Supervised Learning

Linear Regression

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Objective

Objective

Define the set-up of Supervised Learning

Objective

Discuss basic regression models

Supervised Learning

- **The set-up: the given training data consist of <sample, label> pairs, or (x, y); the objective of learning is to figure out a way to predict label y for any new sample x.**

- **Consider two types of problems:**
  - **Regression**: y continuous
  - **Classification**: y is discrete, e.g., class labels.

The Task of Regression

- **Given: A training set of *n* samples <$x^{(i)}$, $y^{(i)}$ > where $y^{(i)}$ is a continuous "label" (or target value) for $x^{(i)}$**

- **To learn a model for predicting y for any new sample x.**

- **A simple model is linear regression: modeling the relation between y and x via a linear function.**

$$y \approx w_0 + w_1 x_1 + \ ... + w_d x_d = \mathbf{w}^t\mathbf{x}$$

(Note: **x** is *augmented* by adding a dimension of constant 1 to the original sample.)

Linear Regression

- We can introduce an error term to capture the residual $\mathbf{y} = \mathbf{w}^t\mathbf{x} + e$

- Applying this to all *n* samples, we have: $\mathbf{y} = \mathbf{X}\,\mathbf{w} + \mathbf{e}$

$$\begin{pmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(n)} \end{pmatrix} \qquad \begin{bmatrix} 1 & x_1^{(1)} & x_2^{(1)} & \cdots & x_d^{(1)} \\ 1 & x_1^{(2)} & x_2^{(2)} & \cdots & x_d^{(2)} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_1^{(n)} & x_2^{(n)} & \cdots & x_d^{(n)} \end{bmatrix} \qquad \begin{pmatrix} e^{(1)} \\ e^{(2)} \\ \vdots \\ e^{(n)} \end{pmatrix}$$

- *Learning* in this case is to figure out a good w.

Linear Regression (cont'd)

- Find an optimal w by minimizing the squared error

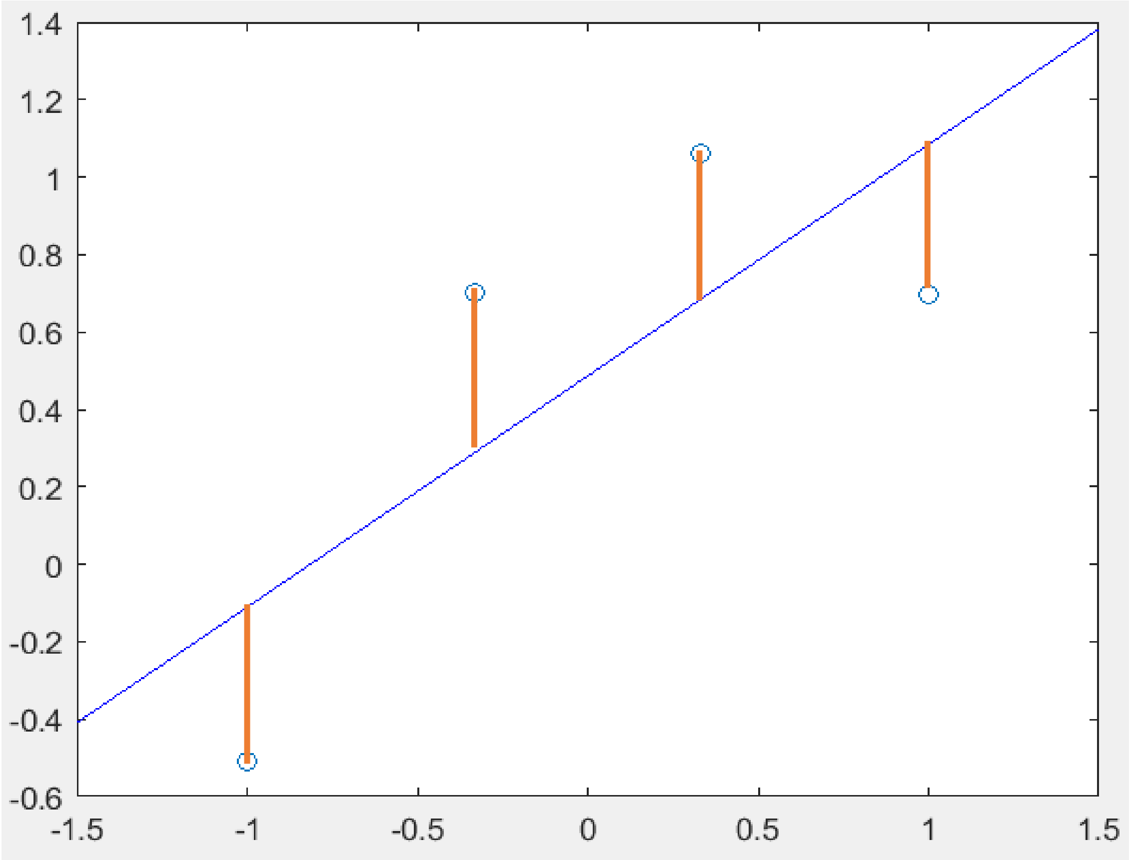
$$||\mathrm{e}||^2 = ||\mathrm{y} - X\,\mathrm{w}||^2$$

