ECE595 / STAT598: Machine Learning I
Lecture 15 Logistic Regression 2

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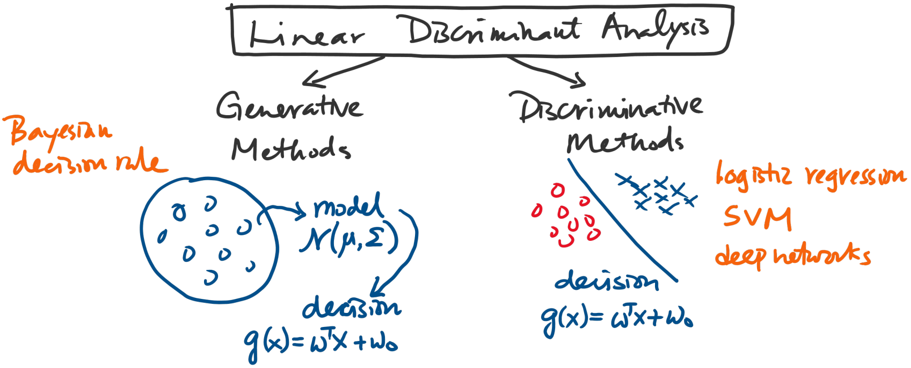
Stanley Chan

School of Electrical and Computer Engineering
Purdue University

Overview



- In linear discriminant analysis (LDA), there are generally two types of approaches
- **Generative approach**: Estimate model, then define the classifier
- **Discriminative approach**: Directly define the classifier

Outline

Discriminative Approaches

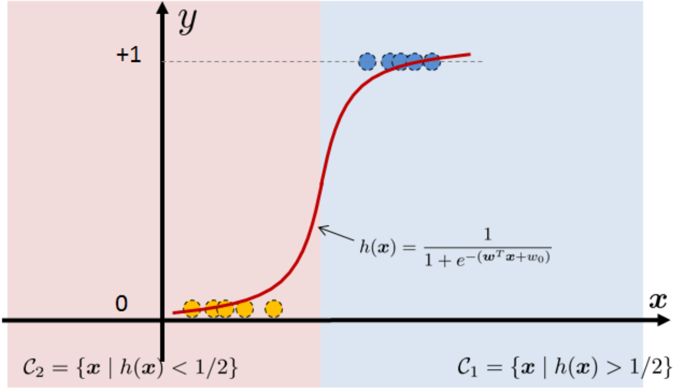
- Lecture 14 Logistic Regression 1
- Lecture 15 Logistic Regression 2

This lecture: Logistic Regression 2

- Gradient Descent
    - Convexity
    - Gradient
    - Regularization
- Connection with Bayes
    - Derivation
    - Interpretation
- Comparison with Linear Regression
    - Is logistic regression better than linear?
    - Case studies

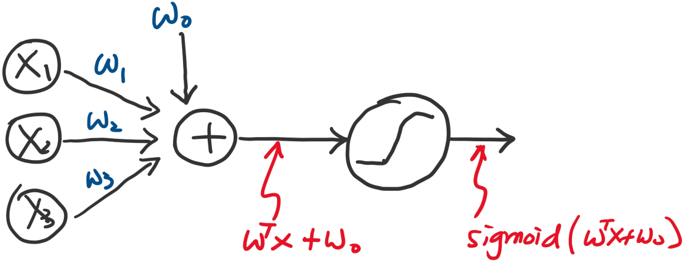
From Linear to Logistic Regression

- Can we replace $g(\boldsymbol{x})$ by $\text{sign}(g(\boldsymbol{x}))$?
- How about a soft-version of $\text{sign}(g(\boldsymbol{x}))$?
- This gives a logistic regression.



