# STA 4273H: <br> Statistical Machine Learning 

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## Lecture 3

## Linear Models for Classification

- So far, we have looked at the linear models for regression that have particularly simple analytical and computational properties.
- We will now look at analogous class of models for solving classification problems.
- We will also look at the Bayesian treatment of linear models for classification.


## Classification

- The goal of classification is to assign an input $\mathbf{x}$ into one of K discrete classes $\mathrm{C}_{\mathrm{k}}$, where $\mathrm{k}=1, . ., \mathrm{K}$.
- Typically, each input is assigned only to one class.
- Example: The input vector $\mathbf{x}$ is the set of pixel intensities, and the output variable $t$ will represent the presence of cancer, class $\mathrm{C}_{1}$, or absence of cancer, class $\mathrm{C}_{2}$.

x -- set of pixel intensities


## Linear Classification

- The goal of classification is to assign an input $\mathbf{x}$ into one of K discrete classes $\mathrm{C}_{\mathrm{k}}$, where $\mathrm{k}=1, . ., \mathrm{K}$.
- The input space is divided into decision regions whose boundaries are called decision boundaries or decision surfaces.
- We will consider linear models for classification. Remember, in the simplest linear regression case, the model is linear in parameters:

adaptive parameters
$y(\mathbf{x}, \mathbf{w})=f\left(\mathbf{x}^{T} \mathbf{w}+w_{0}\right)$
fixed nonlinear function: activation function
- For classification, we need to predict discrete class labels, or posterior probabilities that lie in the range of $(0,1)$, so we use a nonlinear function.


## Linear Classification

$$
y(\mathbf{x}, \mathbf{w})=f\left(\mathbf{x}^{T} \mathbf{w}+w_{0}\right)
$$

- The decision surfaces correspond to $y(\mathbf{x}, \mathbf{w})=$ const, so that $\mathbf{x}^{T} \mathbf{w}+w_{0}=$ const, and hence the decision surfaces are linear functions of $\mathbf{x}$, even if the activation function is nonlinear.
- These class of models are called generalized linear models.
- Note that these models are no longer linear in parameters, due to the presence of nonlinear activation function.
- This leads to more complex analytical and computational properties, compared to linear regression.
- Note that we can make a fixed nonlinear transformation of the input variables using a vector of basis functions $\phi(\mathrm{x})$, as we did for regression models.


## Notation

- In the case of two-class problems, we can use the binary representation for the target value $t \in\{0,1\}$, such that $t=1$ represents the positive class and $t=0$ represents the negative class.
- We can interpret the value of $t$ as the probability of the positive class, and the output of the model can be represented as the probability that the model assigns to the positive class.
- If there are $K$ classes, we use a 1 -of- $K$ encoding scheme, in which $t$ is a vector of length $K$ containing a single 1 for the correct class and 0 elsewhere.
- For example, if we have $\mathrm{K}=5$ classes, then an input that belongs to class 2 would be given a target vector:

$$
t=(0,1,0,0,0)^{T} .
$$

- We can interpret a vector $\mathbf{t}$ as a vector of class probabilities.


## Three Approaches to Classification

- Construct a discriminant function that directly maps each input vector to a specific class.
- Model the conditional probability distribution $p\left(\mathcal{C}_{k} \mid \mathbf{x}\right)$, and then use this distribution to make optimal decisions.
- There are two alternative approaches:
- Discriminative Approach: Model $p\left(\mathcal{C}_{k} \mid \mathbf{x}\right)$, directly, for example by representing them as parametric models, and optimize for parameters using the training set (e.g. logistic regression).
- Generative Approach: Model class conditional densities $p\left(\mathbf{x} \mid \mathcal{C}_{k}\right)$ together with the prior probabilities $p\left(\mathcal{C}_{k}\right)$ for the classes. Infer posterior probability using Bayes' rule:

$$
p\left(\mathcal{C}_{k} \mid \mathbf{x}\right)=\frac{p\left(\mathbf{x} \mid \mathcal{C}_{k}\right) p\left(\mathcal{C}_{k}\right)}{p(\mathbf{x})}
$$

We will consider next.

## Probabilistic Generative Models

- Model class conditional densities $p\left(\mathbf{x} \mid \mathcal{C}_{k}\right)$ separately for each class, as well as the class priors $p\left(\mathcal{C}_{k}\right)$.
- Consider the case of two classes. The posterior probability of class $\mathrm{C}_{1}$ is given by:

$$
\begin{aligned}
p\left(\mathcal{C}_{1} \mid \mathbf{x}\right) & =\frac{p\left(\mathbf{x} \mid \mathcal{C}_{1}\right) p\left(\mathcal{C}_{1}\right)}{p\left(\mathbf{x} \mid \mathcal{C}_{1}\right) p\left(\mathcal{C}_{1}\right)+p\left(\mathbf{x} \mid \mathcal{C}_{2}\right) p\left(\mathcal{C}_{2}\right)} \\
& =\frac{1}{1+\exp (-a)}=\sigma(a)
\end{aligned}
$$

where we defined:

$$
a=\ln \frac{p\left(\mathbf{x} \mid \mathcal{C}_{1}\right) p\left(\mathcal{C}_{1}\right)}{p\left(\mathbf{x} \mid \mathcal{C}_{2}\right) p\left(\mathcal{C}_{2}\right)}=\ln \frac{p\left(\mathcal{C}_{1} \mid \mathbf{x}\right)}{1-p\left(\mathcal{C}_{1} \mid \mathbf{x}\right)}
$$

which is known as the logit function. It represents the log of the ration of probabilities of two classes, also known as the log-odds.

## Sigmoid Function

- The posterior probability of class $\mathrm{C}_{1}$ is given by:

$$
\begin{aligned}
p\left(\mathcal{C}_{1} \mid \mathbf{x}\right)= & \frac{p\left(\mathbf{x} \mid \mathcal{C}_{1}\right) p\left(\mathcal{C}_{1}\right)}{p\left(\mathbf{x} \mid \mathcal{C}_{1}\right) p\left(\mathcal{C}_{1}\right)+p\left(\mathbf{x} \mid \mathcal{C}_{2}\right) p\left(\mathcal{C}_{2}\right)} \\
= & \frac{1}{1+\exp (-a)}=\sigma(a), \\
& \quad \begin{array}{l}
\text { Logistic sigmoid } \\
\text { function }
\end{array}
\end{aligned}
$$

- The term sigmoid means S-shaped: it maps the whole real axis into (0 1).
- It satisfies:

$$
\sigma(-a)=1-\sigma(a), \quad \frac{\mathrm{d}}{\mathrm{~d} a} \sigma(a)=\sigma(a)(1-\sigma(a))
$$

## Softmax Function

- For case of $\mathrm{K}>2$ classes, we have the following multi-class generalization:

$$
p\left(\mathcal{C}_{k} \mid \mathbf{x}\right)=\frac{p\left(\mathbf{x} \mid \mathcal{C}_{k}\right) p\left(\mathcal{C}_{k}\right)}{\sum_{j} p\left(\mathbf{x} \mid \mathcal{C}_{j}\right) p\left(\mathcal{C}_{j}\right.}=\frac{\exp \left(a_{k}\right)}{\sum_{j} \exp \left(a_{j}\right)}, a_{k}=\ln \left[p\left(\mathbf{x} \mid \mathcal{C}_{k}\right) p\left(\mathcal{C}_{k}\right)\right] .
$$

- This normalized exponential is also known as the softmax function, as it represents a smoothed version of the max function:

$$
\text { if } a_{k} \gg a_{j}, \forall j \neq k, \text { then } p\left(\mathcal{C}_{k} \mid \mathbf{x}\right) \approx 1, p\left(\mathcal{C}_{j} \mid \mathbf{x}\right) \approx 0
$$

- We now look at some specific forms of class conditional distributions.


