMATION

- In MLE for BNs, we optimized each parameter independently

- Can we do the same for Bayesian estimation for BNs?

  - Only if the prior also factorizes wrt the BN

- What about the priors? How do we choose them?

  1. Ask the prior for each variable to an expert

  2. Use the same prior for all variables

     - This is called the *K2 prior*

  3. Imagine a dataset D' of imaginary instances

     - The number of imaginary instances for x is $|D'|*P'(x, pa(x))$

     - This is called the *BDe prior*

     - What is P'?

       - Could be anything; e.g., a marginally independent distribution

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BAYESIAN ESTIMATION EXAMPLES

- Try a dataset using
  - MLE
  - Bayesian
    - K2
    - BDe

ICU Alarm network – fig 17.c.1
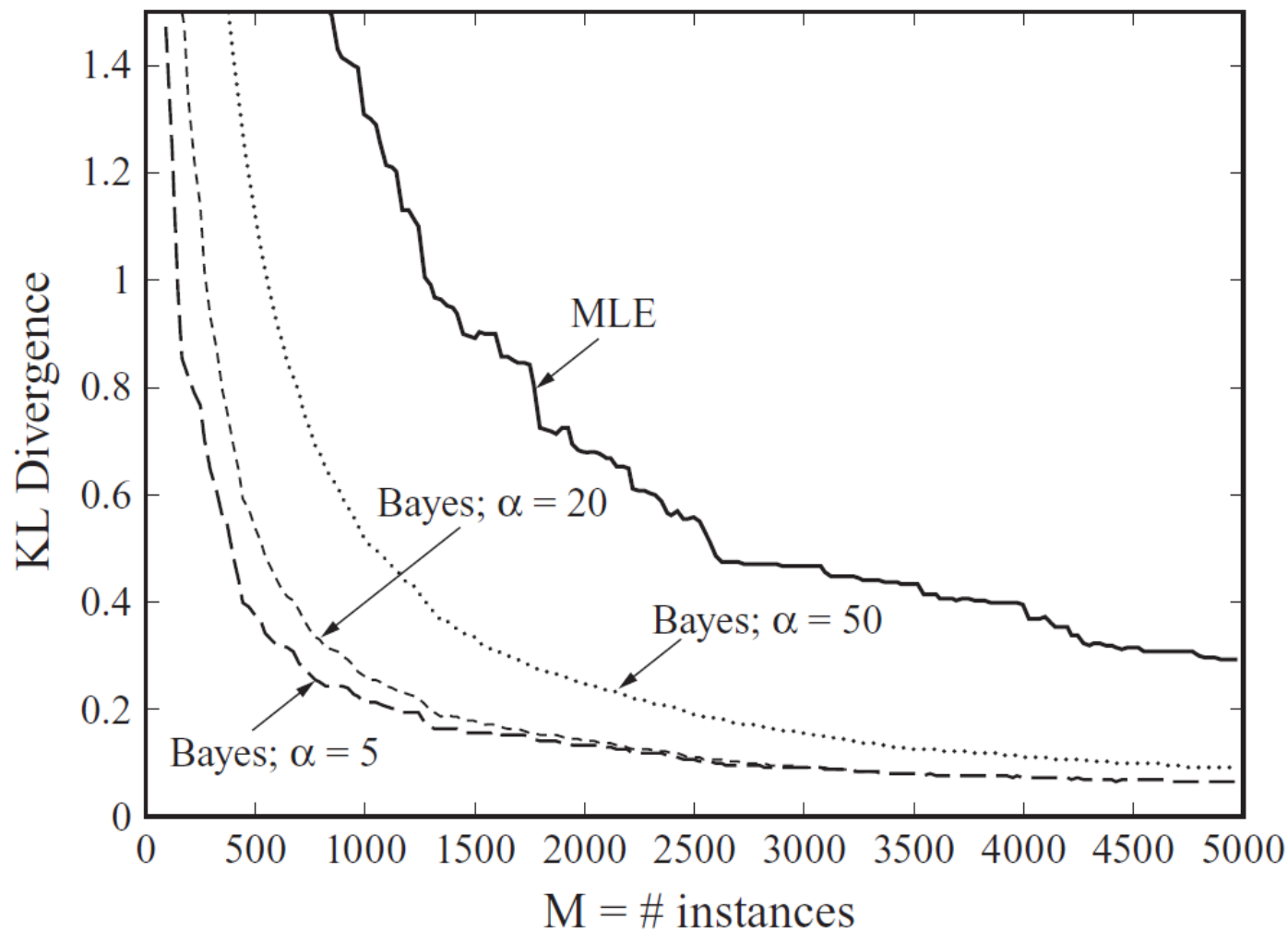
INCOMPLETE DATA
CHAPTER 19

