Lecture 10 (part 1): Iterative Optimization with Gradient Descent

COMP90049 Introduction to Machine Learning

Semester 1, 2024

Ting Dang, CIS

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Acknowledgement: Lea Frermann



Roadmap

So far...

- Naive Bayes Classifier theory and practice
- · MLE estimation of parameters
- · Exact optimization

Now: Quick aside on iterative optimization

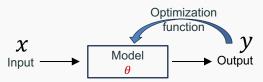
- · Gradient Descent
- · Global and local optima



Finding Optimal Points I

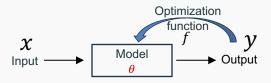
Finding the parameters that optimize a target

- Ex1: Estimate the study time which leads to the **best grade** in COMP90049.
- Ex2: Find the shoe price which leads to maximum profit of our shoe shop.
- Ex3: Predicting **housing prices** from a **weighted** combination of house age and house location
- Ex4: Find the parameters θ of a spam classifier which lead to the **lowest error**
- Ex5: Find the parameters θ of a spam classifier which lead to the **highest** data log likelihood





Recipe for finding Minima / Maxima



- 1. Define your function of interest $f(y|x,\theta)$ (e.g., data log likelihood)
- 2. Compute its first derivative wrt its input θ
- 3. Set the derivative to zero
- 4. Solve for θ



Closed-form vs Iterative Optimization

Closed-form solutions

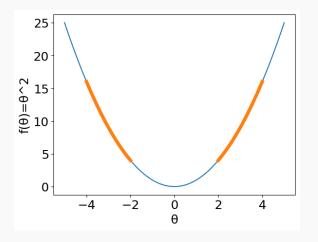
- Previously, we computed the closed form solution for the MLE of the binomial distribution
- · We follow our recipe, and arrive at a single solution

Unfortunately, life is not always as easy

- · Often, no closed-form solution exists
- Instead, we have to **iteratively** improve our estimate of $\hat{\theta}$ until we arrive at a satisfactory solution
- · Gradient descent is one popular iterative optimization method



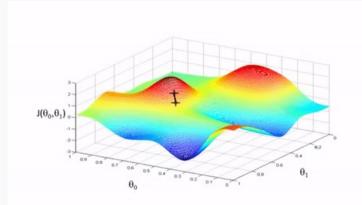
'Descending' the function to find the Optimum



- 1-dimensional case: find parameter θ that minimizes the function
- · follow the curvature of the line step by step



'Descending' the function to find the Optimum



- 2-dimensional case: find parameters $\theta = [\theta_0, \theta_1]$ that minimize the function J
- follow the curvature step by step along the steepest way



Gradient Descent: Intuition

Intuition

- Descending a mountain (aka. our function) as fast as possible: at every position take the next step that takes you most directly into the valley
- We compute a series of solutions θ⁽⁰⁾, θ⁽¹⁾, θ⁽²⁾, ... by 'walking' along the function and taking steps in the direction with the steepest local slope (or gradient).
- · each solution depends on the current location



Gradient Descent: Details

Learn the model parameters θ

- · such that we minimize the error
- traverse over the loss function step by step ('descending into a valley')
- · we would like an algorithm that tells how to update our parameters

$$\theta \leftarrow \theta + \Delta \theta$$



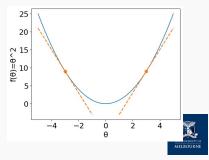
Gradient Descent: Details

Learn the model parameters θ

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- traverse over the loss function step by step ('descending into a valley')
- we would like an algorithm that tells how to update our parameters

$$\theta \leftarrow \theta + \Delta \theta$$

- $\Delta\theta = \frac{\partial f(\theta)}{\partial \theta}$ is the **derivative**, a measure of change in the function f given a change in θ
- the derivative measures the **slope** or **gradient** of a function f at point θ
- for a function $f(\theta)$, $\frac{\partial f(\theta)}{\partial \theta}$ tells us how much f changes in response to a change in θ .