Logistic Regression and Deep Learning

- Logistic regression can be considered as the last layer of a deep network
- Inputs are $\boldsymbol{x}_n$, weights are $\boldsymbol{w}$
- The sigmoid function is the nonlinear activation
- To train the model, you compare the prediction error and minimize the loss by updating the weights



Training Loss Function

$$J(\boldsymbol{\theta}) = \sum_{n=1}^{N} \mathcal{L}(h_\theta(\boldsymbol{x}_n), y_n)$$
$$= \sum_{n=1}^{N} -\Big\{ y_n \log h_{\boldsymbol{\theta}}(\boldsymbol{x}_n) + (1 - y_n) \log(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x}_n)) \Big\}$$

- This is called the cross-entropy loss
- Consider two cases

$$y_n \log h_{\boldsymbol{\theta}}(\boldsymbol{x}_n) = \begin{cases} 0, & \text{if} \quad y_n = 1, \quad \text{and} \quad h_{\boldsymbol{\theta}}(\boldsymbol{x}_n) = 1, \\ -\infty, & \text{if} \quad y_n = 1, \quad \text{and} \quad h_{\boldsymbol{\theta}}(\boldsymbol{x}_n) = 0, \end{cases}$$

$$(1 - y_n)(1 - \log h_{\boldsymbol{\theta}}(\boldsymbol{x}_n)) = \begin{cases} 0, & \text{if} \quad y_n = 0, \quad \text{and} \quad h_{\boldsymbol{\theta}}(\boldsymbol{x}_n) = 0, \\ -\infty, & \text{if} \quad y_n = 0, \quad \text{and} \quad h_{\boldsymbol{\theta}}(\boldsymbol{x}_n) = 1. \end{cases}$$

- No solution if mismatch

Convexity of Logistic Training Loss

Recall that

$$J(\boldsymbol{\theta}) = \sum_{n=1}^{n} -\left\{ y_n \log\left(\frac{h_{\boldsymbol{\theta}}(\boldsymbol{x}_n)}{1 - h_{\boldsymbol{\theta}}(\boldsymbol{x}_n)}\right) + \log(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x}_n)) \right\}$$

- The first term is linear, so it is convex.
- The second term: Gradient:

$$\begin{aligned}
\nabla_{\boldsymbol{\theta}}[-\log(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x}))] &= -\nabla_{\boldsymbol{\theta}}\left[\log\left(1 - \frac{1}{1 + e^{-\boldsymbol{\theta}^T\boldsymbol{x}}}\right)\right] \\
&= -\nabla_{\boldsymbol{\theta}}\left[\log \frac{e^{-\boldsymbol{\theta}^T\boldsymbol{x}}}{1 + e^{-\boldsymbol{\theta}^T\boldsymbol{x}}}\right] = -\nabla_{\boldsymbol{\theta}}\left[\log e^{-\boldsymbol{\theta}^T\boldsymbol{x}} - \log(1 + e^{-\boldsymbol{\theta}^T\boldsymbol{x}})\right] \\
&= -\nabla_{\boldsymbol{\theta}}\left[-\boldsymbol{\theta}^T\boldsymbol{x} - \log(1 + e^{-\boldsymbol{\theta}^T\boldsymbol{x}})\right] = \boldsymbol{x} + \nabla_{\boldsymbol{\theta}}\left[\log\left(1 + e^{-\boldsymbol{\theta}^T\boldsymbol{x}}\right)\right] \\
&= \boldsymbol{x} + \left(\frac{-e^{-\boldsymbol{\theta}^T\boldsymbol{x}}}{1 + e^{-\boldsymbol{\theta}^T\boldsymbol{x}}}\right)\boldsymbol{x} = h_{\boldsymbol{\theta}}(\boldsymbol{x})\boldsymbol{x}.
\end{aligned}$$

Convexity of Logistic Training Loss

- Gradient of second term is

$$\nabla_{\boldsymbol{\theta}}[-\log(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x}))] = h_{\boldsymbol{\theta}}(\boldsymbol{x})\boldsymbol{x}.$$

- Hessian is:

$$\begin{aligned}
\nabla^2_{\boldsymbol{\theta}}[-\log(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x}))] &= \nabla_{\boldsymbol{\theta}}\left[h_{\boldsymbol{\theta}}(\boldsymbol{x})\boldsymbol{x}\right] \\
&= \nabla_{\boldsymbol{\theta}}\left[\left(\frac{1}{1+e^{-\boldsymbol{\theta}^T\boldsymbol{x}}}\right)\boldsymbol{x}\right] \\
&= \left(\frac{1}{(1+e^{-\boldsymbol{\theta}^T\boldsymbol{x}})^2}\right)\left(-e^{-\boldsymbol{\theta}^T\boldsymbol{x}}\right)\boldsymbol{x}\boldsymbol{x}^T \\
&= \left(\frac{1}{1+e^{-\boldsymbol{\theta}^T\boldsymbol{x}}}\right)\left(1 - \frac{1}{1+e^{-\boldsymbol{\theta}^T\boldsymbol{x}}}\right)\boldsymbol{x}\boldsymbol{x}^T \\
&= h_{\boldsymbol{\theta}}(\boldsymbol{x})[1 - h_{\boldsymbol{\theta}}(\boldsymbol{x})]\boldsymbol{x}\boldsymbol{x}^T.
\end{aligned}$$

