#### Announcements

- Quiz 1 due this Thursday, testing mainly lin reg.
- HW0 done, grading in progress. Coding grades looked good.
- HW1 in progress.
- Coming soon:
  - Project format announcements
  - Mid-term preparation materials



# CIS 4190/5190: Lec 05 Mon Sep 16, 2024

### First few mins: Linear Regression Wrap-Up

Robot Image Credit: Viktoriya Sukhanova © 123RF.com

#### **Recap of Linear Regression**

- Lec 01: lin reg model class, loss function, feature maps
  - Asides (broader than lin reg): performance evaluation & metrics, function approx. view of ML, model capacity & overfitting
- Lec 02: Regularized lin reg loss function
  - Asides (broader than lin reg): train and test error, bias and variance, the concept of regularization, hyperparameter tuning & validation data
- Lec 03: Ways to optimize lin reg loss function
  - Both involve measuring the gradient of loss w.r.t parameters.
  - Option 1: set analytical expression of gradient to 0, and solve. Closedform solution.
  - Option 2: iteratively move in the direction of gradient. Gradient descent.
- Today: wrap-up. Feature standardization and  $\ell_1$  regularization

### Indexing: from 0 or 1?

• Our slides mostly follow the math tradition of indexing from 1.

$$L(\beta; Z) = \frac{1}{n} \sum_{i=1}^{n} (y_i - \beta^{\mathsf{T}} x_i)^2 + \lambda \sum_{j=1}^{d} \beta_j^2$$
$$L(\beta; Z) = \frac{1}{n} \sum_{i=1}^{n} (y_i - \beta^{\mathsf{T}} x_i)^2 + \lambda \sum_{j=1}^{d} |\beta_j|$$

• With polynomial functions, our index starts from 0, so that  $\beta_j$  is the coefficients for the j-th order term:

$$f_{\beta}(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4 x^4 + \dots + \beta_{10} x^{10}$$

### Indexing: from 0 or 1?

• With intercept term ( $\phi(x) = \begin{bmatrix} 1 & x_1 & \dots & x_d \end{bmatrix}^{\top}$ ), no penalty on the weight for the intercept term (which is  $\beta_1$  here):

• 
$$L(\beta; Z) = \frac{1}{n} \sum_{i=1}^{n} (y_i - \beta^{\mathsf{T}} x_i)^2 + \lambda \sum_{j=2}^{d} \beta_j^2$$

#### Features in Linear Regression

- Feature Standardization
- Automatic Feature Selection with L1 Regularization

#### **Feature Standardization**

- Unregularized linear regression is invariant to feature scaling
  - Suppose we scale  $x_{ij} \leftarrow 2x_{ij}$  for all examples  $x_i$
  - Without regularization, simply use  $\beta_j \leftarrow \beta_j/2$  to obtain equivalent solution

In particular, 
$$\frac{\beta_j}{2} \cdot 2x_{ij} = \beta_j \cdot x_{ij}$$

• Not true for regularized regression! • Penalty  $(\beta_j/2)^2$  is scaled by 1/4 (not cancelled out!)

• 
$$L(\beta; Z) = \frac{1}{n} \sum_{i=1}^{n} (y_i - \beta^{\mathsf{T}} x_i)^2 + \lambda \left(\beta_2^2 + \dots + \beta_j^2 + \dots + \beta_d^2\right)$$
  
•  $L(\beta; Z) = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - \frac{\beta^{\mathsf{T}}}{2} 2x_i\right)^2 + \lambda \left(\frac{\beta_2^2}{4} + \dots + \frac{\beta_j^2}{4} + \dots + \frac{\beta_d^2}{4}\right)$ 

#### **Feature Standardization**

• Rescale features to zero mean and unit variance

• 
$$x_{i,j} \leftarrow \frac{x_{i,j} - \mu_j}{\sigma_j}$$
  $\mu_j = \frac{1}{N} \sum_{i=1}^N x_{i,j}$   $\sigma_j^2 = \frac{1}{N} \sum_{i=1}^N (x_{i,j} - \mu_j)^2$ 

- Note: When using intercept term, do not rescale  $x_1 = 1$
- Can be sensitive to outliers (fix by dropping outliers)
- Makes it easier to estimate coefficients
- Often better encodes real variations in data
- Common Rookie Error: Must use same transformation during training & prediction
  - Please always compute μ<sub>j</sub> and σ<sub>j</sub> on training data, and use the same values when standardizing test data