Missing Data

1. Accidental
   - E.g., sensor failure

2. Intentional
   - E.g., not all tests are ordered for medical diagnosis

3. Hidden variable
   - E.g., cluster assignment; hidden cause

APPROACHES

1. Ignore the data points with missing values

   - Not economical (throwing data away), not necessarily accurate (if missing intentionally), and might not be possible (hidden variables)

2. Gradient optimization

3. Expectation Maximization

EXPECTATION MAXIMIZATION (EM)

- Initialize θ

- Iterate

  - Expectation

    - $M[x, pa(x)] = \sum P(x, pa(x) \mid observed)$ for each X

  - Maximization

    - $\theta_x = M[x, pa(x)] / M[pa(x)]$ for each X

EM EXAMPLES

- Simple network
  - $X \rightarrow Y$
  - Let's see a few cases:
    - X is missing in a small percentage; sometimes X and sometimes Y is missing; X is a hidden variable

- A more complicated network:
  - A disease (D) variable and three test variables (T_1, T_2 and T_3)
  - A naïve Bayes structure: D is the parent of T_1, T_2 and T_3
  - T_1 is the fastest but least accurate test. T_2 requires more time but is more accurate. T_3 requires the most time but also is the most accurate test.
  - The doctors order T_1 for everyone first. Depending on the results, they might order T_2, and depending on its results, they might order T_3
  - D might be totally hidden or might be observed for only a small subset of the data

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Markov Networks
Chapter 20

OVERVIEW

- Compared with Bayesian networks, the same principles apply but the issues and solutions are quite different

- The most important reason for the differences is the use of global normalization constant Z

- Z couples all parameters together, preventing us from optimizing each parameter independently

- Even simple maximum likelihood parameter estimation does not have a closed form solution

- We often resort to iterative approaches such as gradient ascent

- The good news is that the likelihood objective is concave; iterative approaches converge to global optimum

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SINGLE VARIABLE CASE

- We have a binary variable X with domain(X) = {T, F}.

- Parameters are θ_1 and θ_2
  - Remember, the only constraint on θ_1 and θ_2 is that they need to be non-negative

- Dataset D has a T and b F instances.

- What are the maximum likelihood estimates for θ_1 and θ_2?