Convexity of Logistic Training Loss

- For any $\boldsymbol{v} \in \mathbb{R}^d$, we have that

$$\begin{aligned} \boldsymbol{v}^T \nabla_{\boldsymbol{\theta}}^2 [-\log(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x}))] \boldsymbol{v} &= \boldsymbol{v}^T \left[h_{\boldsymbol{\theta}}(\boldsymbol{x})[1 - h_{\boldsymbol{\theta}}(\boldsymbol{x})] \boldsymbol{x}\boldsymbol{x}^T \right] \boldsymbol{v} \\ &= (h_{\boldsymbol{\theta}}(\boldsymbol{x})[1 - h_{\boldsymbol{\theta}}(\boldsymbol{x})]) \|\boldsymbol{v}^T \boldsymbol{x}\|^2 \geq 0. \end{aligned}$$

- Therefore the Hessian is positive semi-definite.
- So $-\log(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x})$ is convex in $\boldsymbol{\theta}$.
- Conclusion: The training loss function

$$J(\boldsymbol{\theta}) = \sum_{n=1}^{n} - \left\{ y_n \log \left(\frac{h_{\boldsymbol{\theta}}(\boldsymbol{x}_n)}{1 - h_{\boldsymbol{\theta}}(\boldsymbol{x}_n)} \right) + \log(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x}_n)) \right\}$$

  is **convex** in $\boldsymbol{\theta}$.
- So we can use convex optimization algorithms to find $\boldsymbol{\theta}$.

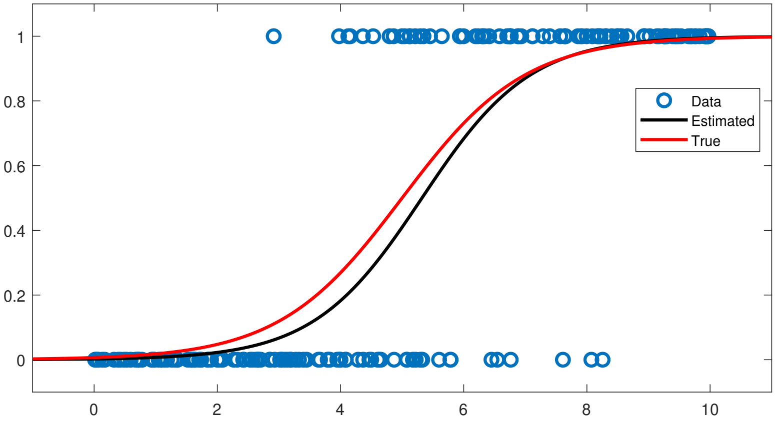
Convex Optimization for Logistic Regression

- We can use CVX to solve the logistic regression problem
- But it requires some re-organization of the equations

$$
\begin{aligned}
J(\boldsymbol{\theta}) &= \sum_{n=1}^{N} -\left\{ y_n \boldsymbol{\theta}^T \boldsymbol{x}_n + \log(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x}_n)) \right\} \\
&= \sum_{n=1}^{N} -\left\{ y_n \boldsymbol{\theta}^T \boldsymbol{x}_n + \log\left(1 - \frac{e^{\boldsymbol{\theta}^T \boldsymbol{x}_n}}{1 + e^{\boldsymbol{\theta}^T \boldsymbol{x}_n}}\right) \right\} \\
&= \sum_{n=1}^{N} -\left\{ y_n \boldsymbol{\theta}^T \boldsymbol{x}_n - \log\left(1 + e^{\boldsymbol{\theta}^T \boldsymbol{x}_n}\right) \right\} \\
&= -\left\{ \left(\sum_{n=1}^{N} y_n \boldsymbol{x}_n \right)^T \boldsymbol{\theta} - \sum_{n=1}^{N} \log\left(1 + e^{\boldsymbol{\theta}^T \boldsymbol{x}_n}\right) \right\}.
\end{aligned}
$$

- The last term is a sum of `log-sum-exp`: $\log(e^0 + e^{\theta^T x})$.