## Example of Continuous Inputs

- Assume that the input vectors for each class are from a Gaussian distribution, and all classes share the same covariance matrix:

$$
p\left(\mathbf{x} \mid \mathcal{C}_{k}\right)=\frac{1}{(2 \pi)^{D / 2}|\boldsymbol{\Sigma}|^{1 / 2}} \exp \left(-\frac{1}{2}\left(\mathbf{x}-\boldsymbol{\mu}_{k}\right)^{T} \boldsymbol{\Sigma}^{-1}\left(\mathbf{x}-\boldsymbol{\mu}_{k}\right)\right) .
$$

- For the case of two classes, the posterior is logistic function:

$$
p\left(\mathcal{C}_{k} \mid \mathbf{x}\right)=\sigma\left(\mathbf{w}^{T} \mathbf{x}+w_{0}\right)
$$

where we have defined:

$$
\begin{aligned}
\mathbf{w} & =\boldsymbol{\Sigma}^{-1}\left(\boldsymbol{\mu}_{1}-\boldsymbol{\mu}_{2}\right), \\
w_{0} & =-\frac{1}{2} \boldsymbol{\mu}_{1}^{T} \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_{1}+\frac{1}{2} \boldsymbol{\mu}_{2}^{T} \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_{2}+\ln \frac{p\left(\mathcal{C}_{1}\right)}{p\left(\mathcal{C}_{2}\right)} .
\end{aligned}
$$

- The quadratic terms in $\mathbf{x}$ cancel (due to the assumption of common covariance matrices).
- This leads to a linear function of $\mathbf{x}$ in the argument of logistic sigmoid. Hence the decision boundaries are linear in input space.


## Example of Two Gaussian Models



Class-conditional densities for two classes


The corresponding posterior probability $p\left(\mathcal{C}_{1} \mid \mathbf{x}\right)$, given by the sigmoid function of a linear function of $\mathbf{x}$.

## Case of K Classes

- For the case of K classes, the posterior is a softmax function:

$$
\begin{aligned}
& p\left(\mathcal{C}_{k} \mid \mathbf{x}\right)=\frac{p\left(\mathbf{x} \mid \mathcal{C}_{k}\right) p\left(\mathcal{C}_{k}\right)}{\sum_{j} p\left(\mathbf{x} \mid \mathcal{C}_{j}\right) p\left(\mathcal{C}_{j}\right)}=\frac{\exp \left(a_{k}\right)}{\sum_{j} \exp \left(a_{j}\right)} \\
& a_{k}=\mathbf{w}_{k}^{T} \mathbf{x}+w_{k 0}
\end{aligned}
$$

where, similar to the 2-class case, we have defined:

$$
\begin{aligned}
& \mathbf{w}_{k}=\boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_{k}, \\
& w_{k 0}=-\frac{1}{2} \boldsymbol{\mu}_{k}^{T} \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_{k}+\ln p\left(\mathcal{C}_{k}\right)
\end{aligned}
$$

- Again, the decision boundaries are linear in input space.
- If we allow each class-conditional density to have its own covariance, we will obtain quadratic functions of $\mathbf{x}$.
- This leads to a quadratic discriminant.


## Quadratic Discriminant

The decision boundary is linear when the covariance matrices are the same and quadratic when they are not.


Class-conditional densities for three classes


The corresponding posterior probabilities for three classes.

## Maximum Likelihood Solution

- Consider the case of two classes, each having a Gaussian classconditional density with shared covariance matrix.
- We observe a dataset $\left\{\mathbf{x}_{n}, t_{n}\right\}, n=1, . ., N$.
- Here $t_{n}=1$ denotes class $C_{1}$, and $t_{n}=0$ denotes class $C_{2}$.
- Also denote $p\left(\mathcal{C}_{1}\right)=\pi, p\left(\mathcal{C}_{2}\right)=1-\pi$.
- The likelihood function takes form:

$$
\begin{aligned}
p\left(\mathbf{t}, \mathbf{X} \mid \pi, \boldsymbol{\mu}_{1}, \boldsymbol{\mu}_{2}, \boldsymbol{\Sigma}\right)= & \prod_{n=1}^{N}\left[\pi \mathcal{N}\left(\mathbf{x}_{n} \mid \boldsymbol{\mu}_{1}, \boldsymbol{\Sigma}\right)\right]^{t_{n}}\left[(1-\pi) \mathcal{N}\left(\mathbf{x}_{n} \mid \boldsymbol{\mu}_{2}, \boldsymbol{\Sigma}\right)\right]^{1-t_{n}} . \\
& \text { Data points } \\
& \text { from class } \mathrm{C}_{1} .
\end{aligned} \quad \begin{aligned}
& \text { Data points } \\
& \text { from class } \mathrm{C}_{2} .
\end{aligned}
$$

- As usual, we will maximize the log of the likelihood function.


## Maximum Likelihood Solution

$$
p\left(\mathbf{t}, \mathbf{X} \mid \pi, \boldsymbol{\mu}_{1}, \boldsymbol{\mu}_{2}, \boldsymbol{\Sigma}\right)=\prod_{n=1}^{N}\left[\pi \mathcal{N}\left(\mathbf{x}_{n} \mid \boldsymbol{\mu}_{1}, \boldsymbol{\Sigma}\right)\right]^{t_{n}}\left[(1-\pi) \mathcal{N}\left(\mathbf{x}_{n} \mid \boldsymbol{\mu}_{2}, \boldsymbol{\Sigma}\right)\right]^{1-t_{n}}
$$

- Maximizing the respect to $\pi$, we look at the terms of the log-likelihood functions that depend on $\pi$ :

$$
\sum_{n}\left[t_{n} \ln \pi+\left(1-t_{n}\right) \ln (1-\pi)\right]+\text { const } .
$$

Differentiating, we get:

$$
\pi=\frac{1}{N} \sum_{n=1}^{N} t_{n}=\frac{N_{1}}{N_{1}+N_{2}}
$$

- Maximizing the respect to $\mu_{1}$, we look at the terms of the log-likelihood functions that depend on $\mu_{1}$ :

$$
\sum_{n} t_{n} \ln \mathcal{N}\left(\mathbf{x}_{n} \mid \boldsymbol{\mu}_{1}, \boldsymbol{\Sigma}\right)=-\frac{1}{2} \sum_{n} t_{n}\left(\mathbf{x}_{n}-\boldsymbol{\mu}_{1}\right)^{T} \boldsymbol{\Sigma}^{-1}\left(\mathbf{x}_{n}-\boldsymbol{\mu}_{1}\right)+\text { const }
$$

Differentiating, we get:

$$
\boldsymbol{\mu}_{1}=\frac{1}{N_{1}} \sum_{n=1}^{N} t_{n} \mathbf{x}_{n} . \quad \boldsymbol{\mu}_{2}=\frac{1}{N_{2}} \sum_{n=1}^{N}\left(1-t_{n}\right) \mathbf{x}_{n} .
$$