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Gradient Ascent

- Find maximum of $f(\theta)$ where there is no closed form solution

- Start with some initial guess θ_0

- While change is not much

  - $\theta_{i+1} = \theta_i + \eta * f'(\theta_i)$

- η is called the learning rate and it is a user specified parameter

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$f = -2x^2 + 8x + 10$

f = -2x^2 + 8x + 10   g = -4x + 8
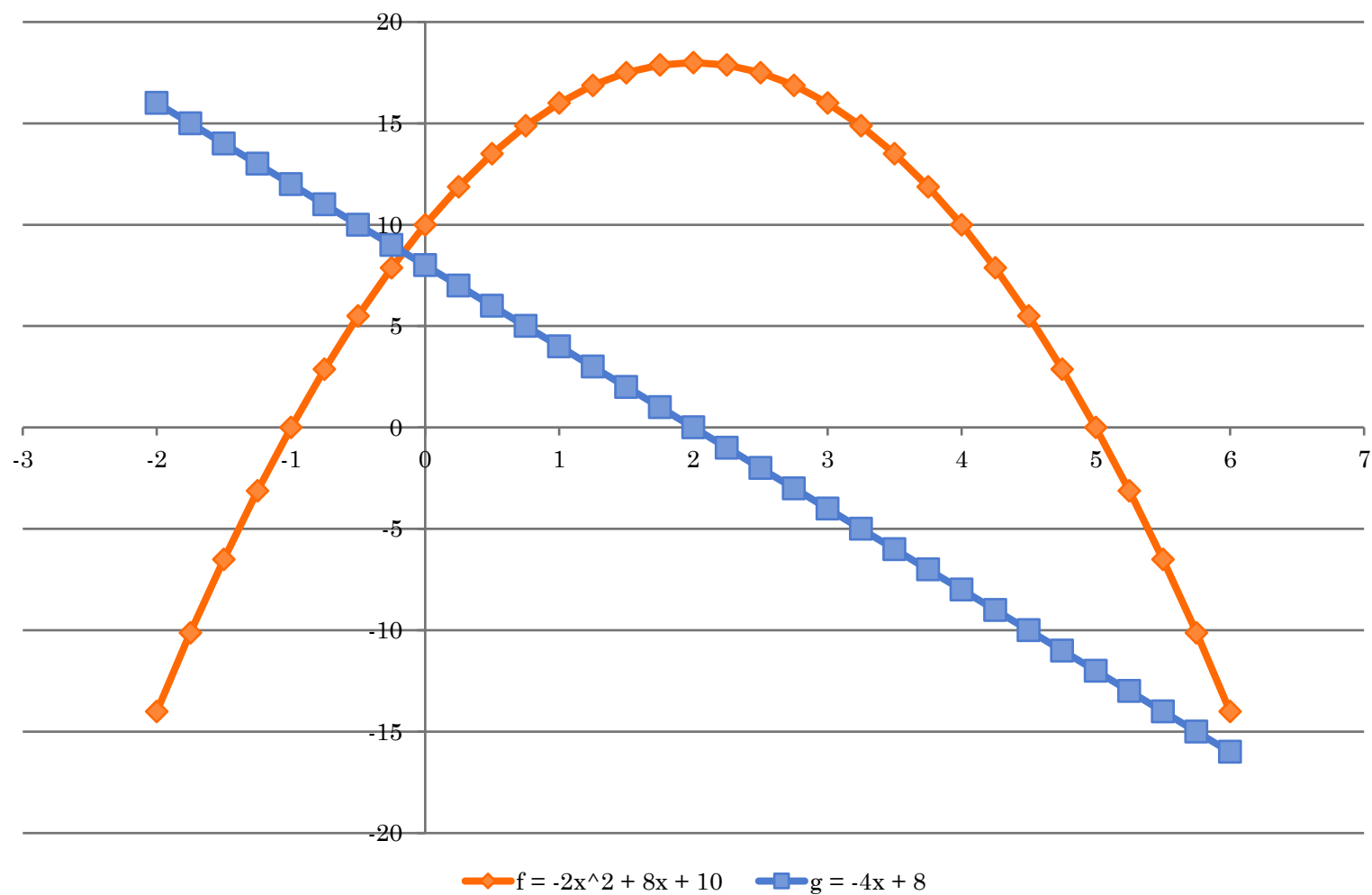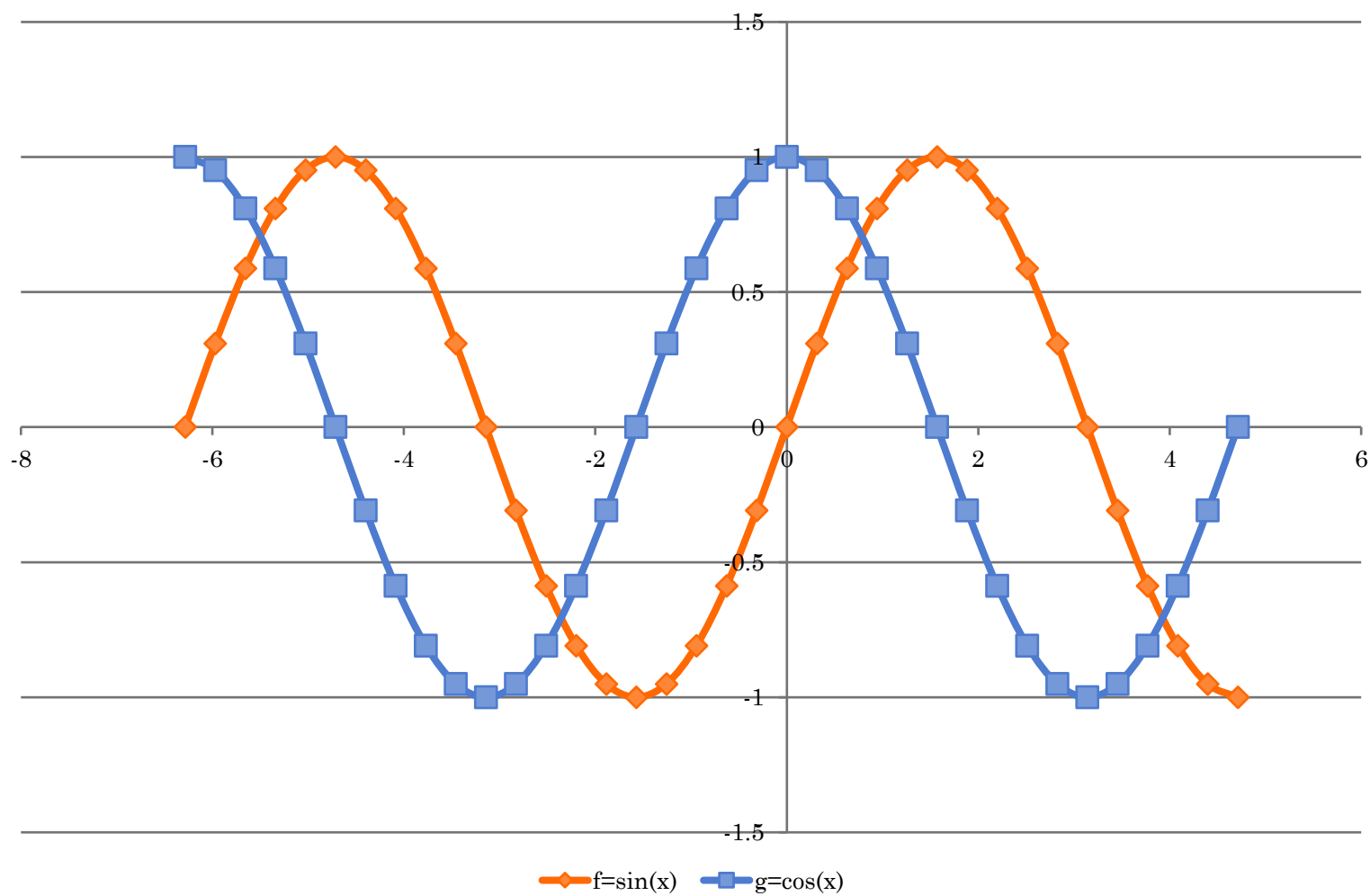
f = sin(x)