Convex Optimization for Logistic Regression



- Black: The true model. You create it.
- Blue circles: Samples drawn from the true distribution.
- Red: Trained model from the samples.

Gradient Descent for Logistic Regression

- The training loss function is

$$J(\boldsymbol{\theta}) = \sum_{n=1}^{n} -\left\{ y_n \boldsymbol{\theta}^T \boldsymbol{x}_n + \log(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x}_n)) \right\}.$$

- Recall that

$$\nabla_{\boldsymbol{\theta}}[-\log(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x}))] = h_{\boldsymbol{\theta}}(\boldsymbol{x})\boldsymbol{x}.$$

- You can run gradient descent

$$\begin{aligned} \boldsymbol{\theta}^{(k+1)} &= \boldsymbol{\theta}^{(k)} - \alpha_k \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}^{(k)}) \\ &= \boldsymbol{\theta}^{(k)} - \alpha_k \left(\sum_{n=1}^{N} (h_{\boldsymbol{\theta}^{(k)}}(\boldsymbol{x}_n) - y_n)\boldsymbol{x}_n \right). \end{aligned}$$

- Since the loss function is convex, guaranteed to find global minimum.

Regularization in Logistic Regression

- The loss function is

$$J(\boldsymbol{\theta}) = \sum_{n=1}^{n} -\left\{ y_n \boldsymbol{\theta}^T \boldsymbol{x}_n + \log(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x}_n)) \right\}$$
$$= \sum_{n=1}^{n} -\left\{ y_n \boldsymbol{\theta}^T \boldsymbol{x}_n + \log\left(1 - \frac{1}{1 + e^{-\boldsymbol{\theta}^T \boldsymbol{x}_n}}\right) \right\}$$

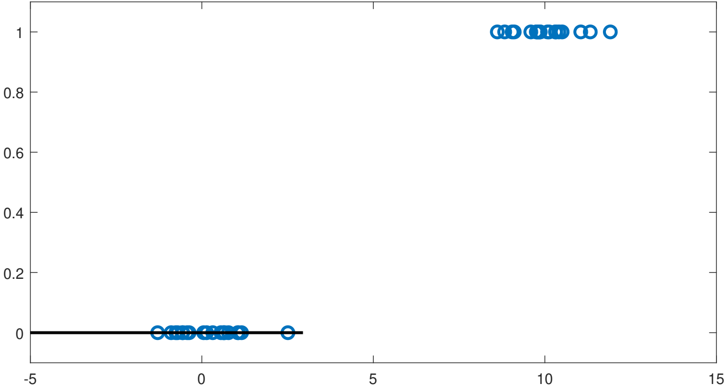
- What if $h_{\boldsymbol{\theta}}(\boldsymbol{x}_n) = 1$? (We need $\boldsymbol{\theta}^T \boldsymbol{x}_n = \infty$.)
- Then we have $\log(1 - 1) = \log 0$, which is $-\infty$.
- Same thing happens in the equivalent form

$$J(\boldsymbol{\theta}) = -\left\{ \left(\sum_{n=1}^{N} y_n \boldsymbol{x}_n \right)^T \boldsymbol{\theta} - \sum_{n=1}^{N} \log\left(1 + e^{\boldsymbol{\theta}^T \boldsymbol{x}_n}\right) \right\}.$$

- When $\boldsymbol{\theta}^T \boldsymbol{x}_n \to \infty$, we have $\log(\infty)$.

