# CEE 616: Probabilistic Machine Learning M2 Linear Methods: L2b Logistic Regression

Jimi Oke

**UMassAmherst** 

College of Engineering

Thu, Sep 25, 2025

#### Outline

- Introduction
- 2 Logistic regression model
- 3 MLE
- 4 Optimization
- Outlook

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Introduction •00000

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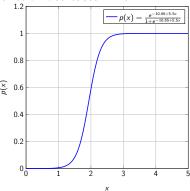
$$S(\mathbf{Wx}) = \left[ \frac{e^{\mathbf{w}_1^{\top} \mathbf{x}}}{\sum_{c'=1}^{C} e^{\mathbf{w}_{c'}^{\top} \mathbf{x}}}, \cdots, \frac{e^{\mathbf{w}_{c}^{\top} \mathbf{x}}}{\sum_{c'=1}^{C} e^{\mathbf{w}_{c'}^{\top} \mathbf{x}}} \right]$$
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where  $\mathbf{W} = [\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_C]$  is a  $C \times D$  weight matrix

For  $w_1 > 0$ , the logistic function increases w.r.t. x.

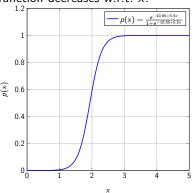
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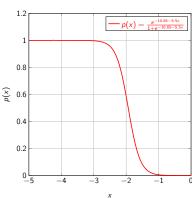
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Introduction

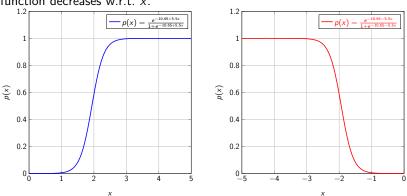
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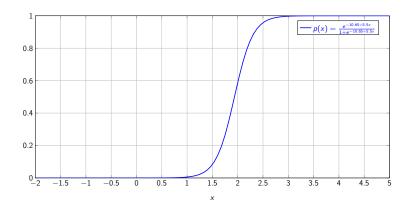
What happens when b is increased or decreased?

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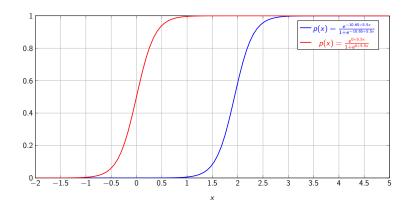
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(x)

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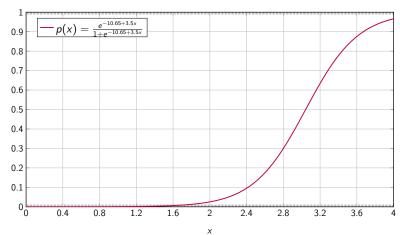
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Introduction

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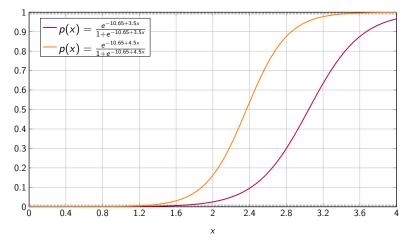


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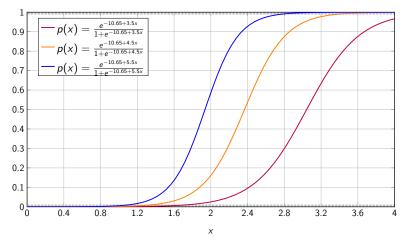
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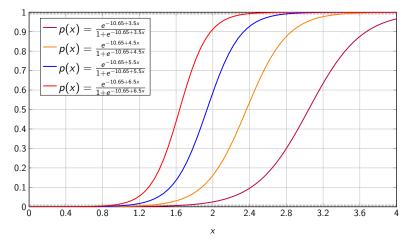
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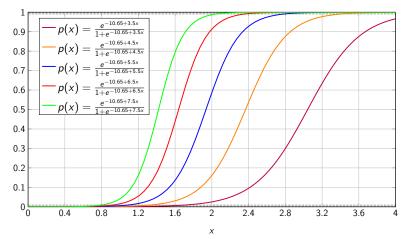
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- In the generalized linear framework, logit is the *link function* between the predictors and the mean response

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The logistic function is a member of the class of **sigmoid** functions (S-shaped curves) and can also be written:

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where  $\mathbf{w}^{\top} = (b, w_1)$ 

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# Credit card defaults

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- balance: The average balance that the customer has remaining on their credit card after making their monthly payment
- income: Income of customer

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Note that the null hypothesis for the tests is:  $H_0$ :  $\mathbf{w}_i = 0$  (i.e. no dependence on the corresponding predictor)

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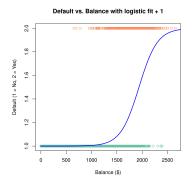
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- 1 How would  $\hat{p}$  (the predicted probability) change if x were to increase by \$100?
- 2 What about if x were to decrease by \$100
- 3 There are 333 defaults out of 10000 observations. What is the impact of b?

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 MLE
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#### Multiple logistic regression

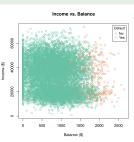
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#### Activity: Binomial logistic regression with multiple predictors

Using the Default dataset, predict the probability of default based on balance and student. Comment on your results and interpret the coefficient estimates.



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### Decision boundary

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Typically,  $\tau = 0.5$ 



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• The likelihood function  $\mathcal{L}(\theta)$  represents the support provided by a sample for a given parameter  $\theta$ :

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• It is also convenient to encode  $c_i$  using a 0/1 response  $y_i$ :

$$y_i = \begin{cases} 1, & \text{when } c_i = \text{Class 1} \\ 0, & \text{when } c_i = \text{Class 2} \end{cases}$$
 (16)

## Log-likelihood function for logistic regression

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In the binomial case, this simplifies to:

$$NLL(\boldsymbol{w}) = -\sum_{i} \left[ y_i \log p(x_i; \boldsymbol{w}) + (1 - y_i) \log(1 - p(x_i; \boldsymbol{w})) \right]$$
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• Recall that we model  $p(x_i; \mathbf{w})$  as:

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• Recall that we model  $p(x_i; \mathbf{w})$  as:

$$p(x_i) = \frac{e^{b + w_1 x_i}}{1 + e^{b + w_1 x_i}} \tag{19}$$

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Substituting (19) into (18), we obtain:

$$\mathsf{NLL}(\boldsymbol{w}) = -\sum_{i} \left[ y_{i} \log \left( \frac{e^{b+w_{1}x_{i}}}{1 + e^{b+w_{1}x_{i}}} \right) + (1 - y_{i}) \log \left( 1 - \frac{e^{b+w_{1}x_{i}}}{1 + e^{b+w_{1}x_{i}}} \right) \right]$$

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To find  $\hat{w}$ , we find the derivative of NLL(w), set it to zero and solve the resulting score equations:

$$\frac{\partial \text{NLL}}{\partial \boldsymbol{w}} = -\frac{\partial}{\partial \boldsymbol{w}} \sum_{i} \left[ y_{i} \left( b + w_{1} x_{i} \right) - \log \left( 1 + e^{b + w_{1} x_{i}} \right) \right]$$

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To find  $\hat{\boldsymbol{w}}$ , we find the derivative of NLL( $\boldsymbol{w}$ ), set it to zero and solve the resulting score equations:

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This is a system of two *nonlinear* equations in  $\boldsymbol{w}$  which can be solved via the **Newton-Raphson** method.

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### Maximizing the log-likelihood

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\begin{pmatrix} \frac{\partial \text{NLL}}{\partial b} \\ \frac{\partial \text{NLL}}{\partial w_{1}} \end{pmatrix} = - \begin{pmatrix} \sum_{i} \left[ y_{i} - p(x_{i}) \right] \\ \sum_{i} \left[ x_{i} \left( y_{i} - p(x_{i}) \right) \right] \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$
(21)

This is a system of two *nonlinear* equations in **w** which can be solved via the **Newton-Raphson** method.

Alternatively, we can use the gradient descent approach to directly minimize NII.

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Also recall the derivative of NLL:

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We can use either Newton-Raphson or gradient descent to minimize NLL.

#### NLL and entropy

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### NLL and entropy

We can show that the NLL is equal to the sum of the **binary cross entropy** of  $y_i$  and  $p(y = 1|x_i)$  over N:

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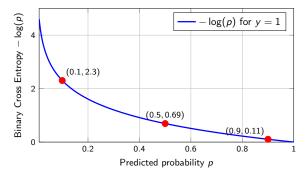
$$\mathbb{H}_{i}(y_{i}, p_{i}) = -[y_{i} \log p_{i} + (1 - y_{i}) \log(1 - p_{i})]$$
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Note that  $p_i = \sigma(\mathbf{w}^{\top} \mathbf{x}_i)$ .

