Probabilistic Models for Classification: Discriminative Classification

Piyush Rai

Probabilistic Machine Learning (CS772A)

Aug 19, 2017

Recap

• A two-step procedure to learn a probabilistic classification model p(y|x)

- A two-step procedure to learn a probabilistic classification model p(y|x)
 - Learn class-conditional distribution p(x|y) and class-prior distribution p(y) using training data

- A two-step procedure to learn a probabilistic classification model p(y|x)
 - Learn class-conditional distribution p(x|y) and class-prior distribution p(y) using training data
 - We usually assume the form of p(x|y) and p(y), but the parameters are unknowns

- A two-step procedure to learn a probabilistic classification model p(y|x)
 - Learn class-conditional distribution p(x|y) and class-prior distribution p(y) using training data
 - We usually assume the form of p(x|y) and p(y), but the parameters are unknowns
 - Parameter estimation can be done via MLE or MAP or fully Bayesian inference

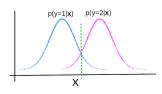
- A two-step procedure to learn a probabilistic classification model p(y|x)
 - **Q** Learn class-conditional distribution p(x|y) and class-prior distribution p(y) using training data
 - We usually assume the form of p(x|y) and p(y), but the parameters are unknowns
 - Parameter estimation can be done via MLE or MAP or fully Bayesian inference
 - **②** Apply Bayes rule to predict the posterior probability of each class for any (test) input x_*

$$p(y_* = k|x_*) = \frac{p(y_* = k)p(x_*|y_* = k)}{p(x_*)}$$

- A two-step procedure to learn a probabilistic classification model p(y|x)
 - Learn class-conditional distribution p(x|y) and class-prior distribution p(y) using training data
 - We usually assume the form of p(x|y) and p(y), but the parameters are unknowns
 - Parameter estimation can be done via MLE or MAP or fully Bayesian inference
 - ② Apply Bayes rule to predict the posterior probability of each class for any (test) input x_*

$$p(y_* = k|x_*) = \frac{p(y_* = k)p(x_*|y_* = k)}{p(x_*)}$$

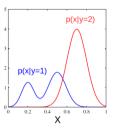
ullet The predicted class for the input x will be the one that has the largest posterior probability

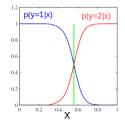


• Generative classification requires modeling the input distribution (for each class)

- Generative classification requires modeling the input distribution (for each class)
- In some cases, this extensive modeling effort may not be worth it (e.g., the case shown below)

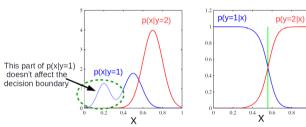




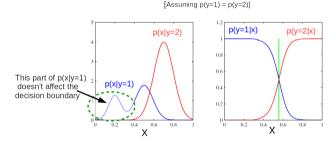


- Generative classification requires modeling the input distribution (for each class)
- In some cases, this extensive modeling effort may not be worth it (e.g., the case shown below)



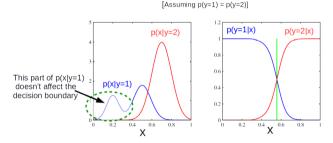


- Generative classification requires modeling the input distribution (for each class)
- In some cases, this extensive modeling effort may not be worth it (e.g., the case shown below)



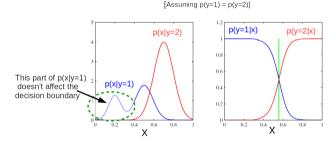
• A better approach would be to directly model p(y|x), i.e., the distribution that makes the decision

- Generative classification requires modeling the input distribution (for each class)
- In some cases, this extensive modeling effort may not be worth it (e.g., the case shown below)



- A better approach would be to directly model p(y|x), i.e., the distribution that makes the decision
 - Such an approach is called Discriminative Classification (today's topic)

- Generative classification requires modeling the input distribution (for each class)
- In some cases, this extensive modeling effort may not be worth it (e.g., the case shown below)



- A better approach would be to directly model p(y|x), i.e., the distribution that makes the decision
 - Such an approach is called Discriminative Classification (today's topic)
- PS: The generative approach is still appealing for many other reasons (as discussed in last lecture)

Probabilistic Models for Discriminative Classification

Probabilistic Models for Discriminative Classification

Note: Many non-probabilistic classification models can be termed as discriminative classifiers (e.g., Support Vector Machine or SVM, which directly learns a separator between classes)

• Models p(y|x) directly using an appropriate discrete distribution

- Models p(y|x) directly using an appropriate discrete distribution
- Parameters of the distribution p(y|x) defined by a linear/nonlinear function of x

- Models p(y|x) directly using an appropriate discrete distribution
- Parameters of the distribution p(y|x) defined by a linear/nonlinear function of x
 - A discriminative model only needs to learn these parameters!

- Models p(y|x) directly using an appropriate discrete distribution
- Parameters of the distribution p(y|x) defined by a linear/nonlinear function of x
 - A discriminative model only needs to learn these parameters!
- For binary classification, p(y|x) would be a Bernoulli

$$p(y|\mathbf{x}) = p(y|\mathbf{x}, f) = \text{Bernoulli}[f(\mathbf{x})]$$

- Models p(y|x) directly using an appropriate discrete distribution
- Parameters of the distribution p(y|x) defined by a linear/nonlinear function of x
 - A discriminative model only needs to learn these parameters!
- For binary classification, p(y|x) would be a Bernoulli

$$p(y|\mathbf{x}) = p(y|\mathbf{x}, f) = \text{Bernoulli}[f(\mathbf{x})]$$

where f() is a function (defined by some params) that maps ${\pmb x}$ to a probability $\mu=p(y=1|{\pmb x})$

- Models p(y|x) directly using an appropriate discrete distribution
- Parameters of the distribution p(y|x) defined by a linear/nonlinear function of x
 - A discriminative model only needs to learn these parameters!
- For binary classification, p(y|x) would be a Bernoulli

$$p(y|\mathbf{x}) = p(y|\mathbf{x}, f) = \text{Bernoulli}[f(\mathbf{x})]$$

where f() is a function (defined by some params) that maps ${\pmb x}$ to a probability $\mu=p(y=1|{\pmb x})$

• For K > 2 class multiclass classification, p(y|x) would be a multinoulli

- Models p(y|x) directly using an appropriate discrete distribution
- Parameters of the distribution p(y|x) defined by a linear/nonlinear function of x
 - A discriminative model only needs to learn these parameters!
- For binary classification, p(y|x) would be a Bernoulli

$$p(y|\mathbf{x}) = p(y|\mathbf{x}, f) = \text{Bernoulli}[f(\mathbf{x})]$$

where f() is a function (defined by some params) that maps ${\pmb x}$ to a probability $\mu=p(y=1|{\pmb x})$

• For K > 2 class multiclass classification, p(y|x) would be a multinoulli

$$p(y|\mathbf{x}) = p(y|\mathbf{x}, f) = \text{multinoulli}[f(\mathbf{x})]$$



- Models p(y|x) directly using an appropriate discrete distribution
- Parameters of the distribution p(y|x) defined by a linear/nonlinear function of x
 - A discriminative model only needs to learn these parameters!
- For binary classification, p(y|x) would be a Bernoulli

$$p(y|\mathbf{x}) = p(y|\mathbf{x}, f) = \text{Bernoulli}[f(\mathbf{x})]$$

where f() is a function (defined by some params) that maps ${\pmb x}$ to a probability $\mu=p(y=1|{\pmb x})$

• For K > 2 class multiclass classification, p(y|x) would be a multinoulli

$$p(y|\mathbf{x}) = p(y|\mathbf{x}, f) = \text{multinoulli}[f(\mathbf{x})]$$

where f() maps ${\pmb x}$ to a probability vector ${\pmb \mu} = [\mu_1, \dots, \mu_K]$ s.t. $p(y=k|{\pmb x}) = \mu_k$



- Models p(y|x) directly using an appropriate discrete distribution
- Parameters of the distribution p(y|x) defined by a linear/nonlinear function of x
 - A discriminative model only needs to learn these parameters!
- For binary classification, p(y|x) would be a Bernoulli

$$p(y|\mathbf{x}) = p(y|\mathbf{x}, f) = \text{Bernoulli}[f(\mathbf{x})]$$

where f() is a function (defined by some params) that maps x to a probability $\mu = p(y=1|x)$