Regularization in Logistic Regression

- Example: Two classes: $\mathcal{N}(0,1)$ and $\mathcal{N}(10,1)$.
- Run CVX



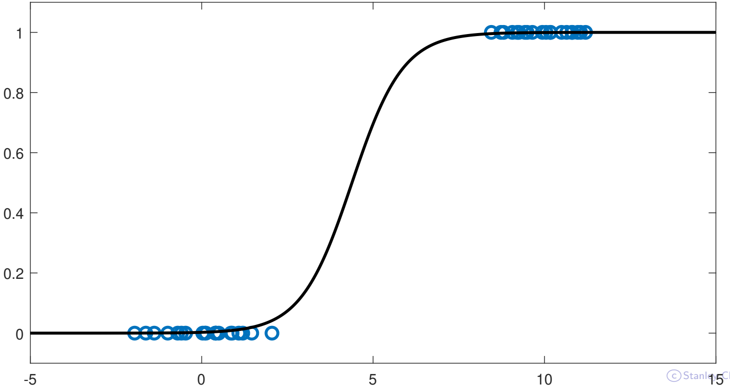
- NaN for $y_n = 1$

Regularization in Logistic Regression

- Add a small regularization

$$J(\boldsymbol{\theta}) = -\left\{ \left(\sum_{n=1}^{N} y_n \boldsymbol{x}_n \right)^T \boldsymbol{\theta} - \sum_{n=1}^{N} \log \left(1 + e^{\boldsymbol{\theta}^T \boldsymbol{x}_n} \right) \right\} + \lambda \|\boldsymbol{\theta}\|^2.$$

- Re-run the same CVX program



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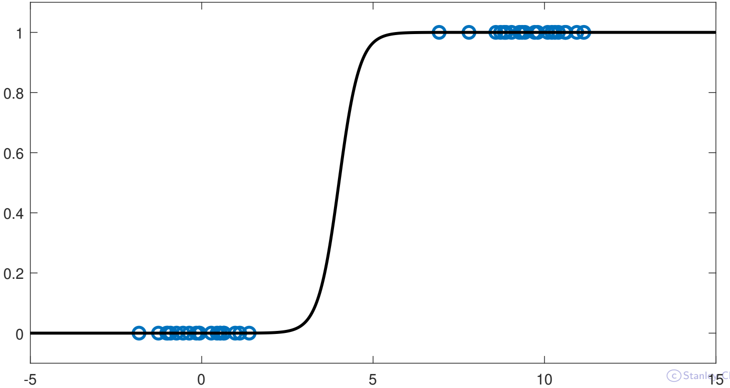
Regularization in Logistic Regression

- If you make λ really really small ...

$$J(\boldsymbol{\theta}) = -\left\{ \left(\sum_{n=1}^{N} y_n \boldsymbol{x}_n \right)^T \boldsymbol{\theta} - \sum_{n=1}^{N} \log \left(1 + e^{\boldsymbol{\theta}^T \boldsymbol{x}_n} \right) \right\} + \lambda \|\boldsymbol{\theta}\|^2.$$

- Re-run the same CVX program



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Try This Online Exercise

- Classify two digits in the MNIST dataset
- http://ufldl.stanford.edu/tutorial/supervised/LogisticRegression/

Exercise 1B

Starter code for this exercise is included in the Starter Code GitHub Repo in the ex1/ directory.

In this exercise you will implement the objective function and gradient computations for logistic regression and use your code to learn to classify images of digits from the MNIST dataset as either "0" or "1". Some examples of these digits are shown below:

Each of the digits is is represented by a 28x28 grid of pixel intensities, which we will reformat as a vector $x^{(i)}$ with 28*28 = 784 elements. The label is binary, so $y^{(i)} \in \{0, 1\}$.

You will find starter code for this exercise in the `ex1/ex1b_logreg.m` file. The starter code file performs the following tasks for you:

1. Calls `ex1_load_mnist.m` to load the MNIST training and testing data. In addition to loading the pixel values into a matrix X (so that that j'th pixel of the i'th example is $X_{ji} = x_j^{(i)}$) and the labels into a row-vector y, it will also perform some simple normalizations of the pixel intensities so that they tend to have zero mean and unit variance. Even though the MNIST dataset contains 10 different digits (0-9), in this exercise we will only load the 0 and 1 digits — the ex1_load_mnist function will do this for you.
2. The code will append a row of 1's so that θ_0 will act as an intercept term.
3. The code calls `minFunc` with the `logistic_regression.m` file as objective function. Your job will be to fill in `logistic_regression.m` to return the objective function value and its gradient.
4. After `minFunc` completes, the classification accuracy on the training set and test set will be printed out.