f = -2x^2 + 8x + 10

- f' = -4x + 8

- Start with x_0 = 6

- Use η = 0.2

- $x_1 = x_0 + \eta * f'(x_0)$
  - x_1 = 6 + 0.2*(-4*6 + 8) = 6 − 0.2*16 = 6 − 3.2 = 2.8

- $x_2 = x_1 + \eta * f'(x_1)$
  - x_2 = 2.8 + 0.2*(-4*2.8 + 8) = 2.8 − 0.2*3.2 = 2.8 − 0.64 = 2.16

- $x_3 = x_2 + \eta * f'(x_2)$
  - x_3 = 2.16 + 0.2*(-4*2.16 + 8) = 2.16 − 0.2*0.64 = 2.16 − 0.128 = 2.032

- $x_4 = x_3 + \eta * f'(x_3)$
  - x_4 = 2.032 + 0.2*(-4*2.032 + 8) = 2.032 − 0.2*0.128 = 2.032 − 0.0256 = 2.0064

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SINGLE VARIABLE CASE – GRADIENT ASCENT

- We have a binary variable X with domain(X) = {T, F}.

- Parameters are θ_1 and θ_2

- Dataset D has 4 T and 6 F instances.

- Solve for θ_1 and θ_2 using $\theta_1=1$ and $\theta_2=1$ as the starting point and

  - learning rate $\lambda=0.1$

  - learning rate $\lambda=0.2$

  - learning rate $\lambda=0.4$

  - learning rate $\lambda=0.5$

LOG-LINEAR MODELS

- A distribution is a *log-linear model* over a Markov network $\mathcal{H}$ is it is associated with

    - A set of features $\mathcal{F} = \{f_1(\mathbf{C}_1), \dots, f_k(\mathbf{C}_k)\}$, where each $\mathbf{C}$ is a complete subgraph in $\mathcal{H}$,

