

CS2109S Tutorial 4

Classification and Logistic Regression

(AY 25/26 Semester 2)

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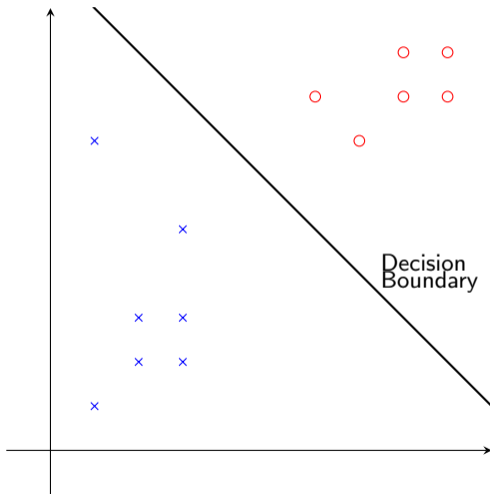
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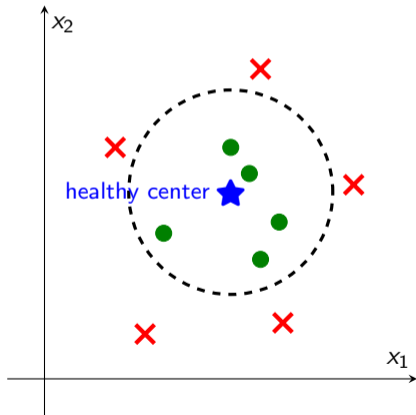
Recap: Classification

Target: Solve **classification** tasks.



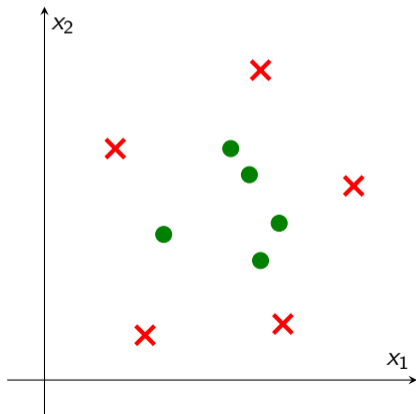
Q1. Tumor Classification

- (a) Describe the geometric pattern exhibited by the two classes.
- ▶ Concentric pattern where distance from the center correlates with tumor type.



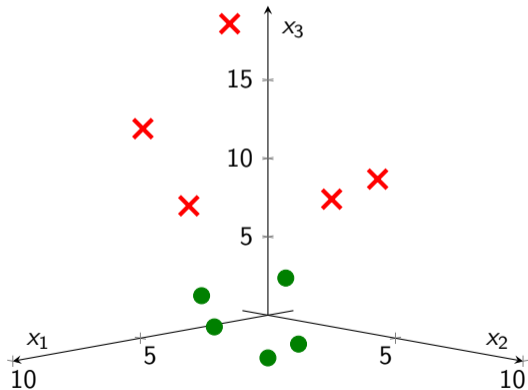
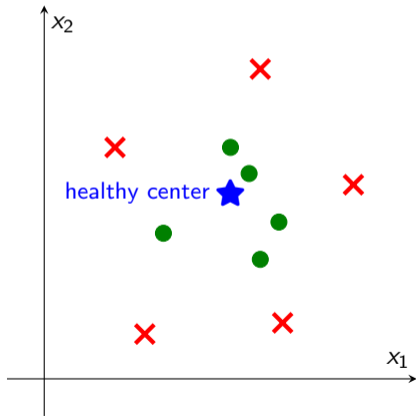
Q1. Tumor Classification

- (b) What if we train a logistic regression classifier using the feature space $[x_1, x_2]$?
- ▶ The two classes are not **linearly separable**.
 - ▶ The model will fail to classify all 10 samples correctly.



Q1. Tumor Classification

- (c) Add a new transformed feature $x_3 = (x_1 - 5)^2 + (x_2 - 5)^2$. What does this mean?
▶ The distance to the healthy center. Exactly what we need!



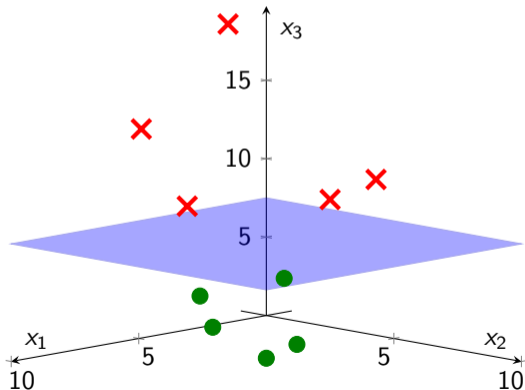
Q1. Tumor Classification

(d) Suggest a decision boundary in the new feature space $[x_1, x_2, x_3]$.

▶ $x_3 = 7.5$ is a possible decision boundary that perfectly classifies the data.

Then, classify a new sample $(x_1, x_2) = (6.0, 7.5)$.

▶ $x_3 = (6.0 - 5.0)^2 + (7.5 - 5.0)^2 = 7.25 < 7.5$, so we classify as Benign.