As for the linear regression exercise, you will need to implement `logistic_regression.m` to loop over all

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Connection with Bayes

- The likelihood is

$$p(\boldsymbol{x}|i) = \frac{1}{\sqrt{(2\pi)^d|\boldsymbol{\Sigma}|}} \exp\left\{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_i)^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu}_i)\right\}$$

- The prior is $p_Y(i) = \pi_i$.
- The posterior is

$$\begin{aligned}
p(1|\boldsymbol{x}) &= \frac{p(\boldsymbol{x}|1)p_Y(1)}{p(\boldsymbol{x}|1)p_Y(1) + p(\boldsymbol{x}|0)p_Y(0)} \\
&= \frac{1}{1 + \frac{p(\boldsymbol{x}|0)p_Y(0)}{p(\boldsymbol{x}|1)p_Y(1)}} = \frac{1}{1 + \exp\left\{-\log\left(\frac{p(\boldsymbol{x}|1)p_Y(1)}{p(\boldsymbol{x}|0)p_Y(0)}\right)\right\}} \\
&= \frac{1}{1 + \exp\left\{-\log\left(\frac{\pi_1}{\pi_0}\right) - \log\left(\frac{p(\boldsymbol{x}|1)}{p(\boldsymbol{x}|0)}\right)\right\}}.
\end{aligned}$$

Connection with Bayes

- We can show that the last term is

$$
\begin{aligned}
&\log\left(\frac{p(\boldsymbol{x}|1)}{p(\boldsymbol{x}|0)}\right) \\
&= \log\left(\frac{\frac{1}{\sqrt{(2\pi)^d|\boldsymbol{\Sigma}|}}\exp\left\{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_1)^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu}_1)\right\}}{\frac{1}{\sqrt{(2\pi)^d|\boldsymbol{\Sigma}|}}\exp\left\{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_0)^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu}_0)\right\}}\right) \\
&= -\frac{1}{2}\left[(\boldsymbol{x}-\boldsymbol{\mu}_1)^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu}_1)-(\boldsymbol{x}-\boldsymbol{\mu}_0)^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu}_0)\right] \\
&= (\boldsymbol{\mu}_1-\boldsymbol{\mu}_0)^T\boldsymbol{\Sigma}^{-1}\boldsymbol{x}-\frac{1}{2}\left(\boldsymbol{\mu}_1^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_1-\boldsymbol{\mu}_0^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_0\right).
\end{aligned}
$$

- Let us define

$$
\begin{aligned}
\boldsymbol{w} &= \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1-\boldsymbol{\mu}_0) \\
w_0 &= -\frac{1}{2}\left(\boldsymbol{\mu}_1^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_1-\boldsymbol{\mu}_0^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_0\right)+\log\left(\frac{\pi_1}{\pi_0}\right)
\end{aligned}
$$

Connection with Bayes

- Then,

$$\begin{aligned}\log\left(\frac{p(\boldsymbol{x}|1)}{p(\boldsymbol{x}|0)}\right) &= (\boldsymbol{\mu}_1-\boldsymbol{\mu}_0)^T\boldsymbol{\Sigma}^{-1}\boldsymbol{x} - \frac{1}{2}\left(\boldsymbol{\mu}_1^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_0\right)\\ &= \boldsymbol{w}^T\boldsymbol{x} + w_0 - \log \pi_1/\pi_0\end{aligned}$$

- Therefore,

$$\begin{aligned}p(1|\boldsymbol{x}) &= \frac{1}{1+\exp\left\{-\log\left(\frac{\pi_1}{\pi_0}\right) - \log\left(\frac{p(\boldsymbol{x}|1)}{p(\boldsymbol{x}|0)}\right)\right\}}\\ &= \frac{1}{1+\exp\{-(\boldsymbol{w}^T\boldsymbol{x}+w_0)\}}\\ &= h_{\boldsymbol{\theta}}(\boldsymbol{x})\end{aligned}$$

Connection with Bayes

- The hypothesis function is the posterior distribution

$$\begin{aligned} p_{Y|\boldsymbol{X}}(1|\boldsymbol{x}) &= \frac{1}{1+\exp\{-(\boldsymbol{w}^T\boldsymbol{x}+w_0)\}} = h_{\theta}(\boldsymbol{x}) \\ p_{Y|\boldsymbol{X}}(0|\boldsymbol{x}) &= \frac{\exp\{-(\boldsymbol{w}^T\boldsymbol{x}+w_0)}{1+\exp\{-(\boldsymbol{w}^T\boldsymbol{x}+w_0)\}} = 1-h_{\theta}(\boldsymbol{x}), \end{aligned} \tag{1}$$

- So logistic regression offers probabilistic reasoning which linear regression does not
- Not true when the covariances are different
- Remark: If the covariances are different, the Bayes returns a quadratic classifier

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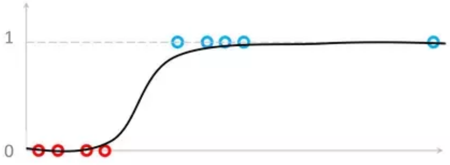
Is Logistic Regression Better than Linear?