• For K > 2 class multiclass classification, p(y|x) would be a multinoulli

$$p(y|\mathbf{x}) = p(y|\mathbf{x}, f) = \text{multinoulli}[f(\mathbf{x})]$$

where f() maps \mathbf{x} to a probability vector $\boldsymbol{\mu} = [\mu_1, \dots, \mu_K]$ s.t. $p(y = k | \mathbf{x}) = \mu_k$

• Many choices of f(x) possible. Lead to different types of discriminative classification models



$$p(y|\mathbf{x}) = \text{Bernoulli}[f(\mathbf{x})]$$
 OR $p(y|\mathbf{x}) = \text{multinoulli}[f(\mathbf{x})]$

• The general form of p(y|x) in these models is given by

$$p(y|\mathbf{x}) = \text{Bernoulli}[f(\mathbf{x})]$$
 OR $p(y|\mathbf{x}) = \text{multinoulli}[f(\mathbf{x})]$

• The function f(x) is composed of two operations

$$p(y|x) = \text{Bernoulli}[f(x)]$$
 OR $p(y|x) = \text{multinoulli}[f(x)]$

- The function f(x) is composed of two operations
 - Compute a score for x (e.g., using a linear model $w^T x$ where w is the param. to be estimated)

$$p(y|\mathbf{x}) = \text{Bernoulli}[f(\mathbf{x})]$$
 OR $p(y|\mathbf{x}) = \text{multinoulli}[f(\mathbf{x})]$

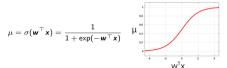
- The function f(x) is composed of two operations
 - Compute a score for x (e.g., using a linear model $w^T x$ where w is the param. to be estimated)
 - Turn this score into a probability of x belonging to each class

$$p(y|\mathbf{x}) = \text{Bernoulli}[f(\mathbf{x})]$$
 OR $p(y|\mathbf{x}) = \text{multinoulli}[f(\mathbf{x})]$

- The function f(x) is composed of two operations
 - Compute a score for x (e.g., using a linear model $w^T x$ where w is the param. to be estimated)
 - Turn this score into a probability of x belonging to each class
- Example: $f(\mathbf{x}) = \mu = \sigma(\mathbf{w}^{\top}\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^{\top}\mathbf{x})} \Rightarrow \text{Logistic Regression}$; used for binary classification

$$p(y|\mathbf{x}) = \text{Bernoulli}[f(\mathbf{x})]$$
 OR $p(y|\mathbf{x}) = \text{multinoulli}[f(\mathbf{x})]$

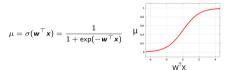
- The function f(x) is composed of two operations
 - Compute a score for x (e.g., using a linear model $w^T x$ where w is the param. to be estimated)
 - Turn this score into a probability of x belonging to each class
- Example: $f(\mathbf{x}) = \mu = \sigma(\mathbf{w}^{\top}\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^{\top}\mathbf{x})} \Rightarrow \text{Logistic Regression}$; used for binary classification



• The general form of p(y|x) in these models is given by

$$p(y|\mathbf{x}) = \text{Bernoulli}[f(\mathbf{x})]$$
 OR $p(y|\mathbf{x}) = \text{multinoulli}[f(\mathbf{x})]$

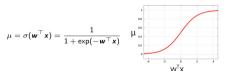
- The function f(x) is composed of two operations
 - Compute a score for x (e.g., using a linear model $w^T x$ where w is the param. to be estimated)
 - Turn this score into a probability of x belonging to each class
- Example: $f(\mathbf{x}) = \mu = \sigma(\mathbf{w}^{\top}\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^{\top}\mathbf{x})} \Rightarrow \text{Logistic Regression}$; used for binary classification



• Another example: $f(\mathbf{x}) = \boldsymbol{\mu}$ where $\mu_k = \frac{\exp(\mathbf{w}_k^{\top} \mathbf{x})}{\sum_{\ell=1}^K \exp(\mathbf{w}_\ell^{\top} \mathbf{x})} \Rightarrow \text{Softmax Regression}$; used for multiclass

$$p(y|\mathbf{x}) = \text{Bernoulli}[f(\mathbf{x})]$$
 OR $p(y|\mathbf{x}) = \text{multinoulli}[f(\mathbf{x})]$

- The function f(x) is composed of two operations
 - Compute a score for x (e.g., using a linear model $w^T x$ where w is the param. to be estimated)
 - Turn this score into a probability of x belonging to each class
- Example: $f(\mathbf{x}) = \mu = \sigma(\mathbf{w}^{\top}\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^{\top}\mathbf{x})} \Rightarrow \text{Logistic Regression}$; used for binary classification



- Another example: $f(\mathbf{x}) = \boldsymbol{\mu}$ where $\mu_k = \frac{\exp(\mathbf{w}_k^{\top} \mathbf{x})}{\sum_{\ell=1}^K \exp(\mathbf{w}_\ell^{\top} \mathbf{x})} \Rightarrow \text{Softmax Regression}$; used for multiclass
- Can also use nonlinear models to compute the scores (e.g., deep NN or Gaussian Process)

Logistic Regression

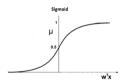
- Perhaps the simplest discriminative model for linear binary classification
- Defines $\mu = p(y = 1|x)$ using the sigmoid function

$$\mu = \sigma(\mathbf{w}^{\top}\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^{\top}\mathbf{x})} = \frac{\exp(\mathbf{w}^{\top}\mathbf{x})}{1 + \exp(\mathbf{w}^{\top}\mathbf{x})}$$

Logistic Regression

- Perhaps the simplest discriminative model for linear binary classification
- Defines $\mu = p(y = 1|x)$ using the sigmoid function

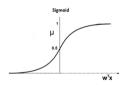
$$\mu = \sigma(\boldsymbol{w}^{\top}\boldsymbol{x}) = \frac{1}{1 + \exp(-\boldsymbol{w}^{\top}\boldsymbol{x})} = \frac{\exp(\boldsymbol{w}^{\top}\boldsymbol{x})}{1 + \exp(\boldsymbol{w}^{\top}\boldsymbol{x})}$$



Logistic Regression

- Perhaps the simplest discriminative model for linear binary classification
- Defines $\mu = p(y = 1|x)$ using the sigmoid function

$$\mu = \sigma(\mathbf{w}^{\top}\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^{\top}\mathbf{x})} = \frac{\exp(\mathbf{w}^{\top}\mathbf{x})}{1 + \exp(\mathbf{w}^{\top}\mathbf{x})}$$

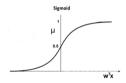


• Here $\mathbf{w}^{\top}\mathbf{x}$ is the score for input \mathbf{x} .

Logistic Regression

- Perhaps the simplest discriminative model for linear binary classification
- Defines $\mu = p(y = 1|x)$ using the sigmoid function

$$\mu = \sigma(\mathbf{w}^{\top}\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^{\top}\mathbf{x})} = \frac{\exp(\mathbf{w}^{\top}\mathbf{x})}{1 + \exp(\mathbf{w}^{\top}\mathbf{x})}$$

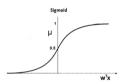


• Here $\mathbf{w}^{\top}\mathbf{x}$ is the score for input \mathbf{x} . The sigmoid turns it into a probability.

Logistic Regression

- Perhaps the simplest discriminative model for linear binary classification
- Defines $\mu = p(y = 1|x)$ using the sigmoid function

$$\mu = \sigma(\mathbf{w}^{\top}\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^{\top}\mathbf{x})} = \frac{\exp(\mathbf{w}^{\top}\mathbf{x})}{1 + \exp(\mathbf{w}^{\top}\mathbf{x})}$$



• Here $\mathbf{w}^{\top}\mathbf{x}$ is the score for input \mathbf{x} . The sigmoid turns it into a probability. Thus we have

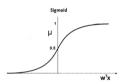
$$\rho(y = 1|\mathbf{x}, \mathbf{w}) = \mu = \sigma(\mathbf{w}^{\top}\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^{\top}\mathbf{x})} = \frac{\exp(\mathbf{w}^{\top}\mathbf{x})}{1 + \exp(\mathbf{w}^{\top}\mathbf{x})}$$
$$\rho(y = 0|\mathbf{x}, \mathbf{w}) = 1 - \mu = 1 - \sigma(\mathbf{w}^{\top}\mathbf{x}) = \frac{1}{1 + \exp(\mathbf{w}^{\top}\mathbf{x})}$$



Logistic Regression

- Perhaps the simplest discriminative model for linear binary classification
- Defines $\mu = p(y = 1|x)$ using the sigmoid function

$$\mu = \sigma(\mathbf{w}^{\top}\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^{\top}\mathbf{x})} = \frac{\exp(\mathbf{w}^{\top}\mathbf{x})}{1 + \exp(\mathbf{w}^{\top}\mathbf{x})}$$



