STA 4273H: Statistical Machine Learning

Russ Salakhutdinov

Department of Statistics rsalakhu@utstat.toronto.edu http://www.utstat.utoronto.ca/~rsalakhu/ Sidney Smith Hall, Room 6002

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 **x** into one of K discrete classes C_k , where k=1,...,K.

• Typically, each input is assigned only to one class.

• Example: The input vector **x** is the set of pixel intensities, and the output variable t will represent the presence of cancer, class C_1 , or absence of cancer, class C_2 .



x -- set of pixel intensities

Linear Classification

• The goal of classification is to assign an input **x** into one of K discrete classes C_k , where k=1,...,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:

$$y(\mathbf{x}, \mathbf{w}) = \mathbf{x}^T \mathbf{w} + w_0.$$
 $y(\mathbf{x}, \mathbf{w}) =$
adaptive parameters

$$y(\mathbf{x}, \mathbf{w}) = f(\mathbf{x}^T \mathbf{w} + w_0).$$

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

 $y(\mathbf{x}, \mathbf{w}) = f(\mathbf{x}^T \mathbf{w} + w_0).$

- The decision surfaces correspond to $y(\mathbf{x}, \mathbf{w}) = \text{const}$, so that $\mathbf{x}^T \mathbf{w} + w_0 = \text{const}$, 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 $\phi(\mathbf{x})$, 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 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 **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 $p(C_k|\mathbf{x})$, and then use this distribution to make optimal decisions.
- There are two alternative approaches:
 - Discriminative Approach: Model $p(C_k|\mathbf{x})$, 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 $p(\mathbf{x}|C_k)$ together with the prior probabilities $p(C_k)$ for the classes. Infer posterior probability using Bayes' rule:

$$p(\mathcal{C}_k|\mathbf{x}) = \frac{p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)}{p(\mathbf{x})}.$$

We will consider next.

Probabilistic Generative Models

• Model class conditional densities $p(\mathbf{x}|C_k)$ separately for each class, as well as the class priors $p(C_k)$.

 \bullet Consider the case of two classes. The posterior probability of class C_1 is given by:



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 C₁ is given by:



- 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 K>2 classes, we have the following multi-class generalization:

$$p(\mathcal{C}_k|\mathbf{x}) = \frac{p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)}{\sum_j p(\mathbf{x}|\mathcal{C}_j)p(\mathcal{C}_j)} = \frac{\exp(a_k)}{\sum_j \exp(a_j)}, \ a_k = \ln[p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)].$$

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

if
$$a_k \gg a_j$$
, $\forall j \neq k$, then $p(\mathcal{C}_k | \mathbf{x}) \approx 1$, $p(\mathcal{C}_j | \mathbf{x}) \approx 0$.

• 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:

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

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

$$p(\mathcal{C}_k|\mathbf{x}) = \sigma(\mathbf{w}^T\mathbf{x} + w_0),$$

where we have defined:

$$\mathbf{w} = \mathbf{\Sigma}^{-1} (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2),$$

$$w_0 = -\frac{1}{2} \boldsymbol{\mu}_1^T \mathbf{\Sigma}^{-1} \boldsymbol{\mu}_1 + \frac{1}{2} \boldsymbol{\mu}_2^T \mathbf{\Sigma}^{-1} \boldsymbol{\mu}_2 + \ln \frac{p(\mathcal{C}_1)}{p(\mathcal{C}_2)}.$$

- The quadratic terms in **x** cancel (due to the assumption of common covariance matrices).
- This leads to a linear function of **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 $p(C_1|\mathbf{x})$, given by the sigmoid function of a linear function of **x**.

Case of K Classes

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

$$p(\mathcal{C}_k | \mathbf{x}) = \frac{p(\mathbf{x} | \mathcal{C}_k) p(\mathcal{C}_k)}{\sum_j p(\mathbf{x} | \mathcal{C}_j) p(\mathcal{C}_j)} = \frac{\exp(a_k)}{\sum_j \exp(a_j)},$$
$$a_k = \mathbf{w}_k^T \mathbf{x} + w_{k0},$$

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

$$\mathbf{w}_{k} = \mathbf{\Sigma}^{-1} \boldsymbol{\mu}_{k},$$

$$w_{k0} = -\frac{1}{2} \boldsymbol{\mu}_{k}^{T} \mathbf{\Sigma}^{-1} \boldsymbol{\mu}_{k} + \ln p(\mathcal{C}_{k}).$$