## Maximum Likelihood Solution

$$
p\left(\mathbf{t}, \mathbf{X} \mid \pi, \boldsymbol{\mu}_{1}, \boldsymbol{\mu}_{2}, \boldsymbol{\Sigma}\right)=\prod_{n=1}^{N}\left[\pi \mathcal{N}\left(\mathbf{x}_{n} \mid \boldsymbol{\mu}_{1}, \boldsymbol{\Sigma}\right)\right]^{t_{n}}\left[(1-\pi) \mathcal{N}\left(\mathbf{x}_{n} \mid \boldsymbol{\mu}_{2}, \boldsymbol{\Sigma}\right)\right]^{1-t_{n}}
$$

- Maximizing the respect to $\Sigma$ :

$$
\begin{aligned}
& -\frac{1}{2} \sum_{n} t_{n} \ln |\boldsymbol{\Sigma}|-\frac{1}{2} \sum_{n} t_{n}\left(\mathbf{x}_{n}-\boldsymbol{\mu}_{1}\right)^{T} \boldsymbol{\Sigma}^{-1}\left(\mathbf{x}_{n}-\boldsymbol{\mu}_{1}\right) \\
& -\frac{1}{2} \sum_{n}\left(1-t_{n}\right) \ln |\boldsymbol{\Sigma}|-\frac{1}{2} \sum_{n}\left(1-t_{n}\right)\left(\mathbf{x}_{n}-\boldsymbol{\mu}_{2}\right)^{T} \boldsymbol{\Sigma}^{-1}\left(\mathbf{x}_{n}-\boldsymbol{\mu}_{2}\right) \\
& =-\frac{N}{2} \ln |\boldsymbol{\Sigma}|-\frac{N}{2} \operatorname{Tr}\left(\boldsymbol{\Sigma}^{-1} \mathbf{S}\right) .
\end{aligned}
$$

- Here we defined:
$\mathbf{S}=\frac{N_{1}}{N} \mathbf{S}_{1}+\frac{N_{2}}{N} \mathbf{S}_{2}$,
$\mathbf{S}_{1}=\frac{1}{N_{1}} \sum_{n \in \mathcal{C}_{1}}\left(\mathbf{x}_{n}-\boldsymbol{\mu}_{1}\right)\left(\mathbf{x}_{n}-\boldsymbol{\mu}_{1}\right)^{T}$,
$\mathbf{S}_{2}=\frac{1}{N_{2}} \sum_{n \in \mathcal{C}_{2}}\left(\mathbf{x}_{n}-\boldsymbol{\mu}_{2}\right)\left(\mathbf{x}_{n}-\boldsymbol{\mu}_{2}\right)^{T}$.
- Using standard results for a Gaussian distribution we have:

$$
\boldsymbol{\Sigma}=\mathbf{S}
$$

- Maximum likelihood solution represents a weighted average of the covariance matrices associated with each of the two classes.


## Example



- For generative fitting, the red mean moves rightwards but the decision boundary moves leftwards! If you believe the data is Gaussian, this is reasonable.
- How can we fix this?


## Three Approaches to Classification

- Construct a discriminant function that directly maps each input vector to a specific class.
- Model the conditional probability distribution $p\left(\mathcal{C}_{k} \mid \mathbf{x}\right)$, and then use this distribution to make optimal decisions.
- There are two approaches:
- Discriminative Approach: Model $p\left(\mathcal{C}_{k} \mid \mathbf{x}\right)$, directly, for example by representing them as parametric models, and optimize for parameters using the training set (e.g. logistic regression).
- Generative Approach: Model class conditional densities $p\left(\mathbf{x} \mid \mathcal{C}_{k}\right)$ together with the prior probabilities $p\left(\mathcal{C}_{k}\right)$ for the classes. Infer posterior probability using Bayes' rule:

$$
p\left(\mathcal{C}_{k} \mid \mathbf{x}\right)=\frac{p\left(\mathbf{x} \mid \mathcal{C}_{k}\right) p\left(\mathcal{C}_{k}\right)}{p(\mathbf{x})}
$$

We will consider next.

## Fixed Basis Functions

- So far, we have considered classification models that work directly in the input space.
- All considered algorithms are equally applicable if we first make a fixed nonlinear transformation of the input space using vector of basis functions $\phi(\mathrm{x})$.
- Decision boundaries will be linear in the feature space $\phi$, but would correspond to nonlinear boundaries in the original input space $\mathbf{x}$.
- Classes that are linearly separable in the feature space $\phi(\mathrm{x})$ need not be linearly separable in the original input space.


## Linear Basis Function Models

Original input space


Corresponding feature space using two Gaussian basis functions


- We define two Gaussian basis functions with centers shown by green the crosses, and with contours shown by the green circles.
- Linear decision boundary (right) is obtained using logistic regression, and corresponds to nonlinear decision boundary in the input space (left, black curve).


## Logistic Regression

- Consider the problem of two-class classification.
- We have seen that the posterior probability of class $\mathrm{C}_{1}$ can be written as a logistic sigmoid function:

$$
p\left(\mathcal{C}_{1} \mid \mathbf{x}\right)=\frac{1}{1+\exp \left(-\mathbf{w}^{T} \mathbf{x}\right)}=\sigma\left(\mathbf{w}^{T} \mathbf{x}\right)
$$

where $p\left(\mathcal{C}_{2} \mid \mathbf{x}\right)=1-p\left(\mathcal{C}_{1} \mid \mathbf{x}\right)$, and we omit the bias term for clarity.

- This model is known as logistic regression (although this is a model for classification rather than regression).

Note that for generative models, we would first determine the class conditional densities and class-specific priors, and then use Bayes' rule to obtain the posterior probabilities.

Here we model $p\left(\mathcal{C}_{k} \mid \mathbf{x}\right)$ directly.


## ML for Logistic Regression

- We observed a training dataset $\left\{\mathbf{x}_{n}, t_{n}\right\}, n=1, . ., N ; t_{n} \in\{0,1\}$.
- Maximize the probability of getting the label right, so the likelihood function takes form:

$$
p(\mathbf{t} \mid \mathbf{X}, \mathbf{w})=\prod_{n=1}^{N}\left[y_{n}^{t_{n}}\left(1-y_{n}\right)^{1-t_{n}}\right], \quad y_{n}=\sigma\left(\mathbf{w}^{T} \mathbf{x}_{n}\right)
$$

- Taking the negative log of the likelihood, we can define cross-entropy error function (that we want to minimize):

$$
E(\mathbf{w})=-\ln p(\mathbf{t} \mid \mathbf{X}, \mathbf{w})=-\sum_{n=1}^{N}\left[t_{n} \ln y_{n}+\left(1-t_{n}\right) \ln \left(1-y_{n}\right)\right]=\sum_{n=1}^{N} E_{n}
$$

- Differentiating and using the chain rule:

$$
\begin{aligned}
& \frac{\mathrm{d}}{\mathrm{~d} y_{n}} E_{n}=\frac{y_{n}-t_{n}}{y_{n}\left(1-y_{n}\right)}, \quad \frac{\mathrm{d}}{\mathrm{~d} \mathbf{w}} y_{n}=y_{n}\left(1-y_{n}\right) \mathbf{x}_{n}, \quad \frac{\mathrm{~d}}{\mathrm{~d} a(a)=\sigma(a)(1-\sigma(a)) .} \\
& \frac{\mathrm{d}}{\mathrm{~d} \mathbf{w}} E_{n}=\frac{\mathrm{d} E_{n}}{\mathrm{~d} y_{n}} \frac{\mathrm{~d} y_{n}}{\mathrm{~d} \mathbf{w}}=\left(y_{n}-t_{n}\right) \mathbf{x}_{n} .
\end{aligned}
$$

- Note that the factor involving the derivative of the logistic function cancelled.