• Here $\mathbf{w}^{\top}\mathbf{x}$ is the score for input \mathbf{x} . The sigmoid turns it into a probability. Thus we have

$$p(y = 1|x, w) = \mu = \sigma(\mathbf{w}^{\top} \mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^{\top} \mathbf{x})} = \frac{\exp(\mathbf{w}^{\top} \mathbf{x})}{1 + \exp(\mathbf{w}^{\top} \mathbf{x})}$$
$$p(y = 0|\mathbf{x}, \mathbf{w}) = 1 - \mu = 1 - \sigma(\mathbf{w}^{\top} \mathbf{x}) = \frac{1}{1 + \exp(\mathbf{w}^{\top} \mathbf{x})}$$

• Note: If we assume $y \in \{-1, +1\}$ instead of $y \in \{0, 1\}$ then $p(y|\mathbf{x}, \mathbf{w}) = \frac{1}{1 + \exp(-y\mathbf{w}^{\top}\mathbf{x})}$

• At the decision boundary where both classes are equiprobable:

$$\begin{array}{lcl} p(y=1|\mathbf{x},\mathbf{w}) & = & p(y=0|\mathbf{x},\mathbf{w}) \\ \frac{\exp(\mathbf{w}^{\top}\mathbf{x})}{1+\exp(\mathbf{w}^{\top}\mathbf{x})} & = & \frac{1}{1+\exp(\mathbf{w}^{\top}\mathbf{x})} \\ \exp(\mathbf{w}^{\top}\mathbf{x}) & = & 1 \\ \mathbf{w}^{\top}\mathbf{x} & = & 0 \end{array}$$

• At the decision boundary where both classes are equiprobable:

$$\begin{array}{lcl} \rho(y=1|\mathbf{x},\mathbf{w}) & = & \rho(y=0|\mathbf{x},\mathbf{w}) \\ \frac{\exp(\mathbf{w}^{\top}\mathbf{x})}{1+\exp(\mathbf{w}^{\top}\mathbf{x})} & = & \frac{1}{1+\exp(\mathbf{w}^{\top}\mathbf{x})} \\ \exp(\mathbf{w}^{\top}\mathbf{x}) & = & 1 \\ \mathbf{w}^{\top}\mathbf{x} & = & 0 \end{array}$$

• Thus the decision boundary of LR is a linear hyperplane, just like Perceptron, SVM, etc.

• At the decision boundary where both classes are equiprobable:

$$\begin{array}{lcl} p(y=1|\mathbf{x},\mathbf{w}) & = & p(y=0|\mathbf{x},\mathbf{w}) \\ \frac{\exp(\mathbf{w}^{\top}\mathbf{x})}{1+\exp(\mathbf{w}^{\top}\mathbf{x})} & = & \frac{1}{1+\exp(\mathbf{w}^{\top}\mathbf{x})} \\ \exp(\mathbf{w}^{\top}\mathbf{x}) & = & 1 \\ \mathbf{w}^{\top}\mathbf{x} & = & 0 \end{array}$$

- Thus the decision boundary of LR is a linear hyperplane, just like Perceptron, SVM, etc.
- Therefore y = 1 if $\mathbf{w}^{\top} \mathbf{x} \ge 0$, otherwise y = 0



• At the decision boundary where both classes are equiprobable:

$$\begin{array}{lcl} \rho(y=1|\mathbf{x},\mathbf{w}) & = & \rho(y=0|\mathbf{x},\mathbf{w}) \\ \frac{\exp(\mathbf{w}^{\top}\mathbf{x})}{1+\exp(\mathbf{w}^{\top}\mathbf{x})} & = & \frac{1}{1+\exp(\mathbf{w}^{\top}\mathbf{x})} \\ \exp(\mathbf{w}^{\top}\mathbf{x}) & = & 1 \\ \mathbf{w}^{\top}\mathbf{x} & = & 0 \end{array}$$

- Thus the decision boundary of LR is a linear hyperplane, just like Perceptron, SVM, etc.
- Therefore y = 1 if $\mathbf{w}^{\top} \mathbf{x} \ge 0$, otherwise y = 0



• High positive (negative) score $\mathbf{w}^{\top}\mathbf{x}$: High (low) probability of label 1

• Each label y_n is binary with probability $\mu_n = \frac{\exp(\mathbf{w}^{\top} \mathbf{x}_n)}{1 + \exp(\mathbf{w}^{\top} \mathbf{x}_n)}$. Since the likelihood is Bernoulli:

$$p(\boldsymbol{y}|\boldsymbol{X},\boldsymbol{w}) = \prod_{n=1}^{N} p(y_n|\boldsymbol{x}_n,\boldsymbol{w}) = \prod_{n=1}^{N} \mu_n^{y_n} (1-\mu_n)^{1-y_n}$$

• Each label y_n is binary with probability $\mu_n = \frac{\exp(\mathbf{w}^{\top} \mathbf{x}_n)}{1 + \exp(\mathbf{w}^{\top} \mathbf{x}_n)}$. Since the likelihood is Bernoulli:

$$p(y|X, w) = \prod_{n=1}^{N} p(y_n|x_n, w) = \prod_{n=1}^{N} \mu_n^{y_n} (1 - \mu_n)^{1-y_n}$$

Negative log-likelihood

$$\mathsf{NLL}(oldsymbol{w}) = -\log p(oldsymbol{y}|oldsymbol{\mathsf{X}},oldsymbol{w}) = -\sum_{n=1}^N (y_n\log \mu_n + (1-y_n)\log(1-\mu_n))$$

• Each label y_n is binary with probability $\mu_n = \frac{\exp(\mathbf{w}^{\top} \mathbf{x}_n)}{1 + \exp(\mathbf{w}^{\top} \mathbf{x}_n)}$. Since the likelihood is Bernoulli:

$$p(\boldsymbol{y}|\boldsymbol{X},\boldsymbol{w}) = \prod_{n=1}^{N} p(y_n|\boldsymbol{x}_n,\boldsymbol{w}) = \prod_{n=1}^{N} \mu_n^{y_n} (1 - \mu_n)^{1 - y_n}$$

Negative log-likelihood

$$\mathsf{NLL}(oldsymbol{w}) = -\log p(oldsymbol{y}|oldsymbol{\mathsf{X}},oldsymbol{w}) = -\sum_{n=1}^N (y_n\log \mu_n + (1-y_n)\log(1-\mu_n))$$

• Plugging in $\mu_n = \frac{\exp(\mathbf{w}^\top \mathbf{x}_n)}{1+\exp(\mathbf{w}^\top \mathbf{x}_n)}$ and chugging, we get (verify yourself)

$$\left| \mathsf{NLL}(\boldsymbol{w}) = -\sum_{n=1}^{N} (y_n \boldsymbol{w}^{\top} \boldsymbol{x}_n - \log(1 + \exp(\boldsymbol{w}^{\top} \boldsymbol{x}_n))) \right|$$

• Each label y_n is binary with probability $\mu_n = \frac{\exp(\mathbf{w}^{\top} \mathbf{x}_n)}{1 + \exp(\mathbf{w}^{\top} \mathbf{x}_n)}$. Since the likelihood is Bernoulli:

$$p(\boldsymbol{y}|\boldsymbol{X},\boldsymbol{w}) = \prod_{n=1}^{N} p(y_n|\boldsymbol{x}_n,\boldsymbol{w}) = \prod_{n=1}^{N} \mu_n^{y_n} (1 - \mu_n)^{1 - y_n}$$

Negative log-likelihood

$$\mathsf{NLL}(oldsymbol{w}) = -\log p(oldsymbol{y}|oldsymbol{\mathsf{X}},oldsymbol{w}) = -\sum_{n=1}^N (y_n\log \mu_n + (1-y_n)\log(1-\mu_n))$$

• Plugging in $\mu_n = \frac{\exp(\mathbf{w}^{\top}\mathbf{x}_n)}{1+\exp(\mathbf{w}^{\top}\mathbf{x}_n)}$ and chugging, we get (verify yourself)

• MLE solution: $\mathbf{w}_{MLE} = \arg\min_{\mathbf{w}} \text{NLL}(\mathbf{w})$



• Each label y_n is binary with probability $\mu_n = \frac{\exp(\mathbf{w}^{\top} \mathbf{x}_n)}{1 + \exp(\mathbf{w}^{\top} \mathbf{x}_n)}$. Since the likelihood is Bernoulli:

$$p(y|X, w) = \prod_{n=1}^{N} p(y_n|x_n, w) = \prod_{n=1}^{N} \mu_n^{y_n} (1 - \mu_n)^{1-y_n}$$