- The solution can be found to be:

$$\hat{\mathrm{w}} = (X^t X)^{-1} X^t \mathrm{y}$$

- In practice, some iterative approaches may be used (e.g., gradient descent search).

A simple example



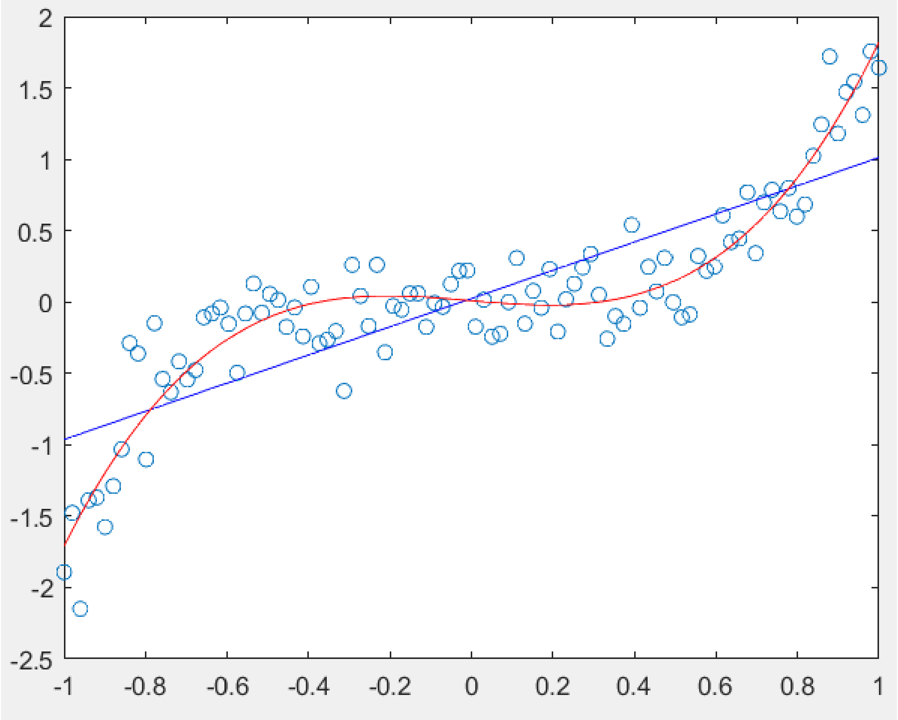
Generalizing Linear Regression

Introducing some basis functions $\phi_j(\mathbf{x})$:

$$y = w_0 + w_1\phi_1(\mathbf{x}) + \ \ldots + w_{M-1}\phi_{M-1}(\mathbf{x})$$

Compare:

- Blue: Linear Regression
- Red: With $\phi_j(x) = x^j$



Regularized Least Squares

- **E.g., use a new error function:** $E_D(\boldsymbol{w}) + \lambda E_W(\boldsymbol{w})$
  - λ is the regularization coefficient
  - $E_D(\mathbf{w})$ is the data-dependent error
  - $E_{\mathbf{W}}(\mathbf{w})$ is the $regularization\ term$, e.g., $\boldsymbol{E}_{\mathbf{W}}(\mathrm{w}) = ||\mathbf{w}||^{\boldsymbol{q}}$

- **Help to alleviate overfitting.**

Supervised Learning

Density Estimation in Supervised Learning

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Objective

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Illustrate classification in Supervised Learning

Objective

Discuss basic density estimation techniques

Supervised Learning

- **The set-up: the given training data consist of <sample, label> pairs, or (x, y); the objective of learning is to figure out a way to predict label y for any new sample x.**

- **Consider two types of problems:**
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  - **Classification**: y is discrete, e.g., class labels.