Automatic Feature Set Selection with L1 Regularization

### $L_0$ Regularization $\rightarrow L_1$ Regularization

- Sparsity: Can we minimize  $\|\beta\|_0 = |\{j \mid \beta_j \neq 0\}|$ , the number of non-zero components? (This is called  $L_0$  regularization)
  - Automatic feature selection!
  - Improves interpretability.

$$L(\beta; Z) = \frac{1}{n} \sum_{i=1}^{n} (y_i - \beta^{\mathsf{T}} x_i)^2 + \lambda ||\beta||_0$$

- Challenge:  $\|\beta\|_0$  is not differentiable, making it hard to optimize
- Solution: *L*<sub>1</sub> Regularization
  - We can instead use an  $L_1$  norm  $\|\beta\|_1$  as the regularizer!
  - Still harder to optimize than  $L_2$  norm, but at least it is convex

## L<sub>1</sub> Regularization



#### L<sub>1</sub> Regularization for Feature Selection

- Step 1: Construct a lot of features and add to feature map
- Step 2: Use L<sub>1</sub> regularized regression to "select" subset of features
   I.e., coefficient β<sub>j</sub> ≠ 0 → feature j is selected)
- Optional: Remove unselected features from the feature map and run vanilla linear regression (a.k.a. ordinary least squares)

#### Optimizing L<sub>1</sub> Regularized Linear Regression?

- Gradient descent still works!
- Specialized algorithms work better in practice
  - Simple one: Gradient descent + soft thresholding
  - Basically, if  $\left|\beta_{t,j}\right| \leq \lambda$ , just set it to zero
  - Good theoretical properties

#### What About Classification Problems?



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## Logistic Regression: Linear Models for Classification

Robot Image Credit: Viktoriya Sukhanova © 123RF.com

#### **Recall: Supervised Learning**



Data 
$$Z = \{(x_i, y_i)\}_{i=1}^n$$
  
PS: sometimes denoted  $D$ 

 $\hat{\beta}(Z) = \arg \min_{\beta} L(\beta; Z)$ L encodes  $y_i \approx f_{\beta}(x_i)$ 

Model  $f_{\widehat{\beta}(Z)}$ 

#### **Recall: Regression**



Model  $f_{\widehat{\beta}(Z)}$ 

Data  $Z = \{(x_i, y_i)\}_{i=1}^n$  $\hat{\beta}(Z) = \arg \min_{\beta} L(\beta; Z)$  $L \text{ encodes } y_i \approx f_{\beta}(x_i)$ 

Label is a **real value**  $y_i \in \mathbb{R}$ 

#### **Recall: Classification**

## 

Model  $f_{\widehat{\beta}(Z)}$ 

Data 
$$Z = \{(x_i, y_i)\}_{i=1}^n$$
  
 $\hat{\beta}(Z) = \arg \min_{\beta} L(\beta; Z)$   
 $L \text{ encodes } y_i \approx f_{\beta}(x_i)$ 

Label is a **discrete value**  $y_i \in \mathcal{Y} = \{1, \dots, k\}$ 

### (Binary) Classification

- Input: Dataset  $Z = \{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$
- **Output:** Model  $y_i \approx f_\beta(x_i)$





Image: https://eyecancer.com/uncategorized/choroidalmetastasis-test/

#### **Example:** Malignant vs. Benign Ocular Tumor

#### Loss Minimization View of ML

- Three design decisions
  - Model family: What are the candidate models f? (E.g., linear functions)
  - Loss function: How to define "approximating"? (E.g., MSE loss)
  - Optimizer: How do we optimize the loss? (E.g., gradient descent)
- How do we adapt to classification?

#### Trying to Come up With A Model Class For Logistic Regression

#### **Repurpose Linear Regression For Classification?**

Given {( $x_1, y_1$ ), ( $x_2, y_2$ ), ..., ( $x_N, y_N$ )} where  $x_i \in \mathbb{R}^D$ ,  $y_i \in \{0, 1\}$ 

Predict  $y_i = \boldsymbol{\beta}^T \boldsymbol{x}_i$ 

Predict  $y_i$  = class 1 if  $\boldsymbol{\beta}^T \boldsymbol{x}_i \ge 0$ Predict  $y_i$  = class 0 if  $\boldsymbol{\beta}^T \boldsymbol{x}_i < 0$ 



#### **Repurpose Linear Regression For Classification?**



What if the data requires a non-linear decision boundary?

#### **Non-Linear Decision Boundaries Thru Feature Expansion**

Can apply basis expansion to features, same as with linear regression



Looks like we have a reasonable model class to start from ...