Negative log-likelihood

$$\mathsf{NLL}(oldsymbol{w}) = -\log p(oldsymbol{y}|oldsymbol{\mathsf{X}},oldsymbol{w}) = -\sum_{n=1}^N (y_n\log \mu_n + (1-y_n)\log(1-\mu_n))$$

• Plugging in $\mu_n = \frac{\exp(\mathbf{w}^{\top}\mathbf{x}_n)}{1+\exp(\mathbf{w}^{\top}\mathbf{x}_n)}$ and chugging, we get (verify yourself)

$$oxed{\mathsf{NLL}(oldsymbol{w}) = -\sum_{n=1}^{N} (y_n oldsymbol{w}^ op oldsymbol{x}_n - \log(1 + \exp(oldsymbol{w}^ op oldsymbol{x}_n)))}$$

- MLE solution: $\mathbf{w}_{MLE} = \arg \min_{\mathbf{w}} \text{NLL}(\mathbf{w})$
- Important note: NLL(w) is convex in w, so global minima can be found



• We have $NLL(w) = -\sum_{n=1}^{N} (y_n w^{\top} x_n - \log(1 + \exp(w^{\top} x_n)))$

- We have $NLL(w) = -\sum_{n=1}^{N} (y_n w^\top x_n \log(1 + \exp(w^\top x_n)))$
- Taking the derivative of NLL(w) w.r.t. w

$$\frac{\partial \text{NLL}(\boldsymbol{w})}{\partial \boldsymbol{w}} = \frac{\partial}{\partial \boldsymbol{w}} \left[-\sum_{n=1}^{N} (y_n \boldsymbol{w}^{\top} \boldsymbol{x}_n - \log(1 + \exp(\boldsymbol{w}^{\top} \boldsymbol{x}_n))) \right]$$

$$= -\sum_{n=1}^{N} \left(y_n \boldsymbol{x}_n - \frac{\exp(\boldsymbol{w}^{\top} \boldsymbol{x}_n)}{(1 + \exp(\boldsymbol{w}^{\top} \boldsymbol{x}_n))} \boldsymbol{x}_n \right)$$

- We have $NLL(w) = -\sum_{n=1}^{N} (y_n w^\top x_n \log(1 + \exp(w^\top x_n)))$
- Taking the derivative of NLL(w) w.r.t. w

$$\frac{\partial \text{NLL}(\boldsymbol{w})}{\partial \boldsymbol{w}} = \frac{\partial}{\partial \boldsymbol{w}} \left[-\sum_{n=1}^{N} (y_n \boldsymbol{w}^{\top} \boldsymbol{x}_n - \log(1 + \exp(\boldsymbol{w}^{\top} \boldsymbol{x}_n))) \right]$$

$$= -\sum_{n=1}^{N} \left(y_n \boldsymbol{x}_n - \frac{\exp(\boldsymbol{w}^{\top} \boldsymbol{x}_n)}{(1 + \exp(\boldsymbol{w}^{\top} \boldsymbol{x}_n))} \boldsymbol{x}_n \right)$$

ullet Can't get a closed form estimate for $oldsymbol{w}$ by setting the derivative to zero

- We have $\text{NLL}(\boldsymbol{w}) = -\sum_{n=1}^{N} (y_n \boldsymbol{w}^{\top} \boldsymbol{x}_n \log(1 + \exp(\boldsymbol{w}^{\top} \boldsymbol{x}_n)))$
- Taking the derivative of NLL(w) w.r.t. w

$$\frac{\partial \text{NLL}(\boldsymbol{w})}{\partial \boldsymbol{w}} = \frac{\partial}{\partial \boldsymbol{w}} \left[-\sum_{n=1}^{N} (y_n \boldsymbol{w}^{\top} \boldsymbol{x}_n - \log(1 + \exp(\boldsymbol{w}^{\top} \boldsymbol{x}_n))) \right]$$

$$= -\sum_{n=1}^{N} \left(y_n \boldsymbol{x}_n - \frac{\exp(\boldsymbol{w}^{\top} \boldsymbol{x}_n)}{(1 + \exp(\boldsymbol{w}^{\top} \boldsymbol{x}_n))} \boldsymbol{x}_n \right)$$

- ullet Can't get a closed form estimate for $oldsymbol{w}$ by setting the derivative to zero
- One solution: Iterative minimization via gradient descent $\mathbf{w}_{t+1} = \mathbf{w}_t \eta_t \mathbf{g}_t$. The gradient is:

$$\mathbf{g} = \frac{\partial \mathsf{NLL}(\boldsymbol{w})}{\partial \boldsymbol{w}} = -\sum_{n=1}^{N} (y_n - \mu_n) \mathbf{x}_n = \mathbf{X}^{\top} (\boldsymbol{\mu} - \boldsymbol{y})$$



- We have $NLL(\boldsymbol{w}) = -\sum_{n=1}^{N} (y_n \boldsymbol{w}^{\top} \boldsymbol{x}_n \log(1 + \exp(\boldsymbol{w}^{\top} \boldsymbol{x}_n)))$
- Taking the derivative of NLL(w) w.r.t. w

$$\frac{\partial \text{NLL}(\boldsymbol{w})}{\partial \boldsymbol{w}} = \frac{\partial}{\partial \boldsymbol{w}} \left[-\sum_{n=1}^{N} (y_n \boldsymbol{w}^{\top} \boldsymbol{x}_n - \log(1 + \exp(\boldsymbol{w}^{\top} \boldsymbol{x}_n))) \right]$$

$$= -\sum_{n=1}^{N} \left(y_n \boldsymbol{x}_n - \frac{\exp(\boldsymbol{w}^{\top} \boldsymbol{x}_n)}{(1 + \exp(\boldsymbol{w}^{\top} \boldsymbol{x}_n))} \boldsymbol{x}_n \right)$$

- ullet Can't get a closed form estimate for $oldsymbol{w}$ by setting the derivative to zero
- One solution: Iterative minimization via gradient descent $\mathbf{w}_{t+1} = \mathbf{w}_t \eta_t \mathbf{g}_t$. The gradient is:

$$\mathbf{g} = \frac{\partial \mathsf{NLL}(\boldsymbol{w})}{\partial \boldsymbol{w}} = -\sum_{n=1}^{N} (y_n - \mu_n) \boldsymbol{x}_n = \boldsymbol{\mathsf{X}}^{\top} (\boldsymbol{\mu} - \boldsymbol{y})$$

• A large error on $x_n \Rightarrow (y_n - \mu_n)$ will be large \Rightarrow large contribution of x_n to the gradient



- We have $NLL(\boldsymbol{w}) = -\sum_{n=1}^{N} (y_n \boldsymbol{w}^{\top} \boldsymbol{x}_n \log(1 + \exp(\boldsymbol{w}^{\top} \boldsymbol{x}_n)))$
- Taking the derivative of NLL(w) w.r.t. w

$$\frac{\partial \text{NLL}(\boldsymbol{w})}{\partial \boldsymbol{w}} = \frac{\partial}{\partial \boldsymbol{w}} \left[-\sum_{n=1}^{N} (y_n \boldsymbol{w}^{\top} \boldsymbol{x}_n - \log(1 + \exp(\boldsymbol{w}^{\top} \boldsymbol{x}_n))) \right]$$

$$= -\sum_{n=1}^{N} \left(y_n \boldsymbol{x}_n - \frac{\exp(\boldsymbol{w}^{\top} \boldsymbol{x}_n)}{(1 + \exp(\boldsymbol{w}^{\top} \boldsymbol{x}_n))} \boldsymbol{x}_n \right)$$

- ullet Can't get a closed form estimate for $oldsymbol{w}$ by setting the derivative to zero
- One solution: Iterative minimization via gradient descent $\mathbf{w}_{t+1} = \mathbf{w}_t \eta_t \mathbf{g}_t$. The gradient is:

$$g = \frac{\partial \mathsf{NLL}(\boldsymbol{w})}{\partial \boldsymbol{w}} = -\sum_{n=1}^{N} (y_n - \mu_n) \boldsymbol{x}_n = \boldsymbol{\mathsf{X}}^{\top} (\boldsymbol{\mu} - \boldsymbol{y})$$

- A large error on $\mathbf{x}_n \Rightarrow (y_n \mu_n)$ will be large \Rightarrow large contribution of \mathbf{x}_n to the gradient
- More sophisticated methods (e.g., Newton's method) can also be used (I'll provide a note)