Examples of Image Classification

- The MNIST training images of hand-written digits

- The Extended Yale B Face Images

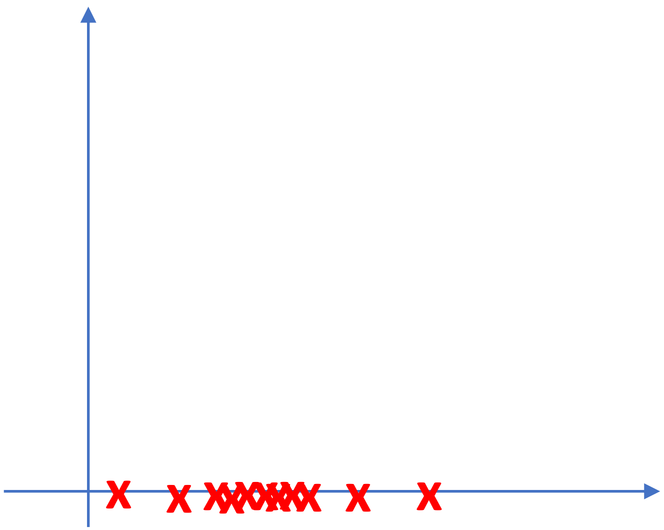
How do we model the training images?

- **Parametric: each class of images (the feature vectors) may be modeled by a density function $p_{\boldsymbol{\theta}}(x)$ with parameter $\boldsymbol{\theta}$.**
  - To emphasize the density is for images from class/label *y*, we may write $p_{\boldsymbol{\theta}}(\mathbf{x}|y)$.
  - We may also use the notation $p(\mathbf{x}|\boldsymbol{\theta})$, if the discussion is true for any y.

  ➔ How to estimate $\boldsymbol{\theta}$ from the training images?

- **Note: We may also consider non-parametric approaches.**

MLE for Density Estimation (1/3)



- **Given some training data; Assuming a parametric model *p*(x|θ); What specific θ will fit/explain the data best?**
  - E.g., Consider a simple 1-D normal density with only a parameter μ (assuming the variance is known)
- **Given a sample x_i, $p(x_i \mid \mu)$ gives an indication of how likely x_i is from $p(x_i \mid \mu)$**

➔the concept of the likelihood function.

MLE for Density Estimation (2/3)

- **The likelihood function: the density function $p(\mathrm{x}|\theta)$ evaluated at the given data sample x_i, and viewed as a function of the parameter θ.**
  - Assessing how likely the parameter $\boldsymbol{\theta}$ (defining the corresponding $p(\mathbf{x}|\boldsymbol{\theta})$) gives arise to the sample $\mathbf{x}_i$.
  - We often use $L(\boldsymbol{\theta})$ to denote the likelihood function, and $l(\boldsymbol{\theta}) = \log(L(\boldsymbol{\theta}))$ is called the log-likelihood.
- **Maximum Likelihood Estimation (MLE): Finding the parameter that maximizes the likelihood function**

$$\widehat{\boldsymbol{\theta}} = \mathrm{argmax}_{\boldsymbol{\theta}}\, p(\mathbf{x}|\boldsymbol{\theta})$$

MLE for Density Estimation (3/3)

- How to consider *all* the given samples $D=\{x_i, i=1,\ldots,n\}$?

- The concept of i.i.d. samples: the samples are assumed to be *independent* and *identically distributed*

- So, the data likelihood is given by

$$L(\boldsymbol{\theta}) = P(D|\boldsymbol{\theta}) =$$

MLE Example 1

- **Tossing a coin for *n* times, observing n_1 times for head.**
  - Estimate the probability θ for head
- **The likelihood function is:**

$$L(\theta) = P(D|\theta) = \theta^{n_1}(1-\theta)^{n-n_1}$$

MLE Example 1 (cont'd)

- We want to find what θ maximizes this likelihood, or equivalently, the log-likelihood

$$l(\theta) = \log P(D|\theta) = \log(\theta^{n_1}(1-\theta)^{n-n_1})$$
$$= \cdots$$