- 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 **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 $\{\mathbf{x}_n, t_n\}, n = 1, ..., N.$
 - Here t_n =1 denotes class C_1 , and t_n =0 denotes class C_2 .
 - Also denote $p(\mathcal{C}_1) = \pi$, $p(\mathcal{C}_2) = 1 \pi$.
- The likelihood function takes form:

$$p(\mathbf{t}, \mathbf{X} | \pi, \boldsymbol{\mu}_{1}, \boldsymbol{\mu}_{2}, \boldsymbol{\Sigma}) = \prod_{n=1}^{N} \begin{bmatrix} \pi \mathcal{N}(\mathbf{x}_{n} | \boldsymbol{\mu}_{1}, \boldsymbol{\Sigma}) \end{bmatrix}^{t_{n}} \begin{bmatrix} (1 - \pi) \mathcal{N}(\mathbf{x}_{n} | \boldsymbol{\mu}_{2}, \boldsymbol{\Sigma}) \end{bmatrix}^{1 - t_{n}}$$

$$Data \text{ points} \text{ from class } \mathbf{C}_{1}.$$
Data points from class $\mathbf{C}_{2}.$

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

Maximum Likelihood Solution

$$p(\mathbf{t}, \mathbf{X} | \pi, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \boldsymbol{\Sigma}) = \prod_{n=1}^{N} \left[\pi \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_1, \boldsymbol{\Sigma}) \right]^{t_n} \left[(1 - \pi) \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_2, \boldsymbol{\Sigma}) \right]^{1 - t_n}$$

• Maximizing the respect to π , we look at the terms of the log-likelihood functions that depend on π :

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

Differentiating, we get:

$$\pi = \frac{1}{N} \sum_{n=1}^{N} t_n = \frac{N_1}{N_1 + N_2}.$$

• Maximizing the respect to μ_1 , we look at the terms of the log-likelihood functions that depend on μ_1 :

$$\sum_{n} t_{n} \ln \mathcal{N}(\mathbf{x}_{n} | \boldsymbol{\mu}_{1}, \boldsymbol{\Sigma}) = -\frac{1}{2} \sum_{n} t_{n} (\mathbf{x}_{n} - \boldsymbol{\mu}_{1})^{T} \boldsymbol{\Sigma}^{-1} (\mathbf{x}_{n} - \boldsymbol{\mu}_{1}) + \text{const.}$$
Differentiating, we get:

$$\boldsymbol{\mu}_{1} = \frac{1}{N_{1}} \sum_{n=1}^{N} t_{n} \mathbf{x}_{n}.$$
And similarly:

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

Maximum Likelihood Solution

$$p(\mathbf{t}, \mathbf{X} | \pi, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \boldsymbol{\Sigma}) = \prod_{n=1}^{N} \left[\pi \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_1, \boldsymbol{\Sigma}) \right]^{t_n} \left[(1 - \pi) \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_2, \boldsymbol{\Sigma}) \right]^{1 - t_n}$$

• Maximizing the respect to Σ :

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

• Here we defined:

$$\mathbf{S} = \frac{N_1}{N} \mathbf{S}_1 + \frac{N_2}{N} \mathbf{S}_2,$$

$$\mathbf{S}_1 = \frac{1}{N_1} \sum_{n \in \mathcal{C}_1} (\mathbf{x}_n - \boldsymbol{\mu}_1) (\mathbf{x}_n - \boldsymbol{\mu}_1)^T,$$

$$\mathbf{S}_2 = \frac{1}{N_2} \sum_{n \in \mathcal{C}_2} (\mathbf{x}_n - \boldsymbol{\mu}_2) (\mathbf{x}_n - \boldsymbol{\mu}_2)^T.$$

• Using standard results for a Gaussian distribution we have:

$$\Sigma = S.$$

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



- 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 $p(C_k|\mathbf{x})$, and then use this distribution to make optimal decisions.
- There are two approaches:
 - Discriminative Approach: Model $p(C_k|\mathbf{x})$, 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 $p(\mathbf{x}|C_k)$ together with the prior probabilities $p(C_k)$ for the classes. Infer posterior probability using Bayes' rule:

$$p(\mathcal{C}_k|\mathbf{x}) = rac{p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)}{p(\mathbf{x})}.$$

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 $\phi(\mathbf{x})$.