MAP Estimation for Logisic Regression

- MLE estimate of w can lead to overfitting. Solution: use a prior p(w) on w
- ullet Just like the linear regression case, let's put a Gausian prior on $oldsymbol{w}$

$$p(\mathbf{w}) = \mathcal{N}(0, \lambda^{-1} \mathbf{I}_D) \propto \exp(-\frac{\lambda}{2} \mathbf{w}^{\top} \mathbf{w})$$

MAP Estimation for Logisic Regression

- MLE estimate of w can lead to overfitting. Solution: use a prior p(w) on w
- ullet Just like the linear regression case, let's put a Gausian prior on $oldsymbol{w}$

$$p(\mathbf{w}) = \mathcal{N}(0, \lambda^{-1} \mathbf{I}_D) \propto \exp(-\frac{\lambda}{2} \mathbf{w}^{\top} \mathbf{w})$$

- MAP objective (log of posterior) = MLE objective + $\log p(w)$
- Leads to the objective (negative of log posterior, ignoring constants):

$$\mathsf{NLL}(\boldsymbol{w}) + \frac{\lambda}{2} \boldsymbol{w}^{\top} \boldsymbol{w}$$

MAP Estimation for Logisic Regression

- MLE estimate of w can lead to overfitting. Solution: use a prior p(w) on w
- ullet Just like the linear regression case, let's put a Gausian prior on $oldsymbol{w}$

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{0}, \lambda^{-1} \mathbf{I}_D) \propto \exp(-\frac{\lambda}{2} \mathbf{w}^{\top} \mathbf{w})$$

- MAP objective (log of posterior) = MLE objective + $\log p(w)$
- Leads to the objective (negative of log posterior, ignoring constants):

$$\mathsf{NLL}(\boldsymbol{w}) + \frac{\lambda}{2} \boldsymbol{w}^{\top} \boldsymbol{w}$$

ullet Estimation of $oldsymbol{w}_{MAP}$ proceeds the same way as MLE using gradient based methods, with

Gradient:
$$\mathbf{g} = \mathbf{X}^{\top}(\boldsymbol{\mu} - \mathbf{y}) + \lambda \mathbf{w}$$



Doing fully Bayesian inference would require computing the posterior

$$p(\mathbf{w}|\mathbf{X},\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{X},\mathbf{w})p(\mathbf{w})}{\int p(\mathbf{y}|\mathbf{X},\mathbf{w})p(\mathbf{w})d\mathbf{w}}$$

Doing fully Bayesian inference would require computing the posterior

$$p(\mathbf{w}|\mathbf{X},\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{X},\mathbf{w})p(\mathbf{w})}{\int p(\mathbf{y}|\mathbf{X},\mathbf{w})p(\mathbf{w})d\mathbf{w}} = \frac{\prod_{n=1}^{N} p(y_n|\mathbf{x}_n,\mathbf{w})p(\mathbf{w})}{\int \prod_{n=1}^{N} p(y_n|\mathbf{x}_n,\mathbf{w})p(\mathbf{w})d\mathbf{w}}$$

• Intractable. Reason: likelihood (logistic-Bernoulli) and prior (Gaussian) here are not conjugate

Doing fully Bayesian inference would require computing the posterior

$$p(\mathbf{w}|\mathbf{X},\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{X},\mathbf{w})p(\mathbf{w})}{\int p(\mathbf{y}|\mathbf{X},\mathbf{w})p(\mathbf{w})d\mathbf{w}} = \frac{\prod_{n=1}^{N} p(y_n|\mathbf{x}_n,\mathbf{w})p(\mathbf{w})}{\int \prod_{n=1}^{N} p(y_n|\mathbf{x}_n,\mathbf{w})p(\mathbf{w})d\mathbf{w}}$$

- Intractable. Reason: likelihood (logistic-Bernoulli) and prior (Gaussian) here are not conjugate
- Need to do approximate inference in this case

Doing fully Bayesian inference would require computing the posterior

$$p(\mathbf{w}|\mathbf{X},\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{X},\mathbf{w})p(\mathbf{w})}{\int p(\mathbf{y}|\mathbf{X},\mathbf{w})p(\mathbf{w})d\mathbf{w}} = \frac{\prod_{n=1}^{N} p(y_n|\mathbf{x}_n,\mathbf{w})p(\mathbf{w})}{\int \prod_{n=1}^{N} p(y_n|\mathbf{x}_n,\mathbf{w})p(\mathbf{w})d\mathbf{w}}$$

- Intractable. Reason: likelihood (logistic-Bernoulli) and prior (Gaussian) here are not conjugate
- Need to do approximate inference in this case
- A crude approximation: Laplace approximation: Approximate a posterior by a Gaussian with mean $= \mathbf{w}_{MAP}$ and covariance = inverse hessian (hessian = second derivative of $\log p(\mathbf{w}|\mathbf{X}, \mathbf{y})$)

$$p(\mathbf{w}|\mathbf{X},\mathbf{y}) = \mathcal{N}(\mathbf{w}_{MAP},\mathbf{H}^{-1})$$



Doing fully Bayesian inference would require computing the posterior

$$\rho(\mathbf{w}|\mathbf{X},\mathbf{y}) = \frac{\rho(\mathbf{y}|\mathbf{X},\mathbf{w})\rho(\mathbf{w})}{\int \rho(\mathbf{y}|\mathbf{X},\mathbf{w})\rho(\mathbf{w})d\mathbf{w}} = \frac{\prod_{n=1}^{N} \rho(y_n|\mathbf{x}_n,\mathbf{w})\rho(\mathbf{w})}{\int \prod_{n=1}^{N} \rho(y_n|\mathbf{x}_n,\mathbf{w})\rho(\mathbf{w})d\mathbf{w}}$$

- Intractable. Reason: likelihood (logistic-Bernoulli) and prior (Gaussian) here are not conjugate
- Need to do approximate inference in this case
- A crude approximation: Laplace approximation: Approximate a posterior by a Gaussian with mean $= \mathbf{w}_{MAP}$ and covariance = inverse hessian (hessian = second derivative of $\log p(\mathbf{w}|\mathbf{X},\mathbf{y})$)

$$p(\mathbf{w}|\mathbf{X},\mathbf{y}) = \mathcal{N}(\mathbf{w}_{MAP},\mathbf{H}^{-1})$$



• Will look at Laplace and other approximate inference methods later during the semester



• When using MLE, the predictive distribution will be

$$p(y_* = 1 | \boldsymbol{x}_*, \boldsymbol{w}_{MLE}) = \sigma(\boldsymbol{w}_{MLE}^{\top} \boldsymbol{x}_*)$$

• When using MLE, the predictive distribution will be

$$p(y_* = 1 | \mathbf{x}_*, \mathbf{w}_{MLE}) = \sigma(\mathbf{w}_{MLE}^{\top} \mathbf{x}_*)$$

$$p(y_* | \mathbf{x}_*, \mathbf{w}_{MLE}) = \text{Bernoulli}(\sigma(\mathbf{w}_{MLE}^{\top} \mathbf{x}_*))$$

When using MLE, the predictive distribution will be

$$p(y_* = 1 | \mathbf{x}_*, \mathbf{w}_{MLE}) = \sigma(\mathbf{w}_{MLE}^{\top} \mathbf{x}_*)$$
$$p(y_* | \mathbf{x}_*, \mathbf{w}_{MLE}) = \text{Bernoulli}(\sigma(\mathbf{w}_{MLE}^{\top} \mathbf{x}_*))$$

• When using MAP, the predictive distribution will be

$$p(y_*|x_*, \boldsymbol{w}_{MAP}) = \text{Bernoulli}(\sigma(\boldsymbol{w}_{MAP}^{\top}x_*))$$

When using MLE, the predictive distribution will be

$$p(y_* = 1 | \mathbf{x}_*, \mathbf{w}_{MLE}) = \sigma(\mathbf{w}_{MLE}^{\top} \mathbf{x}_*)$$
$$p(y_* | \mathbf{x}_*, \mathbf{w}_{MLE}) = \text{Bernoulli}(\sigma(\mathbf{w}_{MLE}^{\top} \mathbf{x}_*))$$

• When using MAP, the predictive distribution will be

$$p(y_*|\mathbf{x}_*, \mathbf{w}_{MAP}) = \text{Bernoulli}(\sigma(\mathbf{w}_{MAP}^{\top}\mathbf{x}_*))$$

$$p(y_* = 1|\mathbf{x}_*, \mathbf{w}_{MAP}) = \sigma(\mathbf{w}_{MAP}^{\top}\mathbf{x}_*)$$