- Take the derivative and set to 0:

$$\frac{d}{d\theta} l(\theta) = 0$$

- This will give us:

$$\hat{\theta} = \frac{n_1}{n}$$

MLE Example 2

- **Given n i.i.d. samples $\{x_i\}$ from the 1-D normal distribution $N(\mu, \sigma^2)$, find the MLE for μ and σ^2**

- **The likelihood function is:**

$$L(\mu,\sigma) = p(D|\mu,\sigma) = \left(\frac{1}{\sigma\sqrt{2\pi}}\right)^n \prod_{i=1}^{n} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

- **The log-likelihood is:**

$$\begin{aligned} l(\mu,\sigma) &= \log P(D|\mu,\sigma) \\ &= \log\left(\left(\frac{1}{\sigma\sqrt{2\pi}}\right)^n \prod_{i=1}^{n} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}\right) \\ &= -n\log\left(\sigma\sqrt{2\pi}\right) - \sum_{i=1}^{n} \frac{(x_i-\mu)^2}{2\sigma^2} \end{aligned}$$

MLE Example 2 (cont'd)

- **The MLE solution for μ**

$$\hat{\mu} = \text{argmax}_{\mu} l(\mu, \sigma)$$
$$= \text{argmax}_{\mu}\{-n \log\left(\sigma\sqrt{2\pi}\right) - \sum_{i=1}^{n} \frac{(x_i - \mu)^2}{2\sigma^2}\}$$

- **Set the derivative to 0:**

$$\frac{\partial}{\partial \mu} l(\mu, \sigma) = 0$$

- **The solution is:**

$$\hat{\mu} = \frac{\sum_{i=1}^{n} x_i}{n}$$

MLE Example 2 (cont'd)

- The MLE solution for μ

$$\hat{\sigma} = \text{argmax}_{\sigma} l(\mu, \sigma)$$
$$= \text{argmax}_{\sigma}\{-n \log\left(\sigma\sqrt{2\pi}\right) - \sum_{i=1}^{n} \frac{(x_i - \mu)^2}{2\sigma^2}\}$$

- Set the derivative to 0:

$$\frac{\partial}{\partial\sigma} l(\mu, \sigma) = 0$$

- The solution is:

$$\widehat{\sigma^2} = \frac{\sum_{i=1}^{n}(x_i - \mu)^2}{n}$$

Supervised Learning

Generative vs Discriminative Models in Supervised Learning

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Objective

Objective

Differentiate between generative and discriminative models of supervised learning

Objective

Discuss challenges in Bayesian learning

Supervised Learning

- **The set-up: the given training data consist of <sample, label> pairs, or (x, y); the objective of learning is to figure out a way to predict label y for any new sample x.**
  - E.g., Given n pairs <$\mathbf{x}^{(i)}$, $y^{(i)}$ >, i=1, …, n; $\mathbf{x}^{(i)}$: i-th sample represented as d-dimensional vectors; $y^{(i)}$: corresponding labels.
- **Equivalently, to find $P(y|x)$**

Two Types of Models

Generative Model

- $P(y|x) \propto P(y)\, p(x|y)$'
- ➔ To learn $P(y)$ and $p(x|y)$.

Discriminative Model

- Directly learn $P(y|x)$
- No assumption made on $p(x|y)$

Two Types of Models

Generative Model

- $P(y|x) \propto P(y)\, p(x|y)$’
- ➔ To learn $P(y)$ and $p(x|y)$.
- ➔ Bayesian learning, Bayes classifiers.
- Example: Naïve Bayes Classifier

Discriminative Model

- Directly learn $P(y|x)$
- No assumption made on $p(x|y)$
- Example: Logistic Regression

Practical Difficulty of Bayesian Learning

Consider doing Bayesian learning without making simplifying assumptions.

- Given n training pairs <$\mathbf{x}^{(i)}$, $y^{(i)}$ >, i=1, …, n. Each $\mathbf{x}^{(i)}$ is d-dimensional.
- We need to learn $P(y)$ and $p(\mathbf{x}|y)$

➔ $p(\mathbf{x}|y)$ can be very difficult to estimate:

➔ Consider a very simple case: binary features, and y is also binary. How many probabilities do we need to estimate?