• Decision boundaries will be linear in the feature space ϕ , but would correspond to nonlinear boundaries in the original input space **x**.

- Classes that are linearly separable in the feature space $\phi({\bf x})$ 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 C_1 can be written as a logistic sigmoid function:

$$p(\mathcal{C}_1|\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^T \mathbf{x})} = \sigma(\mathbf{w}^T \mathbf{x}),$$

where $p(C_2|\mathbf{x}) = 1 - p(C_1|\mathbf{x})$, 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 $p(\mathcal{C}_k|\mathbf{x})$ directly.



ML for Logistic Regression

• We observed a training dataset $\{\mathbf{x}_n, t_n\}, n = 1, ..., N; t_n \in \{0, 1\}.$

• Maximize the probability of getting the label right, so the likelihood function takes form:

$$p(\mathbf{t}|\mathbf{X}, \mathbf{w}) = \prod_{n=1}^{N} \left[y_n^{t_n} (1 - y_n)^{1 - t_n} \right], \quad y_n = \sigma(\mathbf{w}^T \mathbf{x}_n).$$

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

$$E(\mathbf{w}) = -\ln p(\mathbf{t}|\mathbf{X}, \mathbf{w}) = -\sum_{n=1}^{N} \left[t_n \ln y_n + (1 - t_n) \ln(1 - y_n) \right] = \sum_{n=1}^{N} E_n.$$

• Differentiating and using the chain rule:

$$\frac{\mathrm{d}}{\mathrm{d}y_n} E_n = \frac{y_n - t_n}{y_n(1 - y_n)}, \quad \frac{\mathrm{d}}{\mathrm{d}\mathbf{w}} y_n = y_n(1 - y_n)\mathbf{x}_n, \quad \frac{\mathrm{d}}{\mathrm{d}a}\sigma(a) = \sigma(a)(1 - \sigma(a)).$$
$$\frac{\mathrm{d}}{\mathrm{d}\mathbf{w}} E_n = \frac{\mathrm{d}E_n}{\mathrm{d}y_n} \frac{\mathrm{d}y_n}{\mathrm{d}\mathbf{w}} = (y_n - t_n)\mathbf{x}_n.$$

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

ML for Logistic Regression

• We therefore obtain:



- 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 :

$$p(\mathcal{C}_k | \mathbf{x}) = y_k(\mathbf{x}) = \frac{\exp(\mathbf{w}_k^T \mathbf{x})}{\sum_j \exp(\mathbf{w}_j^T \mathbf{x})}.$$

• Unlike in generative models, here we will use maximum likelihood to determine parameters of this discriminative model directly.

• As usual, we observed a dataset $\{\mathbf{x}_n, t_n\}, n = 1, ..., N$, where we use 1-of-K encoding for the target vector \mathbf{t}_n .

• So if \mathbf{x}_n belongs to class C_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 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:

$$p(\mathbf{T}|\mathbf{X}, \mathbf{w}_{1}, ..., \mathbf{w}_{K}) = \prod_{n=1}^{N} \left[\prod_{k=1}^{K} p(\mathcal{C}_{k}|\mathbf{x}_{n})^{t_{nk}} \right] = \prod_{n=1}^{N} \left[\prod_{k=1}^{K} y_{nk}^{t_{nk}} \right]$$

N × K binary matrix of target variables. Only one term corresponding to correct class contributes.

where
$$y_{nk} = p(\mathcal{C}_k | \mathbf{x}_n) = \frac{\exp(\mathbf{w}_k^T \mathbf{x}_n)}{\sum_j \exp(\mathbf{w}_j^T \mathbf{x}_n)}$$
.

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

$$E(\mathbf{w}_1, ..., \mathbf{w}_K) = -\ln p(\mathbf{T} | \mathbf{X}, \mathbf{w}_1, ..., \mathbf{w}_K) = -\sum_{n=1}^N \left[\sum_{k=1}^K t_{nk} \ln y_{nk} \right].$$

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• Taking the gradient:

$$\nabla E_{\mathbf{w}_j}(\mathbf{w}_1, \dots, \mathbf{w}_K) = \sum_{n=1}^N (y_{nj} - t_{nj}) \mathbf{x}_n.$$

Special Case of Softmax

• If we consider a softmax function for two classes:

$$p(\mathcal{C}_1|\mathbf{x}) = \frac{\exp(a_1)}{\exp(a_1) + \exp(a_2)} = \frac{1}{1 + \exp(-(a_1 - a_2))} = \sigma(a_1 - a_2).$$

• 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.

$$p(\mathcal{C}_k|\mathbf{x}) = \frac{p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)}{p(\mathbf{x})}.$$

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

Model $p(\mathcal{C}_k | \mathbf{x})$ directly.