Gradient Descent: Details

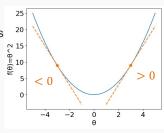
Learn the model parameters θ

- such that we minimize the error
- traverse over the loss function step by step ('descending into a valley')
- we would like an algorithm that tells how to update our parameters

$$\theta \leftarrow \theta + \Delta \theta$$

- if $\frac{\partial f(\theta)}{\partial \theta}$ > 0: $f(\theta)$ increases as θ increases if $\frac{\partial f(\theta)}{\partial \theta}$ < 0: $f(\theta)$ increases as θ decreases
- if $\frac{\partial f(\theta)}{\partial a}$ = 0: we are at a minimum (or maximum)
- so, to approach the minimum:

$$\theta \leftarrow \theta - \eta \ \frac{\partial f}{\partial \theta}$$





Gradient Descent for multiple parameters

- Usually, our models have several parameters which need to be optimized to minimize the error
- We compute **partial derivatives** of $f(\theta)$ wrt. individual θ
- Partial derivatives measure change in a function of multiple parameters given a change in a single parameter, with all others held constant
- For example for $f(\theta_1,\theta_2)$ we can compute $\frac{\partial f}{\partial \theta_1}$ and $\frac{\partial f}{\partial \theta_2}$



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- Partial derivatives measure change in a function of multiple parameters given a change in a single parameter, with all others held constant
- For example for $f(\theta_1, \theta_2)$ we can compute $\frac{\partial f}{\partial \theta_1}$ and $\frac{\partial f}{\partial \theta_2}$
- We then update each parameter individually

$$\theta_1 \leftarrow \theta_1 \cdot \Delta \theta_1$$
 with $\Delta \theta_1 = \eta \frac{\partial f}{\partial \theta_1}$
 $\theta_2 \leftarrow \theta_2 \cdot \Delta \theta_2$ with $\Delta \theta_2 = \eta \frac{\partial f}{\partial \theta_2}$



Gradient Descent: Recipe

Recipe for Gradient Descent (single parameter)

- 1: Define objective function $f(\theta)$
- 2: Initialize parameter $\theta^{(0)}$
- 3: **for** iteration $t \in \{0, 1, 2, ... T\}$ **do**
- 4: Compute the first derivative of f at that point $\theta^{(t)} : \frac{\partial f}{\partial \theta^t}$
- 5: Update your parameter by subtracting the (scaled) derivative

$$\theta^{t+1} \leftarrow \theta^t - \eta \frac{\partial f}{\partial \theta^t}$$

- η is the step size or learning rate, a parameter
- When to stop? Fix number of iterations, or define other criteria

$$f(\theta^{t+1}) - f(\theta^t) < \gamma$$



Gradient Descent: Recipe

Recipe for Gradient Descent (multiple parameters)

- 1: Define objective function $f(\theta)$
- 2: Initialize parameters $\{\theta_1^{(0)}, \theta_2^{(0)}, \theta_3^{(0)}, \ldots\}$
- 3: **for** iteration $t \in \{0, 1, 2, ... T\}$ **do**
- 4: Initialize vector of *gradients* ← []
- 5: **for** parameter $f \in \{1, 2, 3, ...F\}$ **do**
- 6: Compute the first derivative of f at that point $\theta^{(t)}$: $\frac{\partial f}{\partial \theta_i^t}$
- 7: append $\frac{\partial f}{\partial \theta_i^t}$ to *gradients*
- 8: **Update all** parameters by subtracting the (scaled) gradient

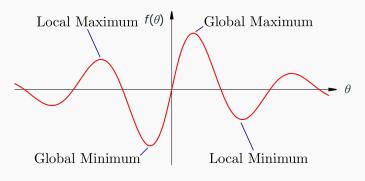
$$\theta_i^{t+1} \leftarrow \theta_i^t - \eta \frac{\partial f}{\partial \theta_i^t}$$



Aside: Global and Local Minima and Maxima

Possible issue: local maxima and minima!