Supervised Learning

Naïve Bayes Classifier

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Objective

Objective

Implement the fundamental learning algorithm Naive Bayes

Naïve Bayesian Classifier

- **The "naive" *conditional independence* assumption: each feature is (conditionally) independent of every other feature, given the label, i.e., $p(x_i | \{x_j \text{ for any } j \neq i\}, y) = p(x_i | y)$**

- **How does this assumption simplify the problem?**
  - Consider the previous example again: d-dimensional binary features, and y is also binary.
  - How many probabilities do we need to estimate now?

$$p(\mathbf{x} | y) = p(x_1, x_2, \ldots, x_d | y) = \ldots$$

Naïve Bayesian Classifier (cont'd)

- The naïve Bayes classifier: the predicted label is given by

$$\hat{y} = \operatorname*{argmax}_{y} P(y) \prod_{i=1}^{d} p(x_i|y)$$

- "Parameters" of the classifier:
  - $P(y)$
  - $p(x_i|y)$ for all i, y

Naïve Bayesian Classifier (cont'd)

- **E.g., estimating the "parameters" of the classifier**
  - $P(y)$ & $p(x_i|y)$ for all i, y -

for the following familiar example

Discrete Feature Example

- $x = <x_1, x_2, \ldots, x_d>$ where each x_i can take only a finite number of values from $\{v_1, v_2, \ldots, v_m\}$:
- In this case, the "parameters" of the classifier are
  - $P(y)$
  - $P(x_i = v_k | y)$, for all i, k, and y
- Given: A training set of n labelled samples $<x^{(i)}, y^{(i)}>$, $i=1, \ldots, n$

  ➔ How to estimate the model parameters?

Discrete Feature Example (cont'd)

Given: A training set of *n* labelled samples <$x^{(i)}$, $y^{(i)}$ >, *i*=1, …, *n*

➔ How to estimate the model parameters?

$P(y) =$

$P(x_i = v_k | y) =$

These are in fact the MLE solutions for the corresponding parameters.

Supervised Learning

Logistic Regression

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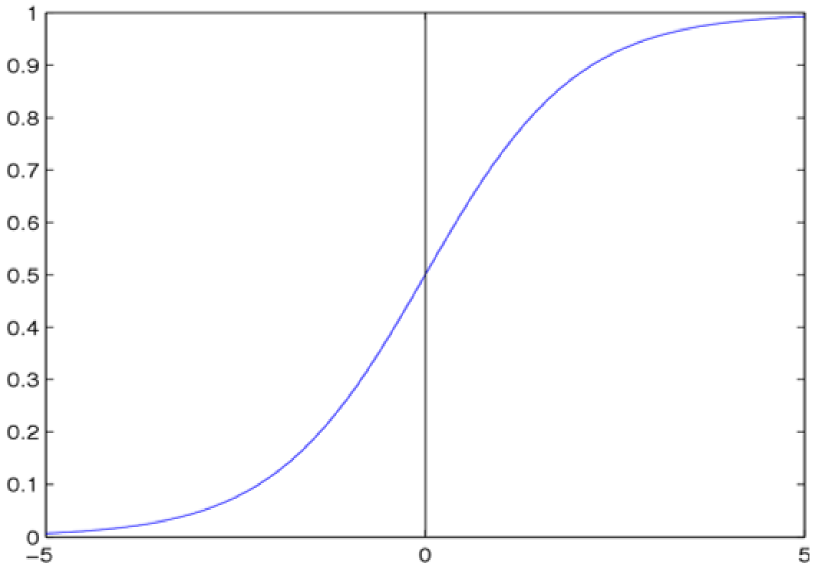
Implement the fundamental learning algorithm Logistic Regression

Discriminative Model: Example

- **Again, we are given a training set of *n* labelled samples <$x^{(i)}$, $y^{(i)}$ >**
- **Why not directly model/learn *P*(y|x)?**
  - Discriminative model
- **Further assume *P*(y|x) takes the form of a logistic sigmoid function**