Bayesian Logistic Regression

- We next look at the Bayesian treatment of logistic regression.
- For the two-class problem, the likelihood takes form:

$$p(\mathbf{t}|\mathbf{X}, \mathbf{w}) = \prod_{n=1}^{N} \left[y_n^{t_n} (1 - y_n)^{1 - t_n} \right], \quad y_n = \frac{1}{1 + \exp(-\mathbf{w}^T \mathbf{x}_n)} = \sigma(\mathbf{w}^T \mathbf{x}_n).$$

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

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_0, \mathbf{S}_0).$$

• However, the posterior distribution

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

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:

 $p(w) \propto \exp(-w^2)\sigma(20w+4).$

- 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.

• We will use the following notation:

$$p(\mathbf{z}) = rac{\widetilde{p}(\mathbf{z})}{\mathcal{Z}}, \ \mathcal{Z} = \int \widetilde{p}(\mathbf{z}) d\mathbf{z}.$$

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

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

• Goal: Find a Gaussian approximation q(z) which is centered on a mode of the distribution p(z).

• We will use the following notation:

$$p(\mathbf{z}) = rac{\widetilde{p}(\mathbf{z})}{\mathcal{Z}}, \ \mathcal{Z} = \int \widetilde{p}(\mathbf{z}) d\mathbf{z}.$$

• At the stationary point z_0 , the gradient $\nabla \tilde{p}(z_0)$ vanishes.

• Consider a Taylor approximation $\ln \tilde{p}(\mathbf{z})$ around \mathbf{z}_0 .

$$\ln \tilde{p}(\mathbf{z}) \approx \ln \tilde{p}(\mathbf{z}_0) - \frac{1}{2} (\mathbf{z} - \mathbf{z}_0)^T A(\mathbf{z} - \mathbf{z}_0),$$

where A is a Hessian matrix:

$$A = - \bigtriangledown \bigtriangledown \ln \tilde{p}(\mathbf{z})|_{\mathbf{z}=\mathbf{z}_0}.$$

• Exponentiating both sides:

$$\tilde{p}(\mathbf{z}) \approx \tilde{p}(\mathbf{z}_0) \exp\left(-\frac{1}{2}(\mathbf{z} - \mathbf{z}_0)^T A(\mathbf{z} - \mathbf{z}_0)\right)$$

• We will use the following notation:

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

• Using Taylor approximation, we get:

$$\tilde{p}(\mathbf{z}) \approx \tilde{p}(\mathbf{z}_0) \exp\left(-\frac{1}{2}(\mathbf{z} - \mathbf{z}_0)^T A(\mathbf{z} - \mathbf{z}_0)\right)$$

• Hence a Gaussian approximation for $p(\mathbf{z})$ is:

$$q(\mathbf{z}) = \frac{|A|^{1/2}}{(2\pi)^{D/2}} \exp\left(-\frac{1}{2}(\mathbf{z} - \mathbf{z}_0)^T A(\mathbf{z} - \mathbf{z}_0)\right),$$

where z_0 is the mode of p(z), and A is the Hessian:

$$A = - \bigtriangledown \bigtriangledown \ln \tilde{p}(\mathbf{z})|_{\mathbf{z}=\mathbf{z}_0}.$$

• We will use the following notation:

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

Using Taylor approximation, we get:

$$\tilde{p}(\mathbf{z}) \approx \tilde{p}(\mathbf{z}_0) \exp\left(-\frac{1}{2}(\mathbf{z} - \mathbf{z}_0)^T A(\mathbf{z} - \mathbf{z}_0)\right)$$

- Bayesian inference: $p(\mathbf{w}|\mathcal{D}) = \frac{p(\mathcal{D}|\mathbf{w})p(\mathbf{w})}{p(\mathcal{D})}$. Identify: $\tilde{p}(\theta|\mathcal{D}) = p(\mathcal{D}|\theta)p(\theta), \ \mathcal{Z} = \int p(\mathcal{D}|\theta)p(\theta)d\theta$.
- The posterior is approximately Gaussian around the MAP estimate:

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

using Laplace approximation:

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

Bayesian Information Criterion

• BIC can be obtained from the Laplace approximation:

$$\ln p(\mathcal{D}) \approx \ln p(\mathcal{D}|\theta_{\text{MAP}}) + \ln P(\theta_{\text{MAP}}) + \frac{D}{2}\ln 2\pi - \frac{1}{2}\ln|A|,$$

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

$$\ln p(\mathcal{D}) \approx \ln p(\mathcal{D}|\theta_{\text{MAP}}) - \frac{1}{2}D\ln N.$$

- 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:

$$p(\mathbf{t}|\mathbf{X}, \mathbf{w}) = \prod_{n=1}^{N} \left[y_n^{t_n} (1 - y_n)^{1 - t_n} \right], \quad y_n = \frac{1}{1 + \exp(-\mathbf{w}^T \mathbf{x}_n)} = \sigma(\mathbf{w}^T \mathbf{x}_n).$$

• And the prior: $p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_0, \mathbf{S}_0).$

• The log of the posterior takes form:

$$\ln p(\mathbf{w}|\mathbf{X}, \mathbf{t}) = -\frac{1}{2} (\mathbf{w} - \mathbf{m}_0)^T \mathbf{S}_0^{-1} (\mathbf{w} - \mathbf{m}_0) + \sum_{n=1}^N \left[t_n \ln y_n + (1 - t_n) \ln(1 - t_n) \right] + \text{const.}$$

Log-prior term

Log-likelihood

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

$$\mathbf{S}_N^{-1} = -\bigtriangledown \bigtriangledown \ln p(\mathbf{w}|\mathbf{X}, \mathbf{t}) = S_0^{-1} + \sum_n y_n (1 - y_n) \mathbf{x}_n \mathbf{x}_n^T.$$

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

$$q(\mathbf{w}) = \mathcal{N}(\mathbf{w} | \mathbf{w}_{\mathrm{MAP}}, \mathbf{S}_N).$$

Predictive Distribution

• The predictive distribution for class C₁, given a new input \mathbf{x}^* is given by marginalizing with respect to posterior distribution $p(\mathbf{w}|\mathbf{X}, \mathbf{t})$, which is itself approximated by a Gaussian distribution:

with the corresponding probability for class C_2 given by:

$$p(\mathcal{C}_1|\mathbf{x}^*, \mathbf{t}, \mathbf{X}) = 1 - p(\mathcal{C}_1|\mathbf{x}^*, \mathbf{t}, \mathbf{X}).$$

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

Predictive Distribution

 $p(\mathcal{C}_1 | \mathbf{x}^*, \mathbf{X}, \mathbf{t}) \approx \int \sigma(\mathbf{w}^T \mathbf{x}^*) q(\mathbf{w}) \mathrm{d}\mathbf{w}.$

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

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

where δ is the Dirac delta function. Hence

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

• Let us characterize p(a).
1-dimensional integral.

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

Predictive Distribution

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

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

$$\mu_{a} = \mathbb{E}[a] = \int ap(a)da = \int \mathbf{w}^{T} \mathbf{x}^{*}q(\mathbf{w})d\mathbf{w} = \mathbf{w}_{MAP}^{T} \mathbf{x}^{*}.$$
 Same form as the predictive distribution for the Bayesian linear $\sigma_{a}^{2} = \operatorname{var}[a] = \int p(a) \left[a^{2} - \mathbb{E}[a]^{2}\right] = \int \left[(\mathbf{w}^{T} \mathbf{x}^{*})^{2} - (\mathbf{w}_{MAP}^{T} \mathbf{x}^{*})^{2}\right] q(\mathbf{w})d\mathbf{w} = \mathbf{x}^{*T} \mathbf{S}_{N} \mathbf{x}^{*}.$ Same form as the predictive distribution for the Bayesian linear regression model.

• Hence we obtain approximate predictive:

$$p(\mathcal{C}_1 | \mathbf{x}^*, \mathbf{X}, \mathbf{t}) \approx \int \sigma(\mathbf{w}^T \mathbf{x}^*) q(\mathbf{w}) d\mathbf{w} = \int \sigma(a) \mathcal{N}(a | \mu_a, \sigma_a^2).$$

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

$$\int \sigma(a) \mathcal{N}(a|\mu_a, \sigma_a^2) \approx \sigma(k\mu_a), \text{ where } k = (1 + \pi \sigma_a^2/8)^{-1/2}.$$

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.