Logistic regression on the other hand can handle this outlier with no issue.



Now let's take a closer look at the logistic regression loss function.

$$f(\mathbf{w}) = \sum_p \log\left(1 + e^{-y_p \mathbf{x}_p^T \mathbf{w}}\right)$$

Here, I'm assuming the labels y_p are in $\{-1, +1\}$. Note that this is equivalent

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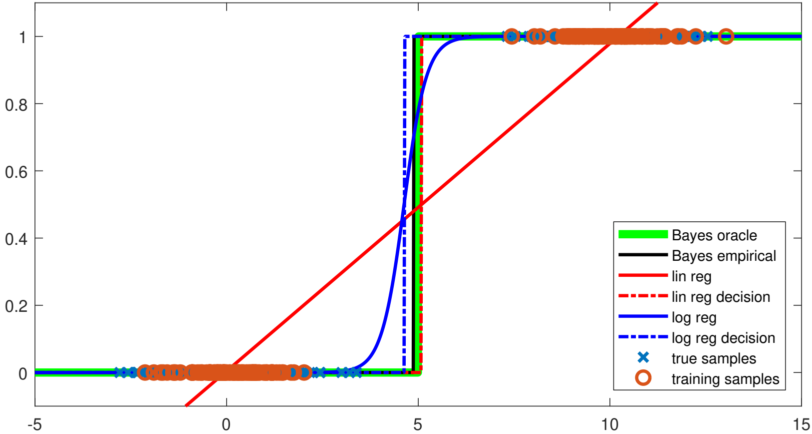
- This is taken from the Internet
- Is that true???

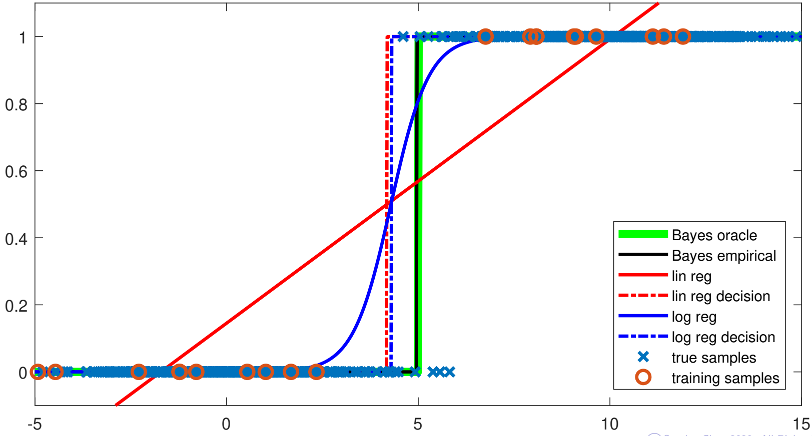
Is Logistic Regression Better than Linear?

- **Scenario 1**: Identical Covariance. Equal Prior. Enough samples.
- $\mathcal{N}(0,1)$ with 100 samples and $\mathcal{N}(10,1)$ with 100 samples.
- Linear and logistic: Not much different.