    - A set of weights $w_1, \dots, w_k$

    $$P\left(X_1, \dots, X_n\right) = \frac{1}{Z(\mathbf{w})} e^{\sum_{i=1}^{k} w_i f_i(\mathbf{C}_i)}$$

    - It is common to have several features over the same scope

LOG-LINEAR MODELS – LOG-LIKELIHOOD

- Given a domain $\mathcal{X}=\{X_1, ..., X_n\}$ and a dataset $\mathcal{D} = \{\xi[1], \xi[2], ..., \xi[M]\}$, where $\xi[i]$ is an instance, i.e., a complete assignment to the variables $\mathcal{X}$

- The log-likelihood is

$$l(\mathbf{w} : D) = \sum_i w_i \left(\sum_m f_i \left(\xi[m] \right) \right) - M \ln Z \left(\mathbf{w} \right)$$

- We are abusing the notation a little for clarity. The feature functions are defined over cliques, but here we passed them the whole instance. They just ignore the irrelevant portions of the instance

- What is $l(\mathbf{w}:D)/M$?

DERIVATIVE OF $l(\mathbf{w}:D)/M$ WRT TO w_i

$$\frac{\partial}{\partial w_i} \frac{1}{M} l\left(\mathbf{w}:D\right) = \mathbf{E}_D\left[f_i\right] - \mathbf{E}_{\mathbf{w}}\left[f_i\right]$$

Let's prove it.

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$\mathbf{E}_D[f_i] - \mathbf{E}_\mathbf{w}[f_i]$

- $\mathbf{E}_D[f_i]$ can be computed by summing f_i over the instances in D and dividing by M

- How can we compute $\mathbf{E}_\mathbf{w}[f_i]$?

- $\mathbf{E}_\mathbf{w}\left[f_i\right] = \sum_{x} P_\mathbf{w}(x) f_i(x)$

- It is impossible to iterate over all possible values of X

- Remember f_i is defined over a set of variables $\mathbf{C}_i$ and it ignores (i.e. equals zero for) the rest of the variables

- $\mathbf{E}_\mathbf{w}\left[f_i\right] = \sum_{\mathbf{c}_i} P_\mathbf{w}(\mathbf{c}_i) f_i(\mathbf{c}_i)$

- Perform inference to compute $P_\mathbf{w}(\mathbf{c}_i)$

- Now we have the gradient, we can optimize $\mathbf{w}$ using gradient ascent

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Bayesian priors

- There was no closed form solution for the maximum likelihood formulation

- There is no closed form solution for full Bayesian approach either

- We instead find the parameters that maximize $P(\theta)P(D|\theta)$

L_2-Regularization

- Assume P($\mathbf{w}$) is zero-mean diagonal Gaussian with equal variances

- In the log space, it gives rise to a penalty of the form

$$\frac{1}{2\sigma^2} \sum_{i=1}^{k} w_i^2$$

- It penalizes large weights

L_1-REGULARIZATION

- Assume P($\mathbf{w}$) is zero-mean Laplacian distribution

- In the log space, it gives rise to a penalty of the form

$$\frac{1}{\beta} \sum_{i=1}^{k} |w_i|$$

- It penalizes large weights

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Why small weights?

- Large weights are more susceptible to the noise in the data

- A small difference in the feature value can cause big changes in the probability

- Small weights give rise to smoother probabilities

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L_2 vs L_1

- L_2 forces the large weights to get closer to zero and places an emphasis on the large weights

  - Even though the weights get closer to zero, they are often not zero

- L_1 also penalizes large weights but the emphasis is not necessarily on the large weights

  - Some of the weights become zero

  - Leads to sparser representation

- Can you see these?

LEARNING RATE

- As we have seen with examples, the learning rate is an important parameter

- If it is too large, then we can overshoot

- If it is too small, then it takes a long time to converge

- There is no single value that works for all datasets and domains

- There are approaches that chooses an appropriate learning rate at each step

  - E.g., line search (more info at the appendix)

MN Parameter estimation summary

- There is no closed form solution for both maximum likelihood estimation and Bayesian estimation

- The likelihood function is concave; there is a single global optimum (note that the objective function has a single global optimum value but there might be many parameter values that achieve the same global optimum)

- Gradient ascent methods are applied to estimate the parameters

- The gradient computation requires running inference, which is costly

- In practice, regularization (L_2, L_1) is used to avoid overfitting

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