→ Logistic Regression



Logistic Regression

- **Logistic regression: use the logistic function for modeling *P*(y|x), considering only the case of y $\in \{0,1\}$**

$$P(y=0|\mathbf{x}) = \frac{1}{1+\exp\left(w_0 + \sum_{i=1}^{d} w_i x_i\right)}$$

$$P(y=1|\mathbf{x}) = \frac{\exp\left(w_0 + \sum_{i=1}^{d} w_i x_i\right)}{1+\exp\left(w_0 + \sum_{i=1}^{d} w_i x_i\right)}$$

- **The *logistic function***

$$\sigma(t) = \frac{1}{1+e^{-t}} = \frac{e^t}{1+e^t}$$

Logistic Regression → Linear Classifier

Given a sample x, we classify it as 0 (i.e., predicting y=0) if

$$P(\mathrm{y}=0|\mathbf{x}) \geq P(\mathrm{y}=1|\mathbf{x})$$

➔ This is a linear classifier.

The Parameters of the Model

- What are the model parameters in logistic regression?
- Given a parameter w, we have P(y|x) =

$$[\sigma(w^t x)]^y [1-\sigma(w^t x)]^{1-y}$$

- Suppose we have two different sets of parameters, $w^{(1)}$ and $w^{(2)}$, whichever giving a larger P(y|x) should be a better parameter.

The Conditional Likelihood

- Given n training samples, $<x^{(i)}, y^{(i)}>$, $i=1,\dots,n$, how can we use them to estimate the parameters?

➔ For a given w, the probability of getting all those $y^{(1)}, y^{(2)} \dots, y^{(n)}$ from the corresponding data $x^{(i)}$, $i=1,\dots,n$, is

$$P[y^{(1)}, y^{(2)}, \dots, y^{(n)} \mid x^{(1)}, x^{(2)}, \dots, x^{(n)}; w] = \prod_{i=1}^{n} P(y^{(i)} \mid x^{(i)}; w)$$

$$= \prod_{i=1}^{n} \left[\sigma(w^t x^{(i)})\right]^{y^{(i)}} \left[1 - \sigma(w^t x^{(i)})\right]^{1-y^{(i)}}$$

➔ Call this L(w), the (conditional) likelihood.

The Conditional Log Likelihood

$$\ell(w) = \log \mathcal{L}(w) = \log \prod_{i=1}^{n} (\cdots)$$

$$= \sum_{i=1}^{n} \log \left[\sigma(w^t x^{(i)})^{y^{(i)}} (1 - \sigma(w^t x^{(i)}))^{1-y^{(i)}} \right]$$

$$= \sum_{i=1}^{n} \left[\log\left(\sigma(w^t x^{(i)})^{y^{(i)}}\right) + \log\left((1 - \sigma(w^t x^{(i)}))^{1-y^{(i)}}\right) \right]$$

Maximizing Conditional Log Likelihood

Optimal parameters

$$\mathbf{w}^* = \mathrm{argmax}_{\mathbf{w}} l(\mathbf{w})$$
$$= \mathrm{argmax}_{\mathbf{w}} \sum_{i=1}^{n} [y^{(i)} \mathbf{w}^t \mathbf{x}^{(i)} - \log\left(1 + \exp\left(\mathbf{w}^t \mathbf{x}^{(i)}\right)\right)]$$

We cannot really solve for w* analytically (no closed-form solution)

- We can use a commonly-used optimization technique, gradient descent/ascent, to find a solution.

Finding the Gradient of $l(w)$

Recall: $\frac{\partial (w^t x)}{\partial w} = x$, $\left(\frac{\partial \log f(x)}{\partial x} = \frac{1}{f(x)} \frac{\partial f(x)}{\partial x} \right.$

$\frac{\partial e^x}{\partial x} = e^x$

$$\nabla_w l(w) = \nabla_w \left[\sum_{i=1}^{n} \left(y^{(i)} w^t x^{(i)} - \log\left(1 + e^{w^t x^{(i)}}\right) \right) \right],$$

$$= \sum_{i=1}^{n} \left[y^{(i)} x^{(i)} - \frac{e^{w^t x^{(i)}} \cdot x^{(i)}}{1 + e^{w^t x^{(i)}}} \right]$$

(Setting this to 0 cannot really give us a closed-form solution for w.

So we will do gradient ascent.)

Gradient Ascent Algorithm

<u>The algorithm</u>

Iterate until converge

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} + \eta \nabla_{\mathbf{w}^{(k)}} l(\mathbf{w})$$

$\eta > 0$ is a constant called the learning rate.