- A global **maximum** is the single highest value of the function
- A global **minimum** is the single lowest value of the function
- A function is convex if a line between any two points of the function lies above the function





Gradient Descent Guarantees

- with an appropriate learning rate, GD will find the global minimum for differentiable convex functions
- with an appropriate learning rate, GD will find a local minimum for differentiable non-convex functions

Equivalently, Gradient Ascent ("GA") would find the global maximum (case 1.) and local maximum (case 2.)



Summary

Now you know:

- What optimization is, and why it's important
- How to do closed-form optimization (aka. "set the derivative of f(θ) to zero and solve for θ)
- That closed-form solutions are not always computable
- · In that case, iterative optimization can help us
- Gradient descent is one instance of an iterative optimization method
- · How gradient descent works!

Next lecture(s)

Logistic Regression



Lecture 10 (part 2): Logistic Regression

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Roadmap

Sofar...

- Decision Trees, Naive Bayes and KNN
- · Optimization (closed-form and iterative)
- Evaluation + Feature Selection

Today: back to classification!

· Logistic Regression



Logistic Regression



Quick Refresher

Recall Naive Bayes

$$P(x,y) = P(y)P(x|y) = \prod_{i=1}^{N} P(y^{i}) \prod_{m=1}^{M} P(x_{m}^{i}|y^{i})$$

- a **probabilistic generative model** of the joint probability P(x,y)
- · optimized to maximize the likelihood of the observed data
- naive due to unrealistic feature independence assumptions



Recall Naive Bayes

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- a **probabilistic generative model** of the joint probability P(x,y)
- · optimized to maximize the likelihood of the observed data
- naive due to unrealistic feature independence assumptions

For prediction, we apply Bayes Rule to obtain the conditional distribution

$$P(x,y) = P(y)P(x|y) = P(x)P(y|x)$$

$$P(y|x) = \frac{P(y)P(x|y)}{P(x)}$$

$$\hat{y} = \underset{y}{\operatorname{argmax}} P(y|x) \approx P(y)P(x|y)$$

How about we model P(y|x) directly? \rightarrow Logistic Regression



Introduction to Logistic Regression

Logistic Regression on a high level

- Is a binary classification model
- Is a **probabilistic discriminative model** because it optimizes P(y|x) directly
- Learns to optimally discriminate between inputs which belong to different classes
- No model of $P(x/y) \rightarrow$ no conditional feature independence assumption