## ML for Logistic Regression

- We therefore obtain:

$$
\nabla E(\mathbf{w})=\sum_{n=1}^{N}\left(y_{n}-t_{n}\right) \mathbf{x}_{n}
$$

- This takes exactly the same form as the gradient of the sum-ofsquares error function for the linear regression model.
- Unlike in linear regression, there is no closed form solution, due to nonlinearity of the logistic sigmoid function.
- The error function is convex and can be optimized using standard gradient-based (or more advanced) optimization techniques.
- Easy to adapt to the online learning setting.


## Multiclass Logistic Regression

- For the multiclass case, we represent posterior probabilities by a softmax transformation of linear functions of input variables :

$$
p\left(\mathcal{C}_{k} \mid \mathbf{x}\right)=y_{k}(\mathbf{x})=\frac{\exp \left(\mathbf{w}_{k}^{T} \mathbf{x}\right)}{\sum_{j} \exp \left(\mathbf{w}_{j}^{T} \mathbf{x}\right)}
$$

- Unlike in generative models, here we will use maximum likelihood to determine parameters of this discriminative model directly.
- As usual, we observed a dataset $\left\{\mathbf{x}_{n}, t_{n}\right\}, n=1, . ., N$, where we use 1 -of-K encoding for the target vector $t_{n}$.
- So if $\mathbf{x}_{\mathrm{n}}$ belongs to class $\mathrm{C}_{\mathrm{k}}$, then t is a binary vector of length K containing a single 1 for element k (the correct class) and 0 elsewhere.
- For example, if we have $\mathrm{K}=5$ classes, then an input that belongs to class 2 would be given a target vector:

$$
t=(0,1,0,0,0)^{T}
$$

## Multiclass Logistic Regression

- We can write down the likelihood function:

$$
\underbrace{p\left(\mathbf{T} \mid \mathbf{X}, \mathbf{w}_{1}, \ldots, \mathbf{w}_{K}\right)=\prod_{n=1}^{N}}_{\begin{array}{c}
\mathrm{N} \times \text { K binary matrix of } \\
\text { target variables. }
\end{array}} \underbrace{\left.\prod_{k=1}^{K} p\left(\mathcal{C}_{k} \mid \mathbf{x}_{n}\right)^{t_{n k}}\right]}_{\begin{array}{l}
\text { Only one term corresponding } \\
\text { to correct class contributes. }
\end{array}}=\prod_{n=1}^{N}\left[\prod_{k=1}^{K} y_{n k}^{t_{n k}}\right]
$$

where $y_{n k}=p\left(\mathcal{C}_{k} \mid \mathbf{x}_{n}\right)=\frac{\exp \left(\mathbf{w}_{k}^{T} \mathbf{x}_{n}\right)}{\sum_{j} \exp \left(\mathbf{w}_{j}^{T} \mathbf{x}_{n}\right)}$.

- Taking the negative logarithm gives the cross-entropy entropy function for multi-class classification problem:

$$
E\left(\mathbf{w}_{1}, \ldots, \mathbf{w}_{K}\right)=-\ln p\left(\mathbf{T} \mid \mathbf{X}, \mathbf{w}_{1}, \ldots, \mathbf{w}_{K}\right)=-\sum_{n=1}^{N}\left[\sum_{k=1}^{K} t_{n k} \ln y_{n k}\right] .
$$

- Taking the gradient:

$$
\nabla E_{\mathbf{w}_{j}}\left(\mathbf{w}_{1}, \ldots \mathbf{w}_{K}\right)=\sum_{n=1}^{N}\left(y_{n j}-t_{n j}\right) \mathbf{x}_{n}
$$

## Special Case of Softmax

- If we consider a softmax function for two classes:

$$
p\left(\mathcal{C}_{1} \mid \mathbf{x}\right)=\frac{\exp \left(a_{1}\right)}{\exp \left(a_{1}\right)+\exp \left(a_{2}\right)}=\frac{1}{1+\exp \left(-\left(a_{1}-a_{2}\right)\right)}=\sigma\left(a_{1}-a_{2}\right)
$$

- So the logistic sigmoid is just a special case of the softmax function that avoids using redundant parameters:
- Adding the same constant to both $a_{1}$ and $a_{2}$ has no effect.
- The over-parameterization of the softmax is because probabilities must add up to one.


## Recap

- Generative approach: Determine the class conditional densities and class-specific priors, and then use Bayes' rule to obtain the posterior probabilities.
- Different models can be trained separately on different machines.
- It is easy to add a new class without retraining all the other classes.

$$
p\left(\mathcal{C}_{k} \mid \mathbf{x}\right)=\frac{p\left(\mathbf{x} \mid \mathcal{C}_{k}\right) p\left(\mathcal{C}_{k}\right)}{p(\mathbf{x})}
$$

- Discriminative approach: Train all of the model parameters to maximize the probability of getting the labels right.

Model $p\left(\mathcal{C}_{k} \mid \mathbf{x}\right)$ directly.

## Bayesian Logistic Regression

-We next look at the Bayesian treatment of logistic regression.

- For the two-class problem, the likelihood takes form:

$$
p(\mathbf{t} \mid \mathbf{X}, \mathbf{w})=\prod_{n=1}^{N}\left[y_{n}^{t_{n}}\left(1-y_{n}\right)^{1-t_{n}}\right], y_{n}=\frac{1}{1+\exp \left(-\mathbf{w}^{T} \mathbf{x}_{n}\right)}=\sigma\left(\mathbf{w}^{T} \mathbf{x}_{n}\right)
$$

- Similar to Bayesian linear regression, we could start with a Gaussian prior:

$$
p(\mathbf{w})=\mathcal{N}\left(\mathbf{w} \mid \mathbf{m}_{0}, \mathbf{S}_{0}\right) .
$$

- However, the posterior distribution

$$
p(\mathbf{w} \mid \mathbf{X}, \mathbf{t}) \propto p(\mathbf{t} \mid \mathbf{X}, \mathbf{w}) p(\mathbf{w})
$$

is no longer Gaussian, and we cannot analytically integrate over model parameters w.

- We need to introduce some approximations.


## Pictorial illustration

- Consider a simple distribution: $p(w) \propto \exp \left(-w^{2}\right) \sigma(20 w+4)$.
- The plot shows the normalized distribution (in yellow), which is not Gaussian.
- The red curve displays the corresponding Gaussian approximation.



## Recap: Computational Challenge of Bayesian Framework

Remember: the big challenge is computing the posterior distribution. There are several main approaches:

- Analytical integration: If we use "conjugate" priors, the posterior distribution can be computed analytically (we saw this for Bayesian linear regression).

We will consider Laplace approximation next.