#### Can We Come Up With A Loss Function?

#### **Loss Function**

• Input: Dataset  $Z = \{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$ 

Training dataset overlay on decision boundary

- Classification:
  - Labels  $y_i \in \{0, 1\}$
  - Predict  $y_i \approx 1(\beta^\top x_i \ge 0)$
  - 1(C) equals 1 if C is true and 0 if C is false  $\propto$
  - How to learn *β*? **Need a loss function!**

Any ideas?



#### Candidate Classification Loss Function: Inaccuracy

• (In)accuracy / Error Rate:

$$L(\beta; Z) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}\left(y_i \neq f_\beta(x_i)\right)$$

- Indeed often captures what we care about in terms of classifier performance. Good *performance metric*.
- But bad loss function, because
   computationally intractable to optimize
  - Discontinuous measures are often hard to optimize. As an example, think about gradient descent ...
- Need to "soften" this in some way ... make more continuous



#### Revisiting the Model Class

#### Making Soft Decisions: Revisiting the Model Class

Predict  $y_i$  = class 1 if  $\beta^T x_i \ge 0$ Predict  $y_i$  = class 0 if  $\beta^T x_i < 0$ 

Predict  $p(y_i = 1 | x_i, \beta)$  based on the value of  $\beta^T x_i$ 

#### Intuition:

if  $\beta^{\top} x_i$  has large positive value, then high  $p(y_i = 1 | x_i, \beta) \rightarrow 1$ large negative value, then low  $p(y_i = 1 | x_i, \beta) \rightarrow 0$ zero, then  $p(y_i = 1 | x_i, \beta) \approx 0.5$ 

#### Logistic Regression

How to convert from  $\beta^{\top} x_i$  which lies in  $(-\infty, \infty)$  to a meaningful probability?

Logistic regression model:  $p(y = 1 | \mathbf{x}; \beta) = \sigma(\beta^{T} \mathbf{x}),$ 

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



 $p(y = 0 | \mathbf{x}; \beta) = 1 - p(y = 1 | \mathbf{x}; \beta)$ 

Provides a score for each possible outcome y = 0 or y = 1

#### Example: Interpretation of Hypothesis Output

Example: Ocular tumor diagnosis from size  $x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ tumorSize \end{bmatrix}$ 

$$p(y = 1 \mid \boldsymbol{x}; \beta) = \sigma(\beta^{\mathsf{T}}\boldsymbol{x}),$$

→ Tumor has a 85% chance of being class 1: malignant



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#### **Decision Boundary?**

Exercise: What happens to *x* at infinite +/- distance from boundary?

$$p(y = 1 \mid \boldsymbol{x}; \beta) = \sigma(\beta^T \boldsymbol{x}) = 0.5$$

So, decision boundary is at:

$$\beta^T \boldsymbol{x} = 0$$

Consistent with:

Predict 
$$y_i$$
 = class 1 if  $\beta^T x_i \ge 0$   
Predict  $y_i$  = class 0 if  $\beta^T x_i < 0$ 



We now have a model class that can predict meaningful binary class probabilities!

#### Soft Non-Linear Decision Boundaries

Same feature expansion trick still works.

$$\boldsymbol{x} = \begin{bmatrix} 1 \\ x_1 \\ x_2 \end{bmatrix} \rightarrow \begin{bmatrix} 1 \\ x_1 x_2 \\ x_1 x_2 \\ x_1^2 \\ x_2^2 \\ x_1^2 x_2 \\ x_1 x_2^2 \\ x_1 x_2^2 \\ x_1 x_2^2 \\ \vdots \end{bmatrix}$$



#### And Now, A Probability-Based Loss Function for Classification

#### "Likelihood" of Data Under a Model

"Likelihood"  $l_D(\beta)$  of data  $D = \{(x_1, y_1), ..., (x_N, y_N)\}$  under some probabilistic model with parameters  $\beta$  describes, loosely:

<u>""" if this model assigned labels to each  $x_i$  in the data, what is the probability</u> <u>that it would assign exactly the true labels  $y_i$  in  $\mathcal{D}$ "?</u>

Which of these datasets has high likelihood under this model?



#### "Likelihood" of Data Under a Model

• In practice, the dataset is fixed, and we are looking to find good models.

Which of these models does the data have high likelihood under?





#### "Likelihood" of Data Under a LogReg Model

"Likelihood"  $l_{\mathcal{D}}(\boldsymbol{\beta})$ : "What is the probability that the model with parameters  $\boldsymbol{\beta}$  would assign labels  $y_i$  to the samples  $\boldsymbol{x}_i$  for all  $(\boldsymbol{x}_i, y_i)_{i=1}^N$  in the dataset  $\mathcal{D}$ ?"