Aside: Linear Regression

• Regression: predict a real-valued quantity *y* given features *x*, e.g.,

```
housing price given {location, size, age, ...}
success of movie ($) given {cast, genre, budget, ...}
air quality given {temperature, timeOfDay, CO2, ...}
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```

- linear regression is the simplet regression model
- a real-valued ŷ is predicted as a linear combination of weighted feature values

$$\hat{y} = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \dots = \theta_0 + \sum_i \theta_i x_i$$

- The weights $\theta_0, \theta_1, \dots$ are model parameters, and need to be optimized during training
- Loss (error) is the sum of squared errors (SSE): $L = \sum_{i=1}^{N} (\hat{y}^i y^i)^2$

- Let's assume a binary classification task, y is true (1) or false (0).
- We model **probabilites** $P(y = 1/x; \theta)$ as a function of observations x under parameters θ .
- We want to use a **regression** approach



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- How about: $P(y = 1/x; \theta)$ as a linear function of x. Problem: probabilities are bounded in 0 and 1, linear functions are not.

$$P(y = 1/x; \theta) = \theta_0 + \theta_1 x_1 + ... \theta_F x_F$$



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- How about: P(y = 1/x;θ) as a linear function of x. Problem: probabilities are bounded in 0 and 1, linear functions are not.
- How about: $log P(y = 1/x; \theta)$ as a linear function of x. Problem: log is bounded in one direction, linear functions are not.

$$\log P(y = 1/x; \theta) = \theta_0 + \theta_1 x_1 + ... \theta_F x_F$$



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- · We want to use a regression approach
- How about: P(y = 1/x; θ) as a linear function of x. Problem: probabilities are bounded in 0 and 1, linear functions are not.
- How about: $log P(y = -1/x; \theta)$ as a linear function of x. Problem: log is bounded in one direction, linear functions are not.
- How about: minimally modifying $log P(y = 1/x; \theta)$ such that is is unbounded, by applying the **logistic** transformation

$$\log \frac{P(y=1|x;\theta)}{1 - P(y=1|x;\theta)} = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_F x_F$$



$$\log \frac{P(y=1|x;\theta)}{1-P(y=1|x;\theta)} = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_F x_F$$

- also called the log odds
- the odds are defined as the fraction of success over the fraction of failures

$$odds = \frac{P(success)}{P(failures)} = \frac{P(success)}{1 - P(success)}$$

• e.g., the odds of rolling a 6 with a fair dice are:

$$\frac{1/6}{1 - (1/6)} = \frac{0.17}{0.83} = 0.2$$

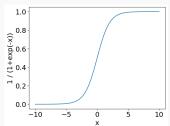


$$\log \frac{P(y=1|x;\theta)}{1 - P(y=1|x;\theta)} = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_F x_F$$

If we rearrange and solve for $P(y = 1|x; \theta)$, we get

$$P(y = 1|x; \theta) = \frac{\exp(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_F x_F)}{1 + \exp(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_F x_F)}$$
$$= \frac{\exp(\theta_0 + \sum_i \theta_i x_i)}{1 + \exp(\theta_0 + \sum_i \theta_i x_i)} = \frac{1}{1 + \exp(-(\theta_0 + \sum_i \theta_i x_i))}$$

- The inverse logit (or logistic function)
- we pass a regression model through the logistic function to obtain a valid probability predicton



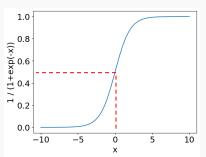


Logistic Regression: Interpretation

$$P(y = 1|x; \theta) = \frac{1}{1 + \exp(-(\theta_0 + \sum_i \theta_i x_i))}$$

A closer look at the logistic function