- Gaussian (Laplace) approximation: Approximate the posterior distribution with a Gaussian. Works well when there is a lot of data compared to the model complexity (as posterior is close to Gaussian).
- Monte Carlo integration: The dominant current approach is Markov Chain Monte Carlo (MCMC) -- simulate a Markov chain that converges to the posterior distribution. It can be applied to a wide variety of problems.
- Variational approximation: A cleverer way to approximate the posterior. It often works much faster, but not as general as MCMC.


## Laplace Approximation



- We will use the following notation:

$$
p(\mathbf{z})=\frac{\tilde{p}(\mathbf{z})}{\mathcal{Z}}, \mathcal{Z}=\int \tilde{p}(\mathbf{z}) \mathrm{d} \mathbf{z}
$$

- We can evaluate $\tilde{p}(\mathbf{z})$ point-wise but cannot evaluate $\mathcal{Z}$.
- For example

$$
p(\mathbf{w} \mid \mathcal{D})=\frac{p(\mathcal{D} \mid \mathbf{w}) p(\mathbf{w})}{p(\mathcal{D})}
$$

- Goal: Find a Gaussian approximation $\mathrm{q}(\mathrm{z})$ which is centered on a mode of the distribution $p(z)$.


## Laplace Approximation



- We will use the following notation:

$$
p(\mathbf{z})=\frac{\tilde{p}(\mathbf{z})}{\mathcal{Z}}, \mathcal{Z}=\int \tilde{p}(\mathbf{z}) \mathrm{d} \mathbf{z}
$$

- At the stationary point $\mathbf{z}_{0}$, the gradient $\nabla \tilde{p}\left(\mathbf{z}_{0}\right)$ vanishes.
- Consider a Taylor approximation $\ln \tilde{p}(\mathbf{z})$ around $\mathbf{z}_{0}$.

$$
\ln \tilde{p}(\mathbf{z}) \approx \ln \tilde{p}\left(\mathbf{z}_{0}\right)-\frac{1}{2}\left(\mathbf{z}-\mathbf{z}_{0}\right)^{T} A\left(\mathbf{z}-\mathbf{z}_{0}\right)
$$

where A is a Hessian matrix:

$$
A=-\left.\nabla \nabla \ln \tilde{p}(\mathbf{z})\right|_{\mathbf{z}=\mathbf{z}_{0}} .
$$

- Exponentiating both sides:

$$
\tilde{p}(\mathbf{z}) \approx \tilde{p}\left(\mathbf{z}_{0}\right) \exp \left(-\frac{1}{2}\left(\mathbf{z}-\mathbf{z}_{0}\right)^{T} A\left(\mathbf{z}-\mathbf{z}_{0}\right)\right) .
$$

## Laplace Approximation



- We will use the following notation:

$$
p(\mathbf{z})=\frac{\tilde{p}(\mathbf{z})}{\mathcal{Z}}, \mathcal{Z}=\int \tilde{p}(\mathbf{z}) \mathrm{d} \mathbf{z}
$$

- Using Taylor approximation, we get:
$\tilde{p}(\mathbf{z}) \approx \tilde{p}\left(\mathbf{z}_{0}\right) \exp \left(-\frac{1}{2}\left(\mathbf{z}-\mathbf{z}_{0}\right)^{T} A\left(\mathbf{z}-\mathbf{z}_{0}\right)\right)$.
- Hence a Gaussian approximation for $p(\mathbf{z})$ is:

$$
q(\mathbf{z})=\frac{|A|^{1 / 2}}{(2 \pi)^{D / 2}} \exp \left(-\frac{1}{2}\left(\mathbf{z}-\mathbf{z}_{0}\right)^{T} A\left(\mathbf{z}-\mathbf{z}_{0}\right)\right)
$$

where $\mathbf{z}_{0}$ is the mode of $p(\mathbf{z})$, and A is the Hessian:

$$
A=-\left.\nabla \nabla \ln \tilde{p}(\mathbf{z})\right|_{\mathbf{z}=\mathbf{z}_{0}}
$$

## Laplace Approximation



- We will use the following notation:

$$
p(\mathbf{z})=\frac{\tilde{p}(\mathbf{z})}{\mathcal{Z}}, \mathcal{Z}=\int \tilde{p}(\mathbf{z}) \mathrm{d} \mathbf{z}
$$

- Using Taylor approximation, we get:
$\tilde{p}(\mathbf{z}) \approx \tilde{p}\left(\mathbf{z}_{0}\right) \exp \left(-\frac{1}{2}\left(\mathbf{z}-\mathbf{z}_{0}\right)^{T} A\left(\mathbf{z}-\mathbf{z}_{0}\right)\right)$.
- Bayesian inference: $p(\mathbf{w} \mid \mathcal{D})=\frac{p(\mathcal{D} \mid \mathbf{w}) p(\mathbf{w})}{p(\mathcal{D})}$.
- Identify: $\tilde{p}(\theta \mid \mathcal{D})=p(\mathcal{D} \mid \theta) p(\theta), \mathcal{Z}=\int p(\mathcal{D} \mid \theta) p(\theta) \mathrm{d} \theta$.
- The posterior is approximately Gaussian around the MAP estimate:

$$
p(\theta \mid \mathcal{D}) \approx \frac{|A|^{1 / 2}}{(2 \pi)^{D / 2}} \exp \left(-\frac{1}{2}\left(\theta-\theta_{\mathrm{MAP}}\right)^{T} A\left(\theta-\theta_{\mathrm{MAP}}\right)\right)
$$

## Laplace Approximation



- We will use the following notation:

$$
p(\mathbf{z})=\frac{\tilde{p}(\mathbf{z})}{\mathcal{Z}}, \mathcal{Z}=\int \tilde{p}(\mathbf{z}) \mathrm{d} \mathbf{z}
$$

- Using Taylor approximation, we get:
$\tilde{p}(\mathbf{z}) \approx \tilde{p}\left(\mathbf{z}_{0}\right) \exp \left(-\frac{1}{2}\left(\mathbf{z}-\mathbf{z}_{0}\right)^{T} A\left(\mathbf{z}-\mathbf{z}_{0}\right)\right)$.

$$
\mathcal{Z}=\int \tilde{p}(\mathbf{z}) \mathrm{d} \mathbf{z} \approx \tilde{p}\left(\mathbf{z}_{0}\right) \int \exp \left(-\frac{1}{2}\left(\mathbf{z}-\mathbf{z}_{0}\right)^{T} A\left(\mathbf{z}-\mathbf{z}_{0}\right)\right)=\tilde{p}\left(\mathbf{z}_{0}\right) \frac{(2 \pi)^{D / 2}}{|A|^{1 / 2}}
$$

- We can approximate Model Evidence: $p(\mathcal{D})=\int p(\mathcal{D} \mid \theta) P(\theta) \mathrm{d} \theta$, using Laplace approximation:

$$
\ln p(\mathcal{D}) \approx \underbrace{\ln p\left(\mathcal{D} \mid \theta_{\mathrm{MAP}}\right)}_{\text {Data fit }}+\underbrace{\ln P\left(\theta_{\mathrm{MAP}}\right)+\frac{D}{2} \ln 2 \pi-\frac{1}{2} \ln |A|}_{\text {Occam factor: penalize model complexity }}
$$

## Bayesian Information Criterion

- BIC can be obtained from the Laplace approximation:

$$
\ln p(\mathcal{D}) \approx \ln p\left(\mathcal{D} \mid \theta_{\mathrm{MAP}}\right)+\ln P\left(\theta_{\mathrm{MAP}}\right)+\frac{D}{2} \ln 2 \pi-\frac{1}{2} \ln |A|
$$

by taking the large sample limit $(N \rightarrow \infty)$ where $N$ is the number of data points.

$$
\ln p(\mathcal{D}) \approx \ln p\left(\mathcal{D} \mid \theta_{\mathrm{MAP}}\right)-\frac{1}{2} D \ln N
$$

- Quick and easy, does not depend on the prior.
- Can use maximum likelihood estimate instead of the MAP estimate.
- D denotes the number of well-determined parameters.
- Danger: Counting parameters can be tricky (e.g. infinite models).