For a single sample dataset  $\mathcal{D} = \{(x_1, y_1)\}$ , this would be:

$$p(y_1|\boldsymbol{x}_1;\boldsymbol{\beta}) = p(y = y_1 | \boldsymbol{x} = \boldsymbol{x}_1;\boldsymbol{\theta}) = \begin{cases} \sigma(\boldsymbol{\beta}^T \boldsymbol{x}_1) & \text{if } y_1 = 1\\ 1 - \sigma(\boldsymbol{\beta}^T \boldsymbol{x}_1) & \text{if } y_1 = 0 \end{cases}$$

For a dataset  $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^N$  with N samples:  $l_{\mathcal{D}}(\boldsymbol{\beta}) = \prod_{i=1}^N p(y_i | \mathbf{x}_i; \boldsymbol{\beta})$ 

> Because independent assignment of y<sub>i</sub>s to x<sub>i</sub>s Recall: joint probability of two "*independent"* events = product of their probabilities.

#### "Maximum Likelihood Estimation"

**"Likelihood"** of a dataset  $\mathcal{D}$  with N samples under model with parameters  $\boldsymbol{\beta}$ :  $l_{\mathcal{D}}(\boldsymbol{\beta}) = \prod_{N} p(y_i \mid \boldsymbol{x_i}; \boldsymbol{\beta})$ 

We are looking for the  $\beta$  that maximizes the likelihood of the training data, so the optimal  $\beta$  is the "maximum likelihood estimate" (MLE):

$$\boldsymbol{\beta}_{MLE} = \arg \max_{\boldsymbol{\beta}} l_{\mathcal{D}}(\boldsymbol{\beta}) = \arg \max_{\boldsymbol{\beta}} \prod_{i=1}^{n} p(y_i \mid \boldsymbol{x}_i; \boldsymbol{\beta})$$

Note: Since each probability is in [0,1], this product is a very small number. What happens if you multiply 0.1 by itself 10,000 times in a computer? Bad things!

#### "Log Likelihood" Objective

Need to solve 
$$\beta_{MLE} = \arg \max_{\beta} l(\beta) = \arg \max_{\beta} \prod_{i=1}^{N} p(y_i | x_i; \beta)$$

Since the logarithm is always higher for higher numbers, we can take the log without changing the optimal  $\beta$ :

$$\boldsymbol{\beta}_{MLE} = \arg \max_{\boldsymbol{\beta}} l(\boldsymbol{\beta}) = \arg \max_{\boldsymbol{\beta}} \prod_{i=1}^{N} p(y_i \mid \boldsymbol{x}_i; \boldsymbol{\beta})$$
  
=  $\arg \max_{\boldsymbol{\beta}} \sum_{i=1}^{N} \log p(y_i \mid \boldsymbol{x}_i; \boldsymbol{\beta})$  This is called the log likelihood  
Sum avoids underflow

Just to avoid writing this expression on two lines, let's write this as:

$$\log p(y_i \mid \boldsymbol{x_i}; \boldsymbol{\beta}) = [y_i \log h_{\boldsymbol{\beta}}(\boldsymbol{x_i}) + (1 - y_i) \log(1 - h_{\boldsymbol{\beta}}(\boldsymbol{x_i}))]$$

#### Summing up the Logistic Regression Loss Function

$$\boldsymbol{\beta}_{MLE} = \arg\min_{\boldsymbol{\beta}} - \sum_{i=1}^{N} \log p(y_i \mid \boldsymbol{x}_i; \boldsymbol{\beta})$$

$$\log p(y_i \mid \boldsymbol{x_i}; \boldsymbol{\beta}) = [y_i \log h_{\boldsymbol{\beta}}(\boldsymbol{x_i}) + (1 - y_i) \log(1 - h_{\boldsymbol{\beta}}(\boldsymbol{x_i}))]$$

Logistic regression maximum likelihood loss function:  

$$\min_{\theta} - \sum_{i=1}^{N} \left[ y_i \log h_{\beta}(x_i) + (1 - y_i) \log(1 - h_{\beta}(x_i)) \right]$$

#### Thought Exercise: Maximum Likelihood More Broadly

- Maximum likelihood estimation is a general framework for thinking about objective function design for ML problems.
- In fact, the linear regression objective (MSE) can also be viewed as the negative log-likelihood of the training dataset under the model.
- Try to think through how: In particular, what form should  $p(y|x;\beta) = \beta^T x$ take so that log likelihood $(\beta) \approx -\frac{1}{N} \sum_{D} (\beta^T x_i - y_i)^2$