When using MLE, the predictive distribution will be

$$p(y_* = 1 | \mathbf{x}_*, \mathbf{w}_{MLE}) = \sigma(\mathbf{w}_{MLE}^{\top} \mathbf{x}_*)$$

$$p(y_* | \mathbf{x}_*, \mathbf{w}_{MLE}) = \text{Bernoulli}(\sigma(\mathbf{w}_{MLE}^{\top} \mathbf{x}_*))$$

• When using MAP, the predictive distribution will be

$$p(y_*|\mathbf{x}_*, \mathbf{w}_{MAP}) = \text{Bernoulli}(\sigma(\mathbf{w}_{MAP}^{\top}\mathbf{x}_*))$$

$$p(y_* = 1|\mathbf{x}_*, \mathbf{w}_{MAP}) = \sigma(\mathbf{w}_{MAP}^{\top}\mathbf{x}_*)$$

• When using Bayesian inference, the posterior predictive distribution, based on posterior averaging

$$p(y_* = 1 | \boldsymbol{x}_*, \boldsymbol{\mathsf{X}}, \boldsymbol{y}) = \int p(y_* = 1 | \boldsymbol{x}_*, \boldsymbol{w}) p(\boldsymbol{w} | \boldsymbol{\mathsf{X}}, \boldsymbol{y}) d\boldsymbol{w}$$

• When using MLE, the predictive distribution will be

$$p(y_* = 1 | \mathbf{x}_*, \mathbf{w}_{MLE}) = \sigma(\mathbf{w}_{MLE}^{\top} \mathbf{x}_*)$$

$$p(y_* | \mathbf{x}_*, \mathbf{w}_{MLE}) = \text{Bernoulli}(\sigma(\mathbf{w}_{MLE}^{\top} \mathbf{x}_*))$$

• When using MAP, the predictive distribution will be

$$p(y_*|\mathbf{x}_*, \mathbf{w}_{MAP}) = \text{Bernoulli}(\sigma(\mathbf{w}_{MAP}^{\top}\mathbf{x}_*))$$

$$p(y_* = 1|\mathbf{x}_*, \mathbf{w}_{MAP}) = \sigma(\mathbf{w}_{MAP}^{\top}\mathbf{x}_*)$$

• When using Bayesian inference, the posterior predictive distribution, based on posterior averaging

$$p(y_* = 1 | \boldsymbol{x}_*, \boldsymbol{\mathsf{X}}, \boldsymbol{y}) = \int p(y_* = 1 | \boldsymbol{x}_*, \boldsymbol{w}) p(\boldsymbol{w} | \boldsymbol{\mathsf{X}}, \boldsymbol{y}) d\boldsymbol{w} = \int \sigma(\boldsymbol{w}^\top \boldsymbol{x}_*) p(\boldsymbol{w} | \boldsymbol{\mathsf{X}}, \boldsymbol{y}) d\boldsymbol{w}$$

When using MLE, the predictive distribution will be

$$p(y_* = 1 | \mathbf{x}_*, \mathbf{w}_{MLE}) = \sigma(\mathbf{w}_{MLE}^{\top} \mathbf{x}_*)$$

$$p(y_* | \mathbf{x}_*, \mathbf{w}_{MLE}) = \text{Bernoulli}(\sigma(\mathbf{w}_{MLE}^{\top} \mathbf{x}_*))$$

• When using MAP, the predictive distribution will be

$$p(y_*|\mathbf{x}_*, \mathbf{w}_{MAP}) = \text{Bernoulli}(\sigma(\mathbf{w}_{MAP}^{\top}\mathbf{x}_*))$$

$$p(y_* = 1|\mathbf{x}_*, \mathbf{w}_{MAP}) = \sigma(\mathbf{w}_{MAP}^{\top}\mathbf{x}_*)$$

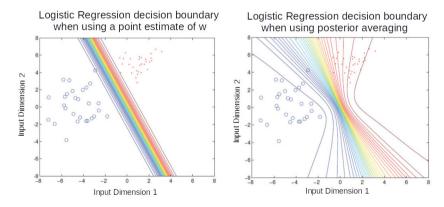
• When using Bayesian inference, the posterior predictive distribution, based on posterior averaging

$$p(y_* = 1 | \boldsymbol{x}_*, \boldsymbol{\mathsf{X}}, \boldsymbol{y}) = \int p(y_* = 1 | \boldsymbol{x}_*, \boldsymbol{w}) p(\boldsymbol{w} | \boldsymbol{\mathsf{X}}, \boldsymbol{y}) d\boldsymbol{w} = \int \sigma(\boldsymbol{w}^\top \boldsymbol{x}_*) p(\boldsymbol{w} | \boldsymbol{\mathsf{X}}, \boldsymbol{y}) d\boldsymbol{w}$$

• Note: Unlike the linear regression case, for logistic regression (and for non-conjugate models in general), posterior averaging can be intractable (and may require approximations)

Logistic Regression: Plug-in Prediction vs Bayesian Averaging

- (Left) Predictive distribution when using a point estimate uses only a single linear hyperplane w
- (Right) Posterior predictive distribution averages over many linear hyperplanes w



Multiclass Logistic (a.k.a. Softmax) Regression

• Also called multinoulli/multinomial regression: Basically, logistic regression for K > 2 classes

Multiclass Logistic (a.k.a. Softmax) Regression

- ullet Also called multinoulli/multinomial regression: Basically, logistic regression for K>2 classes
- In this case, $y_n \in \{1, 2, ..., K\}$ and label probabilities are defined as

$$p(y_n = k | \boldsymbol{x}_n, \boldsymbol{\mathsf{W}}) = \frac{\exp(\boldsymbol{w}_k^{\top} \boldsymbol{x}_n)}{\sum_{\ell=1}^K \exp(\boldsymbol{w}_{\ell}^{\top} \boldsymbol{x}_n)} = \mu_{nk}$$

- ullet Also called multinoulli/multinomial regression: Basically, logistic regression for K>2 classes
- In this case, $y_n \in \{1, 2, \dots, K\}$ and label probabilities are defined as

$$p(y_n = k | \boldsymbol{x}_n, \boldsymbol{\mathsf{W}}) = \frac{\exp(\boldsymbol{w}_k^\top \boldsymbol{x}_n)}{\sum_{\ell=1}^K \exp(\boldsymbol{w}_\ell^\top \boldsymbol{x}_n)} = \mu_{nk} \quad \text{and} \quad \sum_{\ell=1}^K \mu_{n\ell} = 1$$

- ullet Also called multinoulli/multinomial regression: Basically, logistic regression for K>2 classes
- In this case, $y_n \in \{1, 2, \dots, K\}$ and label probabilities are defined as

$$p(y_n = k | \boldsymbol{x}_n, \boldsymbol{\mathsf{W}}) = \frac{\exp(\boldsymbol{w}_k^\top \boldsymbol{x}_n)}{\sum_{\ell=1}^K \exp(\boldsymbol{w}_\ell^\top \boldsymbol{x}_n)} = \mu_{nk} \quad \text{and} \quad \sum_{\ell=1}^K \mu_{n\ell} = 1$$

• $\mathbf{W} = [\mathbf{w}_1 \ \mathbf{w}_2 \ \dots \ \mathbf{w}_K]$ is $D \times K$ weight matrix.

- ullet Also called multinoulli/multinomial regression: Basically, logistic regression for K>2 classes
- ullet In this case, $y_n \in \{1,2,\ldots,K\}$ and label probabilities are defined as

$$p(y_n = k | \boldsymbol{x}_n, \boldsymbol{\mathsf{W}}) = \frac{\exp(\boldsymbol{w}_k^\top \boldsymbol{x}_n)}{\sum_{\ell=1}^K \exp(\boldsymbol{w}_\ell^\top \boldsymbol{x}_n)} = \mu_{nk} \quad \text{and} \quad \sum_{\ell=1}^K \mu_{n\ell} = 1$$

• $\mathbf{W} = [\mathbf{w}_1 \ \mathbf{w}_2 \ \dots \ \mathbf{w}_K]$ is $D \times K$ weight matrix. $\mathbf{w}_1 = \mathbf{0}_{D \times 1}$ (assumed for identifiability)

- Also called multinoulli/multinomial regression: Basically, logistic regression for K > 2 classes
- ullet In this case, $y_n \in \{1,2,\ldots,K\}$ and label probabilities are defined as

$$p(y_n = k | \boldsymbol{x}_n, \boldsymbol{\mathsf{W}}) = \frac{\exp(\boldsymbol{w}_k^\top \boldsymbol{x}_n)}{\sum_{\ell=1}^K \exp(\boldsymbol{w}_\ell^\top \boldsymbol{x}_n)} = \mu_{nk} \quad \text{and} \quad \sum_{\ell=1}^K \mu_{n\ell} = 1$$

- $\mathbf{W} = [\mathbf{w}_1 \ \mathbf{w}_2 \ \dots \ \mathbf{w}_K]$ is $D \times K$ weight matrix. $\mathbf{w}_1 = \mathbf{0}_{D \times 1}$ (assumed for identifiability)
- Called softmax because.. ?