## Bayesian Logistic Regression

- Remember the likelihood:

$$
p(\mathbf{t} \mid \mathbf{X}, \mathbf{w})=\prod_{n=1}^{N}\left[y_{n}^{t_{n}}\left(1-y_{n}\right)^{1-t_{n}}\right], \quad y_{n}=\frac{1}{1+\exp \left(-\mathbf{w}^{T} \mathbf{x}_{n}\right)}=\sigma\left(\mathbf{w}^{T} \mathbf{x}_{n}\right)
$$

- And the prior: $p(\mathbf{w})=\mathcal{N}\left(\mathbf{w} \mid \mathbf{m}_{0}, \mathbf{S}_{0}\right)$.
- The log of the posterior takes form:

$$
\begin{aligned}
\ln p(\mathbf{w} \mid \mathbf{X}, \mathbf{t})= & -\frac{1}{2}\left(\mathbf{w}-\mathbf{m}_{0}\right)^{T} \mathbf{S}_{0}^{-1}\left(\mathbf{w}-\mathbf{m}_{0}\right) \\
& +\sum_{n=1}^{N}\left[t_{n} \ln y_{n}+\left(1-t_{n}\right) \ln \left(1-t_{n}\right)\right]+\text { const. }
\end{aligned}
$$

- We first maximize the log-posterior to get the MAP estimate: $\mathrm{w}_{\text {mAP }}$.
- The inverse of covariance is given by the matrix of second derivatives:

$$
\mathbf{S}_{N}^{-1}=-\nabla \nabla \ln p(\mathbf{w} \mid \mathbf{X}, \mathbf{t})=S_{0}^{-1}+\sum_{n} y_{n}\left(1-y_{n}\right) \mathbf{x}_{n} \mathbf{x}_{n}^{T} .
$$

- The Gaussian approximation to the posterior distribution is given by:

$$
q(\mathbf{w})=\mathcal{N}\left(\mathbf{w} \mid \mathbf{w}_{\mathrm{MAP}}, \mathbf{S}_{N}\right)
$$

## Predictive Distribution

- The predictive distribution for class $\mathrm{C}_{1}$, given a new input $\mathbf{x}^{*}$ is given by marginalizing with respect to posterior distribution $p(\mathbf{w} \mid \mathbf{X}, \mathbf{t})$, which is itself approximated by a Gaussian distribution:

$$
\begin{aligned}
p\left(\mathcal{C}_{1} \mid \mathbf{x}^{*}, \mathbf{t}, \mathbf{X}\right) & =\int p\left(\mathcal{C}_{1} \mid \mathbf{x}^{*}, \mathbf{w}\right) p(\mathbf{w} \mid \mathbf{t}, \mathbf{X}) \mathrm{d} \mathbf{w} \\
& \approx \int \sigma\left(\mathbf{w}^{T} \mathbf{x}^{*}\right) q(\mathbf{w}) \mathrm{d} \mathbf{w}, \quad \sim
\end{aligned}
$$

with the corresponding probability for class $\mathrm{C}_{2}$ given by:

$$
p\left(\mathcal{C}_{1} \mid \mathbf{x}^{*}, \mathbf{t}, \mathbf{X}\right)=1-p\left(\mathcal{C}_{1} \mid \mathbf{x}^{*}, \mathbf{t}, \mathbf{X}\right)
$$

- The convolution of Gaussian with logistic sigmoid cannot be evaluated analytically.


## Predictive Distribution

$$
p\left(\mathcal{C}_{1} \mid \mathbf{x}^{*}, \mathbf{X}, \mathbf{t}\right) \approx \int \sigma\left(\mathbf{w}^{T} \mathbf{x}^{*}\right) q(\mathbf{w}) \mathrm{d} \mathbf{w}
$$

- Note that the logistic function depends on $\mathbf{w}$ only through its projection onto $\mathbf{x}^{*}$. Denoting $a=\mathbf{w}^{T} \mathbf{x}^{*}$, we have:

$$
\sigma\left(\mathbf{w}^{T} \mathbf{x}^{*}\right)=\int \delta\left(a-\mathbf{w}^{T} \mathbf{x}^{*}\right) \sigma(a) \mathrm{d} a
$$

where $\delta$ is the Dirac delta function. Hence
$\int \sigma\left(\mathbf{w}^{T} \mathbf{x}^{*}\right) q(\mathbf{w}) \mathrm{d} \mathbf{w}=\int \sigma(a) p(a) \mathrm{d} a$, where $p(a)=\int \delta\left(a-\mathbf{w}^{T} \mathbf{x}^{*}\right) q(\mathbf{w}) \mathrm{d} \mathbf{w}$.

- Let us characterize $\mathrm{p}(\mathrm{a})$. integral.
- The delta function imposes a linear constraint on w. It forms a marginal distribution from the joint $\mathrm{q}(\mathbf{w})$ by marginalizing out all directions orthogonal to $\mathbf{x}^{*}$.
- Since $q(\mathbf{w})$ is Gaussian, the marginal is also Gaussian.


## Predictive Distribution

$\int \sigma\left(\mathbf{w}^{T} \mathbf{x}^{*}\right) q(\mathbf{w}) \mathrm{d} \mathbf{w}=\int \sigma(a) p(a) \mathrm{d} a$, where $p(a)=\int \delta\left(a-\mathbf{w}^{T} \mathbf{x}^{*}\right) q(\mathbf{w}) \mathrm{d} \mathbf{w}$.

- We can evaluate the mean and variance of the marginal $p(a)$.

$$
\begin{aligned}
& \mu_{a}= \mathbb{E}[a]=\int a p(a) \mathrm{d} a=\int \mathbf{w}^{T} \mathbf{x}^{*} q(\mathbf{w}) \mathrm{d} \mathbf{w}=\mathbf{w}_{\mathrm{MAP}}^{T} \mathbf{x}^{*} . \\
& \sigma_{a}^{2}=\operatorname{var}[a]=\int p(a)\left[a^{2}-\mathbb{E}[a]^{2}\right]= \\
&=\int\left[\left(\mathbf{w}^{T} \mathbf{x}^{*}\right)^{2}-\left(\mathbf{w}_{\mathrm{MAP}}^{T} \mathbf{x}^{*}\right)^{2}\right] q(\mathbf{w}) \mathrm{d} \mathbf{w}=\mathbf{x}^{* T} \mathbf{S}_{N} \mathbf{x}^{*} .
\end{aligned} \begin{aligned}
& \text { } \begin{array}{l}
\text { dame form astive } \\
\text { distribution for the the } \\
\text { regression model }
\end{array}
\end{aligned}
$$