#### Intuition on the Logistic Regression Max-Likelihood Objective

• Loss for example *i* is

$$\begin{cases} -\log(\sigma(\beta^{\mathsf{T}}x_i)) & \text{if } y_i = 1\\ -\log(1 - \sigma(\beta^{\mathsf{T}}x_i)) & \text{if } y_i = 0 \end{cases}$$



Renn Engineering

• Loss for example *i* is

$$\begin{cases} -\log(\sigma(\beta^{\mathsf{T}}x_i)) & \text{if } y_i = 1\\ -\log(1 - \sigma(\beta^{\mathsf{T}}x_i)) & \text{if } y_i = 0 \end{cases}$$



• If 
$$y_i = 1$$
:  
• If  $p_\beta(Y = 1 | x_i) = 1$ , then  $loss = 0$   
• As  $p_\beta(Y = 1 | x_i) \rightarrow 0$ ,  $loss \rightarrow \infty$ 



$$-y_i \cdot \log(\sigma(\beta^{\top} x_i)) - (1 - y_i) \cdot \log(1 - \sigma(\beta^{\top} x_i))$$

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• If 
$$y_i = 1$$
:  
• If  $p_\beta(Y = 1 | x_i) = 1$ , then loss = 0  
• As  $p_\beta(Y = 1 | x_i) \rightarrow 0$ , loss  $\rightarrow \infty$ 

• If 
$$y_i = 0$$
  
• If  $p_\beta(Y = 0 \mid x_i) = 1$ , then loss = 0  
• As  $p_\beta(Y = 0 \mid x_i) \rightarrow 0$ , loss  $\rightarrow \infty$ 



$$y_i \cdot \log(\sigma(\beta^{\mathsf{T}} x_i)) - (1 - y_i) \cdot \log(1 - \sigma(\beta^{\mathsf{T}} x_i))$$

Renn Engineering

#### Optimizing the Logistic Regression Objective

#### **Optimization for Logistic Regression**

• To optimize the NLL loss, we need its gradient:

$$\nabla_{\beta}\ell(\beta;Z) = -\sum_{i=1}^{n} y_{i} \cdot \nabla_{\beta}\log(\sigma(\beta^{\mathsf{T}}x_{i})) + (1-y_{i}) \cdot \nabla_{\beta}\log(1-\sigma(\beta^{\mathsf{T}}x_{i}))$$

$$= -\sum_{i=1}^{n} y_{i} \cdot \frac{\nabla_{\beta}\sigma(\beta^{\mathsf{T}}x_{i})}{\sigma(\beta^{\mathsf{T}}x_{i})} - (1-y_{i}) \cdot \frac{\nabla_{\beta}\sigma(\beta^{\mathsf{T}}x_{i})}{1-\sigma(\beta^{\mathsf{T}}x_{i})}$$

$$= -\sum_{i=1}^{n} y_{i} \cdot \frac{\sigma(\beta^{\mathsf{T}}x_{i})(1-\sigma(\beta^{\mathsf{T}}x_{i})) \cdot x_{i}}{\sigma(\beta^{\mathsf{T}}x_{i})} - (1-y_{i}) \cdot \frac{\sigma(\beta^{\mathsf{T}}x_{i})(1-\sigma(\beta^{\mathsf{T}}x_{i})) \cdot x_{i}}{1-\sigma(\beta^{\mathsf{T}}x_{i})}$$

$$= -\sum_{i=1}^{n} y_{i} \cdot (1-\sigma(\beta^{\mathsf{T}}x_{i})) \cdot x_{i} - (1-y_{i}) \cdot \sigma(\beta^{\mathsf{T}}x_{i}) \cdot x_{i}$$

$$= -\sum_{i=1}^{n} (y_{i} - \sigma(\beta^{\mathsf{T}}x_{i})) \cdot x_{i}$$

#### **Optimization for Logistic Regression**

• Gradient of NLL:

$$\nabla_{\beta} \ell(\beta; \mathbf{Z}) = \sum_{i=1}^{n} (\sigma(\beta^{\mathsf{T}} \mathbf{x}_{i}) - \mathbf{y}_{i}) \cdot \mathbf{x}_{i}$$

- Surprisingly similar to the gradient for linear regression!
   Only difference is the σ
- Gradient descent works as before
  - No closed-form solution for  $\hat{\beta}(Z)$

#### **Gradient Descent for Logistic Regression**