Most inputs lead to P(y/x)=0 or P(y/x)=1. That is intended, because all true labels are either 0 or 1.



- $(\theta_0 + \sum_i \theta_i x_i) > 0$ means y=1
- $(\theta_0 + \sum_i \theta_i x_i) \approx 0$ means most uncertainty
- $(\theta_0 + \sum_i \theta_i x_i) < 0$ means y=0



Example!

$$P(y=1|x;\theta) = \frac{1}{1 + \exp(-(\theta_0 + \sum_i \theta_i x_i))} = \frac{1}{1 + \exp(-(\boldsymbol{\theta}^T \boldsymbol{X}))} = \sigma(\boldsymbol{\theta}^T \boldsymbol{X})$$

Model parameters

$$\theta = [0.1, -3.5, 0.7, 2.1]$$
 $\theta_0 \quad \theta_1 \quad \theta_2 \quad \theta_3$

Feature Function

$$x_0 = 1 \text{ (bias term)}$$

$$x_1 = \begin{cases} 1 \text{ if outlook} = sunny \\ 2 \text{ if outlook} = overcast \\ 3 \text{ if outlook} = rainy \end{cases}$$

$$\begin{cases} 1 \text{ if temp} = hot \end{cases}$$

$$x_2 = \begin{cases} 1 & \text{if } temp = hot \\ 2 & \text{if } temp = mild \\ 3 & \text{if } temp = cool \end{cases}$$

$$x_3 = \begin{cases} 1 & \text{if } humidity = normal \\ 2 & \text{if } humidity = high \end{cases}$$

(Small) Test Data set

`	Outlook	Temp	Humidity	Class
	rainy	cool	normal	0
	sunny	hot	high	1



Parameter Estimation

What are the four steps we would follow in finding the optimal parameters?



Objective Function

Mimimize the Negative conditional log likelihood

$$L(\theta) = -P(y|x;\theta) = -\prod_{i=1}^{N} P(y_i|x_i;\theta)$$

note that

$$P(y = 1|x; \theta) = \sigma(\theta^{T}X)$$

$$P(y = 0|x; \theta) = 1 - \sigma(\theta^{T}X)$$



Objective Function

Mimimize the Negative conditional log likelihood

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SO

$$L(\theta) = -P(y|x;\theta) = -\prod_{i=1}^{N} P(y_i|x_i;\theta)$$
$$= -\prod_{i=1}^{N} \left(\sigma(\boldsymbol{\theta}^T \boldsymbol{X})\right)^{y_i} \left(1 - \sigma(\boldsymbol{\theta}^T \boldsymbol{X})\right)^{1-y_i}$$

take the log of this function

$$\log L(\theta) = -\sum_{i=1}^{N} \left[y_i log \sigma(\theta^T X) + (1 - y_i) \log \left(1 - \sigma(\theta^T X) \right) \right]$$



$$\log L(\theta) = -\sum_{i=1}^{N} \left[y_i log \sigma(\boldsymbol{\theta}^T \boldsymbol{X}) + (1 - y_i) \log \left(1 - \sigma(\boldsymbol{\theta}^T \boldsymbol{X}) \right) \right]$$

- The derivative of the logistic (sigmoid) function is $\frac{\partial \sigma(z)}{\partial z} = \sigma(z)[1 \sigma(z)]$
- The chain rule tells us that $\frac{\partial A}{\partial D} = \frac{\partial A}{\partial B} \times \frac{\partial B}{\partial C} \times \frac{\partial C}{\partial D}$



$$L = \log L(\theta) = -\sum_{i=1}^{N} \left[y_i log \sigma(\boldsymbol{\theta}^T \boldsymbol{X}) + (1 - y_i) \log \left(1 - \sigma(\boldsymbol{\theta}^T \boldsymbol{X}) \right) \right]$$

Preliminaries

- The derivative of the logistic (sigmoid) function is $\frac{\partial \sigma(z)}{\partial z} = \sigma(z)[1 \sigma(z)]$
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Also

- Derivative of sum = sum of derivatives → focus on 1 training input
- Compute $\frac{\partial I}{\partial \theta_j}$ for each θ_j individually, so focus on 1 θ_j



$$L = \log L(\theta) = -\sum_{i=1}^{N} \left[y_i \log \sigma(\boldsymbol{\theta}^T \boldsymbol{X}) + (1 - y_i) \log \left(1 - \sigma(\boldsymbol{\theta}^T \boldsymbol{X}) \right) \right]$$

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$$\frac{\partial \log L(\theta)}{\partial \theta_j} = \frac{\partial \log L(\theta)}{\partial P} \times \frac{\partial P}{\partial z} \times \frac{\partial Z}{\partial \theta_j} \quad where \ P = \sigma(\boldsymbol{\theta}^T \boldsymbol{X}) \ and \quad z = \boldsymbol{\theta}^T \boldsymbol{X}$$