- ullet Also called multinoulli/multinomial regression: Basically, logistic regression for K>2 classes
- ullet In this case, $y_n \in \{1,2,\ldots,K\}$ and label probabilities are defined as

$$p(y_n = k | \boldsymbol{x}_n, \boldsymbol{\mathsf{W}}) = \frac{\exp(\boldsymbol{w}_k^\top \boldsymbol{x}_n)}{\sum_{\ell=1}^K \exp(\boldsymbol{w}_\ell^\top \boldsymbol{x}_n)} = \mu_{nk} \quad \text{and} \quad \sum_{\ell=1}^K \mu_{n\ell} = 1$$

- $\mathbf{W} = [\mathbf{w}_1 \ \mathbf{w}_2 \ \dots \ \mathbf{w}_K]$ is $D \times K$ weight matrix. $\mathbf{w}_1 = \mathbf{0}_{D \times 1}$ (assumed for identifiability)
- Called softmax because.. ?
- Each likelihood $p(y_n|\mathbf{x}_n,\mathbf{W})$ is a multinoulli. Therefore

$$p(\mathbf{y}|\mathbf{X},\mathbf{W}) = \prod_{n=1}^{N} \prod_{\ell=1}^{K} \mu_{n\ell}^{y_{n\ell}}$$

- Also called multinoulli/multinomial regression: Basically, logistic regression for K > 2 classes
- ullet In this case, $y_n \in \{1,2,\ldots,K\}$ and label probabilities are defined as

$$p(y_n = k | \boldsymbol{x}_n, \boldsymbol{\mathsf{W}}) = \frac{\exp(\boldsymbol{w}_k^\top \boldsymbol{x}_n)}{\sum_{\ell=1}^K \exp(\boldsymbol{w}_\ell^\top \boldsymbol{x}_n)} = \mu_{nk} \quad \text{and} \quad \sum_{\ell=1}^K \mu_{n\ell} = 1$$

- $\mathbf{W} = [\mathbf{w}_1 \ \mathbf{w}_2 \ \dots \ \mathbf{w}_K]$ is $D \times K$ weight matrix. $\mathbf{w}_1 = \mathbf{0}_{D \times 1}$ (assumed for identifiability)
- Called softmax because.. ?
- Each likelihood $p(y_n|\mathbf{x}_n,\mathbf{W})$ is a multinoulli. Therefore

$$p(\mathbf{y}|\mathbf{X},\mathbf{W}) = \prod_{n=1}^{N} \prod_{\ell=1}^{K} \mu_{n\ell}^{\mathbf{y}_{n\ell}}$$

where $y_{n\ell}=1$ if true class of example n is ℓ and $y_{n\ell'}=0$ for all other $\ell'\neq\ell$



- Also called multinoulli/multinomial regression: Basically, logistic regression for K > 2 classes
- In this case, $y_n \in \{1, 2, \dots, K\}$ and label probabilities are defined as

$$p(y_n = k | \mathbf{x}_n, \mathbf{W}) = \frac{\exp(\mathbf{w}_k^{ op} \mathbf{x}_n)}{\sum_{\ell=1}^K \exp(\mathbf{w}_\ell^{ op} \mathbf{x}_n)} = \mu_{nk} \quad \text{and} \quad \sum_{\ell=1}^K \mu_{n\ell} = 1$$

- $\mathbf{W} = [\mathbf{w}_1 \ \mathbf{w}_2 \ \dots \ \mathbf{w}_K]$ is $D \times K$ weight matrix. $\mathbf{w}_1 = \mathbf{0}_{D \times 1}$ (assumed for identifiability)
- Called softmax because.. ?
- Each likelihood $p(y_n|\mathbf{x}_n,\mathbf{W})$ is a multinoulli. Therefore

$$p(\mathbf{y}|\mathbf{X},\mathbf{W}) = \prod_{n=1}^{N} \prod_{\ell=1}^{K} \mu_{n\ell}^{y_{n\ell}}$$

where $y_{n\ell}=1$ if true class of example n is ℓ and $y_{n\ell'}=0$ for all other $\ell'\neq\ell$

• Can do MLE/MAP/fully Bayesian estimation for W similar to the logistic regression model



- Also called multinoulli/multinomial regression: Basically, logistic regression for K > 2 classes
- In this case, $y_n \in \{1, 2, \dots, K\}$ and label probabilities are defined as

$$p(y_n = k | \boldsymbol{x}_n, \boldsymbol{\mathsf{W}}) = \frac{\exp(\boldsymbol{w}_k^\top \boldsymbol{x}_n)}{\sum_{\ell=1}^K \exp(\boldsymbol{w}_\ell^\top \boldsymbol{x}_n)} = \mu_{nk} \quad \text{and} \quad \sum_{\ell=1}^K \mu_{n\ell} = 1$$

- $\mathbf{W} = [\mathbf{w}_1 \ \mathbf{w}_2 \ \dots \ \mathbf{w}_K]$ is $D \times K$ weight matrix. $\mathbf{w}_1 = \mathbf{0}_{D \times 1}$ (assumed for identifiability)
- Called softmax because.. ?
- Each likelihood $p(y_n|\mathbf{x}_n,\mathbf{W})$ is a multinoulli. Therefore

$$p(\mathbf{y}|\mathbf{X},\mathbf{W}) = \prod_{n=1}^{N} \prod_{\ell=1}^{K} \mu_{n\ell}^{y_{n\ell}}$$

where $y_{n\ell}=1$ if true class of example n is ℓ and $y_{n\ell'}=0$ for all other $\ell'\neq\ell$

- Can do MLE/MAP/fully Bayesian estimation for W similar to the logistic regression model
- Doing MLE is like minimizing the cross-entropy loss: $-\sum_{n=1}^{N}\sum_{\ell=1}^{L}y_{n\ell}\log\mu_{n\ell}$



• Both logistic and softmax classification are discriminative model for linear classification

- Both logistic and softmax classification are discriminative model for linear classification
- These are special cases of the more general form of discriminative models for classification

$$p(y|x) = \text{Bernoulli}(f(x))$$
 OR $p(y|x) = \text{multinoulli}(f(x))$

- Both logistic and softmax classification are discriminative model for linear classification
- These are special cases of the more general form of discriminative models for classification

$$p(y|\mathbf{x}) = \text{Bernoulli}(f(\mathbf{x}))$$
 OR $p(y|\mathbf{x}) = \text{multinoulli}(f(\mathbf{x}))$

Logistic and softmax also belong to the class of "Generalized Linear Models" (GLM)

- Both logistic and softmax classification are discriminative model for linear classification
- These are special cases of the more general form of discriminative models for classification

$$p(y|x) = Bernoulli(f(x))$$
 OR $p(y|x) = multinoulli(f(x))$

- Logistic and softmax also belong to the class of "Generalized Linear Models" (GLM)
 - GLM can model outputs of various types, e.g., real, categorical, counts, positive reals, etc.