- 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|a, b)p(a, b) = p(c|a, b)p(b|a)p(a)

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

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

$$p(a, b, c) = p(c|a, b)p(a, b) = p(c|a, b)p(b|a)p(a)$$

• 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 $p(c \vert a, b),$ there will be links from nodes a and b to node c.
- For the factor p(a), there will be no incoming links.

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

$$p(a, b, c) = p(c|a, b)p(a, b) = p(c|a, b)p(b|a)p(a)$$

• 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:

$$p(x_1, \ldots, x_K) = p(x_K | x_1, \ldots, x_{K-1}) \ldots p(x_2 | x_1) p(x_1)$$

• 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.

• 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 x_1, \ldots, x_7 can be written as a product of a set of conditional distributions.

 $p(x_1, \dots, x_7) = p(x_1)p(x_2)p(x_3)p(x_4|x_1, x_2, x_3)$ $p(x_5|x_1, x_3)p(x_6|x_4)p(x_7|x_4, x_5)$

• Note that according to the graph, x_5 will be conditioned only on x_1 and 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:

$$p(\mathbf{x}) = \prod_{k=1}^{K} p(x_k | \mathrm{pa}_k)$$

where pa_k denotes a set of parents for the node x_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.

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

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

• 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 K^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 M(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 $p(\mathbf{x}_1)$ requires K-1 parameters.
- The remaining conditional distributions $p(\mathbf{x}_i | \mathbf{x}_{i-1}), i = 2, ..., M$ require K(K-1) parameters.
- Total number of parameters: K-1 + (M-1)(K-1)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.

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.

• 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:

$$p(x_i | pa_i) = \mathcal{N}\left(x_i \left| \sum_{j \in pa_i} w_{ij} x_j + b_i, v_i \right)\right)$$

where w_{ij} and b_i are parameters governing the mean, and v_i is the variance.

Linear Gaussian Models

• The log of the joint distribution takes form:

$$\ln p(\mathbf{x}) = \sum_{i=1}^{D} \ln p(x_i | \mathbf{pa}_i) = -\sum_{i=1}^{D} \frac{1}{2v_i} \left(x_i - \sum_{j \in \mathbf{pa}_i} w_{ij} x_j - b_i \right)^2 + \text{const},$$

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: (

$$p(x_i | \mathrm{pa}_i) = \mathcal{N}\left(x_i \left| \sum_{j \in \mathrm{pa}_i} w_{ij} x_j + b_i, v_i \right. \right)$$

hence

$$x_i = \sum_{j \in pa_i} w_{ij} x_j + b_i + \sqrt{v_i} \epsilon_i, \qquad \epsilon_i \sim \mathcal{N}(0, 1),$$

so its expected value:

$$\mathbb{E}[x_i] = \sum_{j \in \mathrm{pa}_i} w_{ij} \mathbb{E}[x_j] + b_i.$$

• Hence we can find components: $\mathbb{E}[\mathbf{x}] = [\mathbb{E}[x_1], ..., \mathbb{E}[x_D]]$ by doing ancestral pass: start at the top and proceed in order (see example):

Computing the Covariance

• We can obtain the i,j element of the covariance matrix in the form of a recursion relation:

$$\begin{aligned} \operatorname{cov}[x_i, x_j] &= \mathbb{E}\left[(x_i - \mathbb{E}[x_i])(x_j - \mathbb{E}[x_j]) \right] \\ &= \mathbb{E}\left[\left(x_i - \mathbb{E}[x_i] \right) \left(\sum_{k \in \operatorname{pa}_j} w_{jk}(x_k - \mathbb{E}[x_k]) + \sqrt{v_i} \epsilon_j \right) \right] \\ &= \sum_{k \in \operatorname{pa}_j} w_{jk} \operatorname{cov}[x_i, x_k] + I_{ij} v_j. \end{aligned}$$

- Consider two cases:
- There are no links in the graph (graph is fully factorized), so that w_{ij} 's are zero. In this case: $\mathbb{E}[\mathbf{x}] = [b_1, ..., b_D]^T$, and the covariance is diagonal $\operatorname{diag}(v_1, ..., v_D)$. 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

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

Hierarchical Models