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$$\frac{\partial \log L(\theta)}{\partial \theta_{j}} = \frac{\partial \log L(\theta)}{\partial P} \times \frac{\partial P}{\partial z} \times \frac{\partial z}{\partial \theta_{j}} \quad where \ P = \sigma(\boldsymbol{\theta}^{T}\boldsymbol{X}) \ and \quad z = \boldsymbol{\theta}^{T}\boldsymbol{X}$$

$$\downarrow \qquad \qquad \qquad \frac{\partial \log L(\theta)}{\partial P} = -(\frac{y}{P} - \frac{1 - y}{1 - P})$$

because
$$\log L(\theta) = -[ylogP + (1-y)\log(1-P)]$$



$$\log L(\theta) = -\sum_{i=1}^{N} y_i \log \sigma(\boldsymbol{\theta}^T \boldsymbol{X}_i) + (1 - y_i) \log(1 - \sigma(\boldsymbol{\theta}^T \boldsymbol{X}_i))$$

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$$\frac{\partial P}{\partial z} = \frac{\partial \sigma(z)}{\partial z} = \sigma(z)(1 - \sigma(z))$$



$$\log L(\theta) = -\sum_{i=1}^{N} y_i log \sigma(\theta^T X_i) + (1 - y_i) \log(1 - \sigma(\theta^T X_i))$$

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$$\frac{\partial z}{\partial \theta_{j}} = \frac{\partial \theta^{T}X}{\partial \theta_{j}} = x^{j}$$



$$\log L(\theta) = -\sum_{i=1}^{N} y_i log \sigma(\theta^T X_i) + (1 - y_i) \log(1 - \sigma(\theta^T X_i))$$

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$$\begin{split} \frac{\partial \log L(\theta)}{\partial \theta_{j}} &= \frac{\partial \log L(\theta)}{\partial P} \times \frac{\partial P}{\partial z} \times \frac{\partial Z}{\partial \theta_{j}} & where \ P = \sigma(\theta^{T}X) \ and \quad z = \theta^{T}X \\ &= -\left(\frac{y}{P} - \frac{1 - y}{1 - P}\right) \times \sigma(z) \left(1 - \sigma(z)\right) \times x^{j} \end{split}$$



$$\log L(\theta) = -\sum_{i=1}^{N} y_i log \sigma(\theta^T X_i) + (1 - y_i) \log(1 - \sigma(\theta^T X_i))$$

- The derivative of the logistic (sigmoid) function is $\frac{\partial \sigma(z)}{\partial z} = \sigma(z)[1 \sigma(z)]$
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Logistic Regression: Parameter Estimation III

The derivative of the log likelihood wrt. a single parameter θ_i for **all** training examples

$$\frac{\partial \log L(\theta)}{\partial \theta_j} = \sum_{i=1}^{N} (\sigma(\theta^T x^i) - y^i) x_j^i$$

- Now, we would set derivatives to zero (Step 3) and solve for θ (Step 4)
- Unfortunately, that's not straightforward here (as for Naive Bayes)
- Instead, we will use iterative method: Gradient Descent



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- Unfortunately, that's not straightforward here (as for Naive Bayes)
- Instead, we will use an iterative method: Gradient Descent

$$\theta_{j}^{(new)} \leftarrow \theta_{j}^{(old)} - \eta \frac{\partial \log L(\theta)}{\partial \theta_{j}}$$



Multinomial Logistic Regression

• So far we looked at problems where either y = 0 or y = 1 (e.g., spam classification: $y \in \{\text{play}, \text{not play}\}\)$

$$P(y = 1/x; \theta) = o(\theta^{T} x) = \frac{exp(\theta^{T} x)}{1 + exp(\theta^{T} x)}$$

$$P(y = 0/x; \theta) = 1 - o(\theta^{T} x) = 1 - \frac{exp(\theta^{T} x)}{1 + exp(\theta^{T} x)}$$



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- But what if we have more than 2 classes, e.g., y ∈{positive, negative, neutral}
- we predict the probability of each class c by passing the input representation through the softmax function, a generalization of the sigmoid

$$P(y = c | x; \theta) = \frac{\exp(\theta_c x)}{\sum_k \exp(\theta_k x)}$$