- Hence we obtain approximate predictive:

$$
p\left(\mathcal{C}_{1} \mid \mathbf{x}^{*}, \mathbf{X}, \mathbf{t}\right) \approx \int \sigma\left(\mathbf{w}^{T} \mathbf{x}^{*}\right) q(\mathbf{w}) \mathrm{d} \mathbf{w}=\int \sigma(a) \mathcal{N}\left(a \mid \mu_{a}, \sigma_{a}^{2}\right)
$$

- The integral is 1 -dimensional and can further be approximated via:

$$
\int \sigma(a) \mathcal{N}\left(a \mid \mu_{a}, \sigma_{a}^{2}\right) \approx \sigma\left(k \mu_{a}\right), \quad \text { where } k=\left(1+\pi \sigma_{a}^{2} / 8\right)^{-1 / 2}
$$

## Graphical Models

- Probabilistic graphical models provide a powerful framework for representing dependency structure between random variables.
- Graphical models offer several useful properties:
- They provide a simple way to visualize the structure of a probabilistic model and can be used to motivate new models.
- They provide various insights into the properties of the model, including conditional independence.
- Complex computations (e.g. inference and learning in sophisticated models) can be expressed in terms of graphical manipulations.


## Graphical Models

- A graph contains a set of nodes (vertices) connected by links (edges or arcs)

- In a probabilistic graphical model, each node represents a random variable, and links represent probabilistic dependencies between random variables.
- The graph specifies the way in which the joint distribution over all random variables decomposes into a product of factors, where each factor depends on a subset of the variables.
- Two types of graphical models:
- Bayesian networks, also known as Directed Graphical Models (the links have a particular directionality indicated by the arrows)
- Markov Random Fields, also known as Undirected Graphical Models (the links do not carry arrows and have no directional significance).
- Hybrid graphical models that combine directed and undirected graphical models, such as Deep Belief Networks.


## Bayesian Networks

- Directed Graphs are useful for expressing causal relationships between random variables.
- Let us consider an arbitrary joint distribution $p(a, b, c)$ over three random variables $a, b$, and $c$.
- Note that at this point, we do not need to specify anything else about these variables (e.g. whether they are discrete or continuous).
- By application of the product rule of probability (twice), we get

$$
p(a, b, c)=p(c \mid a, b) p(a, b)=p(c \mid a, b) p(b \mid a) p(a)
$$

- This decomposition holds for any choice of the joint distribution.


## Bayesian Networks

- By application of the product rule of probability (twice), we get

$$
p(a, b, c)=p(c \mid a, b) p(a, b)=p(c \mid a, b) p(b \mid a) p(a)
$$

- Represent the joint distribution in terms of a simple graphical model:

- Introduce a node for each of the random variables.
- Associate each node with the corresponding conditional distribution in above equation.
- For each conditional distribution we add directed links to the graphs from the nodes corresponding to the variables on which the distribution is conditioned.
- Hence for the factor $p(c \mid a, b)$, there will be links from nodes $\mathbf{a}$ and $\mathbf{b}$ to node c.
- For the factor $p(a)$, there will be no incoming links.


## Bayesian Networks

- By application of the product rule of probability (twice), we get

$$
p(a, b, c)=p(c \mid a, b) p(a, b)=p(c \mid a, b) p(b \mid a) p(a)
$$

- If there is a link going from node a to node $b$, then we say that:

- node $a$ is a parent of node $b$.
- node $b$ is a child of node $a$.
- For the decomposition, we choose a specific ordering of the random variables: $a, b, c$.
- If we chose a different ordering, we would get a different graphical representation (we will come back to that point later).
- The joint distribution over K variables factorizes:

$$
p\left(x_{1}, \ldots, x_{K}\right)=p\left(x_{K} \mid x_{1}, \ldots, x_{K-1}\right) \ldots p\left(x_{2} \mid x_{1}\right) p\left(x_{1}\right)
$$

- If each node has incoming links from all lower numbered nodes, then the graph is fully connected; there is a link between all pairs of nodes.


## Bayesian Networks

- Absence of links conveys certain information about the properties of the class of distributions that the graph conveys.

- Note that this graph is not fully connected (e.g. there is no link from $x_{1}$ to $x_{2}$.
- The joint distribution over $\mathrm{x}_{1}, \ldots, \mathrm{x}_{7}$ can be written as a product of a set of conditional distributions.

$$
\begin{aligned}
p\left(x_{1}, \ldots, x_{7}\right)= & p\left(x_{1}\right) p\left(x_{2}\right) p\left(x_{3}\right) p\left(x_{4} \mid x_{1}, x_{2}, x_{3}\right) \\
& p\left(x_{5} \mid x_{1}, x_{3}\right) p\left(x_{6} \mid x_{4}\right) p\left(x_{7} \mid x_{4}, x_{5}\right)
\end{aligned}
$$

- Note that according to the graph, $\mathrm{x}_{5}$ will be conditioned only on $\mathrm{x}_{1}$ and $\mathrm{x}_{3}$.


## Factorization Property

- The joint distribution defined by the graph is given by the product of a conditional distribution for each node conditioned on its parents:


$$
p(\mathbf{x})=\prod_{k=1}^{K} p\left(x_{k} \mid \mathrm{pa}_{k}\right)
$$

where $p a_{k}$ denotes a set of parents for the node $\mathrm{X}_{\mathrm{k}}$.

- This equation expresses a key factorization property of the joint distribution for a directed graphical model.
- Important restriction: There must be no directed cycles!
- Such graphs are also called directed acyclic graphs (DAGs).


## Discrete Variables

- General joint distribution: K²-1 parameters.


$$
p\left(\mathbf{x}_{1}, \mathbf{x}_{2} \mid \boldsymbol{\mu}\right)=\prod_{k=1}^{K} \prod_{l=1}^{K} \mu_{k l}^{x_{1 k} x_{2 l}}
$$

- Independent joint distribution: 2(K-1) parameters.


$$
\hat{p}\left(\mathbf{x}_{1}, \mathbf{x}_{2} \mid \boldsymbol{\mu}\right)=\prod_{k=1}^{K} \mu_{1 k}^{x_{1 k}} \prod_{l=1}^{K} \mu_{2 l}^{x_{2 l}}
$$

- We dropped the link between the nodes, so each variables is described by a separate multinomial distribution.


## Discrete Variables

- In general:
- Fully connected graphs have completely general distributions and have exponential $\mathrm{K}^{\mathrm{M}}$-1 number of parameters (too complex).
- If there are no links, the joint distribution fully factorizes into the product of the marginals, and have $\mathrm{M}(\mathrm{K}-1)$ parameters (too simple).
- Graphs that have an intermediate level of connectivity allow for more general distributions compared to the fully factorized one, while requiring fewer parameters than the general joint distribution.
- Let us look at the example of the chain graph.


## Chain Graph

- Consider an M-node Markov chain:

- The marginal distribution $p\left(\mathbf{x}_{1}\right)$ requires K-1 parameters.
- The remaining conditional distributions $p\left(\mathbf{x}_{i} \mid \mathbf{x}_{i-1}\right), i=2, \ldots, M$ require $\mathrm{K}(\mathrm{K}-1)$ parameters.
- Total number of parameters: $\mathrm{K}-1+(\mathrm{M}-1)(\mathrm{K}-1) \mathrm{K}$, which is quadratic in $K$ and linear in the length $M$ of the chain.
- This graphical model forms the basis of a simple Hidden Markov Model.