- Both logistic and softmax classification are discriminative model for linear classification
- These are special cases of the more general form of discriminative models for classification

$$p(y|x) = Bernoulli(f(x))$$
 OR $p(y|x) = multinoulli(f(x))$

- Logistic and softmax also belong to the class of "Generalized Linear Models" (GLM)
 - GLM can model outputs of various types, e.g., real, categorical, counts, positive reals, etc.
 - Will look at GLM when we discuss exponential families

- Both logistic and softmax classification are discriminative model for linear classification
- These are special cases of the more general form of discriminative models for classification

$$p(y|\mathbf{x}) = \text{Bernoulli}(f(\mathbf{x}))$$
 OR $p(y|\mathbf{x}) = \text{multinoulli}(f(\mathbf{x}))$

- Logistic and softmax also belong to the class of "Generalized Linear Models" (GLM)
 - GLM can model outputs of various types, e.g., real, categorical, counts, positive reals, etc.
 - Will look at GLM when we discuss exponential families
- Logistic/softmax can also be extended to handle nonlinear classification, e.g.,

- Both logistic and softmax classification are discriminative model for linear classification
- These are special cases of the more general form of discriminative models for classification

$$p(y|\mathbf{x}) = \text{Bernoulli}(f(\mathbf{x}))$$
 OR $p(y|\mathbf{x}) = \text{multinoulli}(f(\mathbf{x}))$

- Logistic and softmax also belong to the class of "Generalized Linear Models" (GLM)
 - GLM can model outputs of various types, e.g., real, categorical, counts, positive reals, etc.
 - Will look at GLM when we discuss exponential families
- Logistic/softmax can also be extended to handle nonlinear classification, e.g.,
 - Using a deep neural network + sigmoid/softmax to model f(x)

- Both logistic and softmax classification are discriminative model for linear classification
- These are special cases of the more general form of discriminative models for classification

$$p(y|x) = Bernoulli(f(x))$$
 OR $p(y|x) = multinoulli(f(x))$

- Logistic and softmax also belong to the class of "Generalized Linear Models" (GLM)
 - GLM can model outputs of various types, e.g., real, categorical, counts, positive reals, etc.
 - Will look at GLM when we discuss exponential families
- Logistic/softmax can also be extended to handle nonlinear classification, e.g.,
 - Using a deep neural network + sigmoid/softmax to model f(x)
 - Using Gaussian Processes (GP) which are essentially Bayesian kernel methods

- Both logistic and softmax classification are discriminative model for linear classification
- These are special cases of the more general form of discriminative models for classification

$$p(y|\mathbf{x}) = \text{Bernoulli}(f(\mathbf{x}))$$
 OR $p(y|\mathbf{x}) = \text{multinoulli}(f(\mathbf{x}))$

- Logistic and softmax also belong to the class of "Generalized Linear Models" (GLM)
 - GLM can model outputs of various types, e.g., real, categorical, counts, positive reals, etc.
 - Will look at GLM when we discuss exponential families
- Logistic/softmax can also be extended to handle nonlinear classification, e.g.,
 - Using a deep neural network + sigmoid/softmax to model f(x)
 - Using Gaussian Processes (GP) which are essentially Bayesian kernel methods
 - We will look at such nonlinear classification models later..



• Number of parameters: Discriminative models have fewer parameters to be learned (e.g., just the weight vector/matrix **w/W** in case of logistic/softmax classification

- Number of parameters: Discriminative models have fewer parameters to be learned (e.g., just the weight vector/matrix \mathbf{w}/\mathbf{W} in case of logistic/softmax classification
- Ease of parameter estimation: Debatable as to which one is easier

- Number of parameters: Discriminative models have fewer parameters to be learned (e.g., just the weight vector/matrix \mathbf{w}/\mathbf{W} in case of logistic/softmax classification
- Ease of parameter estimation: Debatable as to which one is easier
 - For "simple" class-conditionals (e.g., naïve Bayes assumption, diagonal covariance for Gaussian p(x|y)), it is easier for generative classification model (often closed-form solution)

- Number of parameters: Discriminative models have fewer parameters to be learned (e.g., just the weight vector/matrix \mathbf{w}/\mathbf{W} in case of logistic/softmax classification
- Ease of parameter estimation: Debatable as to which one is easier
 - For "simple" class-conditionals (e.g., naïve Bayes assumption, diagonal covariance for Gaussian p(x|y)), it is easier for generative classification model (often closed-form solution)
 - Parameter estimation for discriminative models (logistic/softmax) usually requires iterative methods (although objective functions usually have global optima)

- Number of parameters: Discriminative models have fewer parameters to be learned (e.g., just the weight vector/matrix \mathbf{w}/\mathbf{W} in case of logistic/softmax classification
- Ease of parameter estimation: Debatable as to which one is easier
 - For "simple" class-conditionals (e.g., naïve Bayes assumption, diagonal covariance for Gaussian p(x|y)), it is easier for generative classification model (often closed-form solution)
 - Parameter estimation for discriminative models (logistic/softmax) usually requires iterative methods (although objective functions usually have global optima)
- Dealing with missing features in the inputs: Generative models can handle this easily (e.g., by integrating out the missing features while estimating the parameters)

- Number of parameters: Discriminative models have fewer parameters to be learned (e.g., just the weight vector/matrix \mathbf{w}/\mathbf{W} in case of logistic/softmax classification
- Ease of parameter estimation: Debatable as to which one is easier
 - For "simple" class-conditionals (e.g., naïve Bayes assumption, diagonal covariance for Gaussian p(x|y)), it is easier for generative classification model (often closed-form solution)
 - Parameter estimation for discriminative models (logistic/softmax) usually requires iterative methods (although objective functions usually have global optima)
- Dealing with missing features in the inputs: Generative models can handle this easily (e.g., by integrating out the missing features while estimating the parameters)
- Inputs with features having mixed types: Naturally handled by a generative model using an appropriate p(x|y) for each type of feature in the input. Difficult for discriminative models

• Leveraging <u>unlabeled data</u>: Generative models can handle this easily by treating the missing labels are latent variables and ideal for Semi-supervised Learning. Discriminative models can't do it easily

- Leveraging <u>unlabeled data</u>: Generative models can handle this easily by treating the missing labels are latent variables and ideal for <u>Semi-supervised Learning</u>. Discriminative models can't do it easily
- Adding data from <u>new classes</u>: Discriminative model will need to be re-trained. Generative model will just require estimating the class-conditionals of newly added classes

- Leveraging <u>unlabeled data</u>: Generative models can handle this easily by treating the missing labels are latent variables and ideal for Semi-supervised Learning. Discriminative models can't do it easily
- Adding data from <u>new classes</u>: Discriminative model will need to be re-trained. Generative model will just require estimating the class-conditionals of newly added classes
- Have lots of labeled data: Discriminative models usually work very well

- Leveraging <u>unlabeled data</u>: Generative models can handle this easily by treating the missing labels are latent variables and ideal for Semi-supervised Learning. Discriminative models can't do it easily
- Adding data from <u>new classes</u>: Discriminative model will need to be re-trained. Generative model will just require estimating the class-conditionals of newly added classes
- Have lots of labeled data: Discriminative models usually work very well
- Final Verdict? Despite generative classification having some clear advantages, both methods can be equally powerful (the actual choice may be dictated by the problem)

- Leveraging <u>unlabeled data</u>: Generative models can handle this easily by treating the missing labels are latent variables and ideal for Semi-supervised Learning. Discriminative models can't do it easily
- Adding data from <u>new classes</u>: Discriminative model will need to be re-trained. Generative model will just require estimating the class-conditionals of newly added classes
- Have lots of labeled data: Discriminative models usually work very well
- Final Verdict? Despite generative classification having some clear advantages, both methods can be equally powerful (the actual choice may be dictated by the problem)
 - Important to be aware of their strengths/weaknesses, and also the connections between these models

- Leveraging <u>unlabeled data</u>: Generative models can handle this easily by treating the missing labels are latent variables and ideal for Semi-supervised Learning. Discriminative models can't do it easily
- Adding data from <u>new classes</u>: Discriminative model will need to be re-trained. Generative model will just require estimating the class-conditionals of newly added classes
- Have lots of labeled data: Discriminative models usually work very well
- Final Verdict? Despite generative classification having some clear advantages, both methods can be equally powerful (the actual choice may be dictated by the problem)
 - Important to be aware of their strengths/weaknesses, and also the connections between these models
- Possibility of a <u>Hybrid Design</u>? Yes, Generative and Discriminative models also be <u>combined</u>, e.g.,

- Leveraging <u>unlabeled data</u>: Generative models can handle this easily by treating the missing labels are latent variables and ideal for Semi-supervised Learning. Discriminative models can't do it easily
- Adding data from <u>new classes</u>: Discriminative model will need to be re-trained. Generative model will just require estimating the class-conditionals of newly added classes
- Have <u>lots of labeled data</u>: Discriminative models usually work very well
- Final Verdict? Despite generative classification having some clear advantages, both methods can be equally powerful (the actual choice may be dictated by the problem)
 - Important to be aware of their strengths/weaknesses, and also the connections between these models
- Possibility of a <u>Hybrid Design</u>? Yes, Generative and Discriminative models also be <u>combined</u>, e.g.,
 - "Principled Hybrids of Generative and Discriminative Models" (Lassere et al, 2006)
 - "Deep Hybrid Models: Bridging Discriminative & Generative Approaches" (Kuleshov & Ermon, 2017)