• we learn a parameter vector θ_c for each class c



Example! Multi-class with 1-hot features

$$P(y = c|x; \theta) = \frac{\exp(\theta_c x)}{\sum_k \exp(\theta_k x)}$$

(Small) Test Data set

Outlook	Temp	Humidity	Class
rainy	cool	normal	0 (don't play)
sunny	cool	normal	1 (maybe play)
sunny	hot	high	2 (play)

Feature Function

$$x_0 = 1 \text{ (bias term)}$$

$$x_1 = \begin{cases} 1 & if \ outlook = sunny \\ 2 & if \ outlook = overcast \\ 3 & if \ outlook = rainy \end{cases}$$

$$x_2 = \begin{cases} 1 & \text{if } temp = hot \\ 2 & \text{if } temp = mild \\ 3 & \text{if } temp = cool \end{cases}$$

$$x_3 = \left\{ \begin{array}{l} 1 \ if \ humidity = normal \\ 2 \ if \ humidity = high \end{array} \right.$$



Example! Multi-class with 1-hot features

$$P(y = c|x; \theta) = \frac{\exp(\theta_c x)}{\sum_k \exp(\theta_k x)}$$

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Outlook	Temp	Humidity	Class
rainy	cool	normal	0 (don't play)
sunny	cool	normal	1 (maybe play)
sunny	hot	high	2 (play)

Feature Function

Model parameters

$$x_{0} = 1 \text{ (bias term)} \qquad \theta_{c0}$$

$$x_{1} = \begin{cases} 1 \text{ if outlook} = \text{sunny} \\ 2 \text{ if outlook} = \text{overcast} \\ 3 \text{ if outlook} = \text{rainy} \end{cases} \qquad [0.1, 0.7, 0.2, -3.5, -3.5, 0.7, 2.1]$$

$$x_{2} = \begin{cases} 1 \text{ if temp} = \text{hot} \\ 2 \text{ if temp} = \text{mild} \\ 3 \text{ if temp} = \text{cool} \end{cases} \qquad [0.6, 0.1, 0.9, 2.5, 2.5, 2.5, 2.7, -2.1]$$

$$x_{3} = \begin{cases} 1 \text{ if humidity} = \text{normal} \\ 2 \text{ if humidity} = \text{high} \end{cases}$$



Logistic Regression: Final Thoughts

Pros

- · Probabilistic interpretation
- No restrictive assumptions on features
- · Often outperforms Naive Bayes
- · Particularly suited to frequency-based features (so, popular in NLP)

Cons

- · Can only learn linear feature-data relationships
- · Some feature scaling issues
- · Often needs a lot of data to work well
- Regularisation a nuisance, but important since overfitting can be a big problem



Summary

- · Derivation of logistic regression
- Prediction
- · Derivation of maximum likelihood



References

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 $\underline{\text{https://www.stat.cmu.edu/}}{\sim} \underline{\text{cshalizi/ADAfaEPoV/ADAfaEPoV.pdf}}$

Dan Jurafsky and James H. Martin. *Speech and Language Processing*. Chapter 5. Online Draft V3.0.

https://web.stanford.edu/~jurafsky/slp3/



Step 2 Differentiate the loglikelihood wrt. the parameters

$$\log L(\theta) = -\sum_{i=1}^{N} y_i \log \sigma(\boldsymbol{\theta}^T \boldsymbol{X}_i) + (1 - y_i) \log(1 - \sigma(\boldsymbol{\theta}^T \boldsymbol{X}_i))$$

- The derivative of the logistic (sigmoid) function is $\frac{\partial \sigma(z)}{\partial z} = \sigma(z)[1 \sigma(z)]$
- The chain rule tells us that $\frac{\partial A}{\partial D} = \frac{\partial A}{\partial B} \times \frac{\partial B}{\partial C} \times \frac{\partial C}{\partial D}$



$$\log L(\theta) = -\sum_{i=1}^{N} y_i \log \sigma(\theta^T X_i) + (1 - y_i) \log(1 - \sigma(\theta^T X_i))$$

Preliminaries

- The derivative of the logistic (sigmoid) function is $\frac{\partial \sigma(z)}{\partial z} = \sigma(z)[1 \sigma(z)]$
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Also

- Derivative of sum = sum of derivatives → focus on 1 training input
- Compute $\frac{\partial L}{\partial \theta_j}$ for each θ_j individually, so focus on 1 θ_j