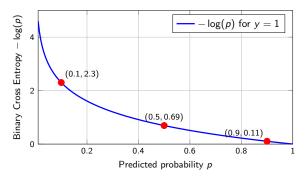
 Binary cross-entropy quantifies how far your predicted probabilities are from the actual binary labels.

For a true label y = 1, the binary cross entropy is  $\mathbb{H}(1, p) = -\log(p)$ .

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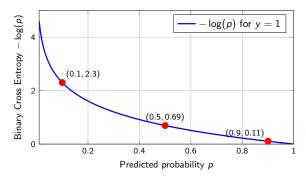


L2b: Logistic Regression

#### **Key observations:**

• As  $p \to 1$ : cross entropy  $\to 0$  (low penalty for correct prediction)

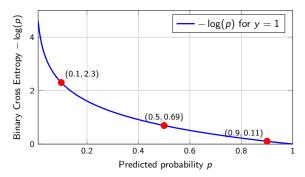
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#### **Key observations:**

- As  $p \to 1$ : cross entropy  $\to 0$  (low penalty for correct prediction)
- As p o 0: cross entropy  $o \infty$  (high penalty for incorrect prediction)
- The function is convex, ensuring unique minimum in optimization

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$$BCE = -[1 \times \log(0.1) + 0 \times \log(0.9)] = -\log(0.1) \approx 2.303$$
 (high loss - bad!)

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#### Note

- The gradient descent method does not require a second derivative
- However, it may require more iterations to converge than Newton-Raphson

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$$\mathbf{w}_{k+1} = \mathbf{w}_k - \left[ \left( \frac{\partial^2 \mathsf{NLL}(\mathbf{w})}{\partial \mathbf{w} \partial \mathbf{w}^\top} \right)^{-1} \frac{\partial \mathsf{NLL}(\mathbf{w})}{\partial \mathbf{w}} \right]_{\dots}$$
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In this form, the estimation is also called iteratively reweighted least squares (IRLS).

Jimi Oke (UMass Amherst)

### OLS, WLS and IRLS

Jimi Oke (UMass Amherst) L2b: Logistic Regression Thu, Sep 25, 2025

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- Note that the update step is identical in form to the WLS estimator
- However, W and z change in each iteration, hence the name iteratively reweighted least squares (IRLS)

#### Summary

• The binary logistic regression model is given by:

$$p(y=1|\mathbf{x};\boldsymbol{\theta}) = \frac{1}{1+e^{-\mathbf{w}^{\top}\mathbf{x}}}$$
(45)

 The negative log-likelihood of a sample of N observations in the binomial response case is:

$$NLL(\mathbf{w}) = \sum_{i} \left[ y_i \left( b + w_1 x_i \right) - \log \left( 1 + e^{b + w_1 x_i} \right) \right]$$
 (46)

- Based on the principle of maximum likelihood, the estimate  $\hat{\pmb{w}}$  is given by the minimizing NLL.
- This can be solved via gradient descent or Newton-Raphson.

# Summary (cont.)

#### Gradient descent update for logistic regression

$$\mathbf{w}_{k+1} = \mathbf{w}_k - \lambda \nabla \mathsf{NLL}(\mathbf{w}_k) \tag{47}$$

Newton-Raphson update for logistic regression

$$\mathbf{w}_{k+1} = \mathbf{w}_k - \mathbf{H}_{\mathbf{w}_k}^{-1}(\mathsf{NLL})\nabla_{\mathbf{w}_k}\mathsf{NLL}(\mathbf{w}_k)$$
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Jimi Oke (UMass Amherst) L2b: Logistic Regression Thu, Sep 25, 2025

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 MAP estimation: weight decay/regularization to make NLL convex (have unique solution). We define the **penalized negative log-likelihood** PNLL as:

$$PNLL(\boldsymbol{w}) = NLL(\boldsymbol{w}) + \lambda \boldsymbol{w}^{\top} \boldsymbol{w}$$
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# Reading assignments

- **PMLCE** 9.2
- **PMLI** 10.1-3
- ESL 4.4