## Adding Priors

- We can turn a graph over discrete random variables into a Bayesian model by introducing Dirichlet priors for the parameters
- From a graphical point of view, each node acquires an additional parent representing the Dirichlet distribution over parameters.

$p\left(\left\{\mathbf{x}_{m}, \boldsymbol{\mu}_{m}\right\}\right)=p\left(\mathbf{x}_{1} \mid \boldsymbol{\mu}_{1}\right) p\left(\boldsymbol{\mu}_{1}\right) \prod_{m=2}^{M} p\left(\mathbf{x}_{m} \mid \mathbf{x}_{m-1}, \boldsymbol{\mu}_{m}\right) p\left(\boldsymbol{\mu}_{m}\right)$

$$
p\left(\boldsymbol{\mu}_{m}\right)=\operatorname{Dir}\left(\boldsymbol{\mu}_{m} \mid \boldsymbol{\alpha}_{m}\right)
$$

## Shared Prior

- We can further share the common prior over the parameters governing the conditional distributions.



## Parameterized Models

- We can use parameterized models to control exponential growth in the number of parameters.

$$
\begin{aligned}
& \text { If } x_{1}, \ldots, x_{M} \text { are discrete, } \mathrm{K} \text {-state } \\
& \text { variables, } p\left(y=1 \mid x_{1}, \ldots, x_{M}\right) \\
& \text { in general has } \mathrm{O}\left(\mathrm{~K}^{\mathrm{M}}\right) \text { parameters. }
\end{aligned}
$$

- We can obtain a more parsimonious form of the conditional distribution by using a logistic function acting on a linear combination of the parent variables:

$$
p\left(y=1 \mid x_{1}, \ldots, x_{M}\right)=\sigma\left(w_{0}+\sum_{i=1}^{M} w_{i} x_{i}\right)=\sigma\left(\mathbf{w}^{\mathrm{T}} \mathbf{x}\right)
$$

- This is a more restricted form of conditional distribution, but it requires only M+1 parameters (linear growth in the number of parameters).


## Linear Gaussian Models

- So far we worked with joint probability distributions over a set of discrete random variables (expressed as nodes in directed acyclic graphs).
- We now show how a multivariate Gaussian distribution can be expressed as a directed graph corresponding to a linear Gaussian model.
- Consider an arbitrary acyclic graph over D random variables, in which each node represent a single continuous Gaussian distribution with its mean given by the linear function of the parents:

$$
p\left(x_{i} \mid \mathrm{pa}_{i}\right)=\mathcal{N}\left(x_{i} \mid \sum_{j \in \mathrm{pa}_{i}} w_{i j} x_{j}+b_{i}, v_{i}\right)
$$

where $\mathrm{w}_{\mathrm{ij}}$ and $\mathrm{b}_{\mathrm{i}}$ are parameters governing the mean, and $\mathrm{v}_{\mathrm{i}}$ is the variance.

## Linear Gaussian Models

- The log of the joint distribution takes form:

$$
\ln p(\mathbf{x})=\sum_{i=1}^{D} \ln p\left(x_{i} \mid \mathrm{pa}_{i}\right)=-\sum_{i=1}^{D} \frac{1}{2 v_{i}}\left(x_{i}-\sum_{j \in \mathrm{pa}_{i}} w_{i j} x_{j}-b_{i}\right)^{2}+\text { const },
$$

where 'const' denotes terms independent of $x$.

- This is a quadratic function of $x$, and hence the joint distribution $p(x)$ is a multivariate Gaussian.
- For example, consider a directed graph over three Gaussian variables with one missing link:



## Computing the Mean

- We can determine the mean and covariance of the joint distribution.

Remember:
hence

$$
p\left(x_{i} \mid \mathrm{pa}_{i}\right)=\mathcal{N}\left(x_{i} \mid \sum_{j \in \mathrm{pa}_{i}} w_{i j} x_{j}+b_{i}, v_{i}\right)
$$

$$
x_{i}=\sum_{j \in \operatorname{pa}_{i}} w_{i j} x_{j}+b_{i}+\sqrt{v_{i}} \epsilon_{i}, \quad \epsilon_{i} \sim \mathcal{N}(0,1),
$$

so its expected value:

$$
\mathbb{E}\left[x_{i}\right]=\sum_{j \in \mathrm{pa}_{i}} w_{i j} \mathbb{E}\left[x_{j}\right]+b_{i}
$$

- Hence we can find components: $\mathbb{E}[\mathbf{x}]=\left[\mathbb{E}\left[x_{1}\right], \ldots, \mathbb{E}\left[x_{D}\right]\right]$ by doing ancestral pass: start at the top and proceed in order (see example):



## Computing the Covariance

- We can obtain the $\mathrm{i}, \mathrm{j}$ element of the covariance matrix in the form of a recursion relation:

$$
\begin{aligned}
\operatorname{cov}\left[x_{i}, x_{j}\right] & =\mathbb{E}\left[\left(x_{i}-\mathbb{E}\left[x_{i}\right]\right)\left(x_{j}-\mathbb{E}\left[x_{j}\right]\right)\right] \\
& =\mathbb{E}\left[\left(x_{i}-\mathbb{E}\left[x_{i}\right]\right)\left(\sum_{k \in \operatorname{pa}_{j}} w_{j k}\left(x_{k}-\mathbb{E}\left[x_{k}\right]\right)+\sqrt{v_{i}} \epsilon_{j}\right)\right] \\
& =\sum_{k \in \mathrm{pa}_{j}} w_{j k} \operatorname{cov}\left[x_{i}, x_{k}\right]+I_{i j} v_{j} .
\end{aligned}
$$

- Consider two cases:
- There are no links in the graph (graph is fully factorized), so that $\mathrm{w}_{\mathrm{ij}}$ 's are zero. In this case: $\mathbb{E}[\mathbf{x}]=\left[b_{1}, \ldots, b_{D}\right]^{T}$, and the covariance is diagonal $\operatorname{diag}\left(v_{1}, \ldots, v_{D}\right)$. The joint distribution represents $D$ independent univariate Gaussian distributions.
- The graph is fully connected. The total number of parameters is $D+D(D-1) / 2$. The covariance corresponds to a general symmetric covariance matrix.


## Bilinear Gaussian Model

－Consider the following model：

$u \sim \mathcal{N}(0,1)$,
$v \sim \mathcal{N}(0,1)$,
$r \sim \mathcal{N}(u v, 1)$.


Gaussian terms

|  | d | d | J | dJ | d |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 1 |  | ？ | ？ | 市市的 | 市市 |
| 9 | ？ | 办为全 | ＊ | ？ | 亦交 |
| $\bullet$ | 市交方 | ？ | 亦交它 |  | ？ |



$$
\begin{aligned}
& u_{i} \sim \mathcal{N}(0,1), i=1, \ldots, N \\
& v_{j} \sim \mathcal{N}(0,1), j=1, \ldots, M \\
& r_{i j} \sim \mathcal{N}\left(u_{i} v_{j}, 1\right) .
\end{aligned}
$$

－The mean is given by the product of two Gaussians．

## Hierarchical Models