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$$L = \log L(\theta) = -\sum_{i=1}^{N} \left[y_i log \sigma(\boldsymbol{\theta}^T \boldsymbol{X}) + (1 - y_i) \log \left(1 - \sigma(\boldsymbol{\theta}^T \boldsymbol{X}) \right) \right]$$

Preliminaries

- The derivative of the logistic (sigmoid) function is $\frac{\partial \sigma(z)}{\partial z} = \sigma(z)[1 \sigma(z)]$
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$$\frac{\partial \log L(\theta)}{\partial \theta_{j}} = \frac{\partial \log L(\theta)}{\partial P} \times \frac{\partial P}{\partial z} \times \frac{\partial z}{\partial \theta_{j}} \quad where \ P = \sigma(\boldsymbol{\theta}^{T}\boldsymbol{X}) \ and \quad z = \boldsymbol{\theta}^{T}\boldsymbol{X}$$

$$\frac{\partial \log L(\theta)}{\partial P} = -\frac{y}{P} - \frac{1 - y}{1 - P}$$

because $\log L(\theta) = -[ylogP + (1-y)\log(1-P)]$



$$\log L(\theta) = -\sum_{i=1}^{N} y_i log \sigma(\boldsymbol{\theta}^T \boldsymbol{X}_i) + (1 - y_i) \log(1 - \sigma(\boldsymbol{\theta}^T \boldsymbol{X}_i))$$

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$$\frac{\partial \log L(\theta)}{\partial \theta_j} = \frac{\partial \log L(\theta)}{\partial P} \times \frac{\partial P}{\partial z} \times \frac{\partial z}{\partial \theta_j} \quad \text{where } P = \sigma(\boldsymbol{\theta}^T \boldsymbol{X}) \text{ and } \quad z = \boldsymbol{\theta}^T \boldsymbol{X}$$

$$\frac{\partial P}{\partial z} = \frac{\partial \sigma(z)}{\partial z} = \sigma(z)(1 - \sigma(z))$$



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$$\frac{\partial z}{\partial \theta_{i}} = \frac{\partial \theta^{T}X}{\partial \theta_{i}} = x^{j}$$



$$\log L(\theta) = -\sum_{i=1}^{N} y_i log \sigma(\boldsymbol{\theta}^T \boldsymbol{X}_i) + (1 - y_i) \log(1 - \sigma(\boldsymbol{\theta}^T \boldsymbol{X}_i))$$

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$$\begin{split} \frac{\partial \log L(\theta)}{\partial \theta_{j}} &= \frac{\partial \log L(\theta)}{\partial P} \times \frac{\partial P}{\partial z} \times \frac{\partial Z}{\partial \theta_{j}} & where \ P = \sigma(\theta^{T}X) \ and \quad z = \theta^{T}X \\ &= -\left(\frac{y}{P} - \frac{1 - y}{1 - P}\right) \times \sigma(z) \left(1 - \sigma(z)\right) \times x^{j} \end{split}$$



Step 2 Differentiate the loglikelihood wrt. the parameters

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Preliminaries

 $= -(v(1-P) - P(1-v)) \times x^{j}$

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$$= -\left(\frac{y}{P} - \frac{1 - y}{1 - P}\right) \times \sigma(z)(1 - \sigma(z)) \times x^{j} \quad \text{[[combine 3 derivatives]]}$$

$$= -\left(\frac{y(1 - P)}{P(1 - P)} - \frac{P(1 - y)}{P(1 - P)}\right) \times P(1 - P) \times x^{j} \quad \text{[[} o(z) = p]\text{]}$$

$$= -\left(\frac{y(1 - P)}{P(1 - P)} - \frac{P(1 - y)}{P(1 - P)}\right) \times P(1 - P) \times x^{j} \quad \text{[[} x \times \frac{P(1 - P)}{P(1 - P)}\text{]]}$$



[[cancel terms]]

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$$\begin{split} \frac{\partial \log L(\theta)}{\partial \theta_{j}} &= \frac{\partial \log L(\theta)}{\partial P} \times \frac{\partial P}{\partial z} \times \frac{\partial Z}{\partial \theta_{j}} & \text{where } p = o(\theta^{T}x) \text{ and } z = \theta^{T}x \\ &= -(y(1-P)-P(1-y)) \times x^{j} & \text{[[copy from last slide]]} \\ &= -(y-yP-P+yP) \times x^{j} & \text{[[multiply out]]} \\ &= -(y-P) \times x^{j} & \text{[[-yP+yP=0]]} \\ &= (P-y) \times x^{j} & \text{[[-(y-P)=-y+P=P-y]]} \\ &= (\sigma(\theta^{T}X)-y) \times x^{j} & \text{[[P=\sigma(z), z=\theta^{T}x]]} \end{split}$$