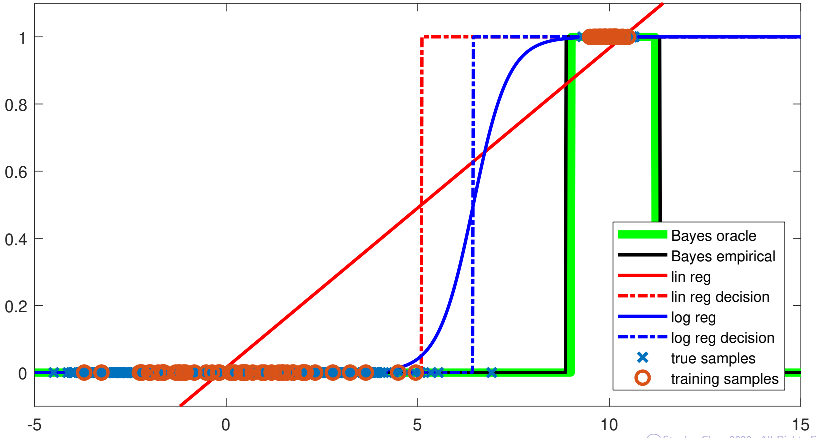
The False Sense of Good Fitting

- **Scenario 2**: Identical Covariance. Equal Prior. Not a lot of samples.
- $\mathcal{N}(0, 2)$ with 10 samples and $\mathcal{N}(10, 2)$ with 10 samples.
- Linear and logistic: Not much different.



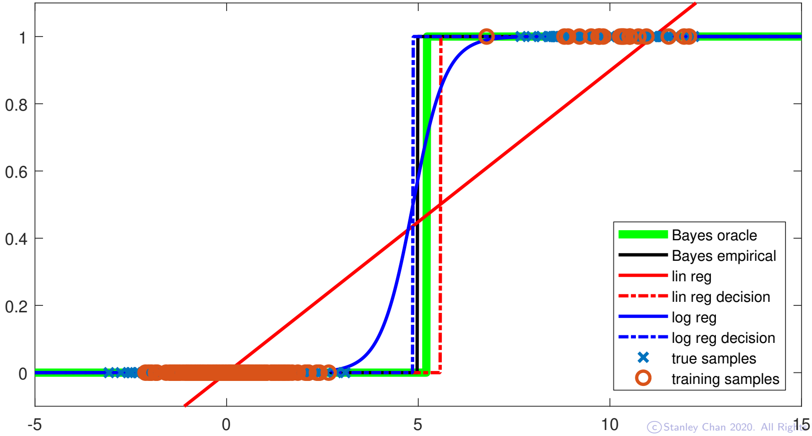
Is Logistic Regression Better than Linear?

- **Scenario 3**: Different Covariance. Equal Prior.
- $\mathcal{N}(0, 2)$ with 50 samples and $\mathcal{N}(10, 0.2)$ with 50 samples.
- Linear and logistic: Equally bad.



Is Logistic Regression Better than Linear?

- **Scenario 4**: Identical Covariance. Unequal Prior.
- Training size proportional to prior: 180 samples and 20 samples.
- $\mathcal{N}(0,1)$ with $\pi_0 = 0.9$ and $\mathcal{N}(10,1)$ with $\pi_1 = 0.1$.
- Linear and logistic: Not much different.



So what can we say about Logistic Regression?

- Logistic regression empowers a discriminative method with probabilistic reasonings.
- The hypothesis function is the posterior probability

$$p(1|\boldsymbol{x}) = \frac{1}{1+\exp\{-(\boldsymbol{w}^T\boldsymbol{x}+w_0)\}} = h_{\boldsymbol{\theta}}(\boldsymbol{x})$$
$$p(0|\boldsymbol{x}) = \frac{\exp\{-(\boldsymbol{w}^T\boldsymbol{x}+w_0)}{1+\exp\{-(\boldsymbol{w}^T\boldsymbol{x}+w_0)\}} = 1 - h_{\boldsymbol{\theta}}(\boldsymbol{x}),$$

- Logistic is yet another special case of Bayesian
- More or less the same performance as linear regression
- Logistic can give lower training error — which looks better on plots.
- But its generalization is similar to linear regression

Reading List

Logistic Regression (Machine Learning Perspective)

- Chris Bishop's *Pattern Recognition*, Chapter 4.3
- Hastie-Tibshirani-Friedman's *Elements of Statistical Learning*, Chapter 4.4
- Stanford CS 229 Discriminant Algorithms http://cs229.stanford.edu/notes/cs229-notes1.pdf
- CMU Lecture https://www.stat.cmu.edu/~cshalizi/uADA/12/lectures/ch12.pdf
- Stanford Language Processing https://web.stanford.edu/~jurafsky/slp3/ (Lecture 5)

Logistic Regression (Statistics Perspective)

- Duke Lecture https://www2.stat.duke.edu/courses/Spring13/sta102.001/Lec/Lec20.pdf
- Princeton Lecture https://data.princeton.edu/wws509/notes/c3.pdf