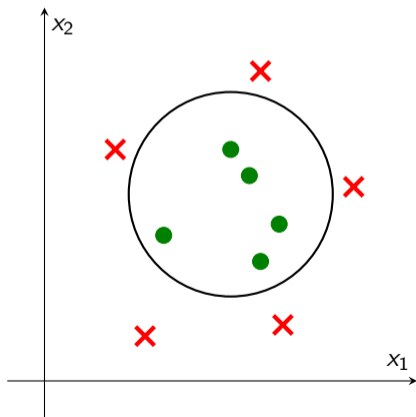


Sample	x_1	x_2	x_3	Label
A	5.5	5.5	0.50	Benign
B	5.0	6.2	1.44	Benign
C	3.2	3.9	4.45	Benign
D	5.8	3.2	3.88	Benign
E	6.3	4.2	2.33	Benign
F	8.3	5.2	10.93	Malignant
G	5.8	8.3	11.53	Malignant
H	1.9	6.2	11.05	Malignant
I	2.7	1.2	19.73	Malignant
J	6.4	1.5	14.21	Malignant

Q1. Tumor Classification

(e) Draw the decision boundary back in the original plot.

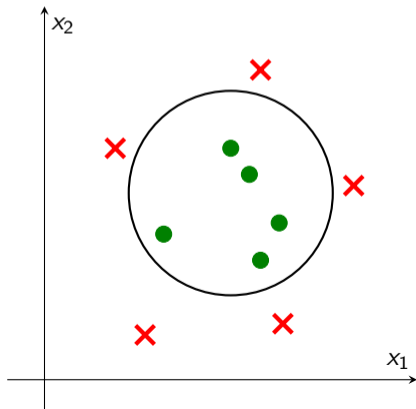
- ▶ $(x_1 - 5)^2 + (x_2 - 5)^2 = 7.5$.
- ▶ This is a circle! (i.e. non-linear decision boundary)



Discussion Question

The transformed feature x_3 added in this question is sort of idealized – we already “guessed” the pattern of the data correctly. In a practical scenario, if we realise this dataset is not linearly separable, what transformed features will we add instead?

- ▶ Usually we will add x_1^2 and x_2^2 .
- ▶ The model will learn the correct weights (coefficients) to produce the same circle.



Recap: Logistic Regression

Target: Solve **classification** tasks (output a **probability** between 0 and 1).

▶ First Try (regression): $p = \mathbf{w} \cdot \mathbf{x}$

▶ FAIL: $\mathbf{w} \cdot \mathbf{x}$ can be outside $[0, 1]$.

▶ Second Try (odds ratio): $\frac{p}{1-p} = \mathbf{w} \cdot \mathbf{x}$

▶ FAIL: $\frac{p}{1-p}$ is always non-negative, but $\mathbf{w} \cdot \mathbf{x}$ can be outside $[0, \infty)$.

▶ Third Try (logits): $\log\left(\frac{p}{1-p}\right) = \mathbf{w} \cdot \mathbf{x}$ (works!)

▶ Rearrange terms: $p = \frac{1}{1 + e^{-\mathbf{w} \cdot \mathbf{x}}}$

Recap: Logistic Regression

Hypothesis:

$$h_{\mathbf{w}}(x) = \frac{1}{1 + e^{-\mathbf{w}^T \mathbf{x}}} = \sigma(\mathbf{w}^T \mathbf{x})$$

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

Loss function:

- ▶ **Mean Squared Error** is not convex under logistic regression \Rightarrow gradient descent might not reach global minimum.
- ▶ Use **binary cross entropy loss** instead:

$$\begin{aligned} BCE(p) &= \begin{cases} -\log(p) & \text{if } y = 1 \\ -\log(1 - p) & \text{if } y = 0 \end{cases} \\ &= -y \log(p) - (1 - y) \log(1 - p) \end{aligned}$$

“surprisal” in entropy!

Q2. Loss function of Logistic Regression

Hypothesis:

$$h_{\mathbf{w}}(x) = p(y = 1 | x) = \sigma(\mathbf{w}^T \mathbf{x})$$

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

(a) Show that $p(y = 1 | x) = \sigma(z)$ where $z = \ln \left(\frac{p(y = 1 | x)}{p(y = 0 | x)} \right)$. **log odds ratio!**

$$z = \ln \left(\frac{p}{1 - p} \right)$$

$$e^z = \frac{p}{1 - p}$$

$$(1 - p)e^z = p$$

$$e^z = p(e^z + 1)$$

$$p = \frac{e^z}{e^z + 1} = \frac{1}{1 + e^{-z}}$$

Q2. Loss Function of Logistic Regression

Derivative of Sigmoid Function

Let $\sigma(z) = \frac{1}{1 + e^{-z}}$. We have $\sigma'(z) = \sigma(z)(1 - \sigma(z))$.

(b) Show that $\frac{\partial}{\partial w_j} BCE(y, \sigma(z)) = (\sigma(z) - y)x_j$, where

$$BCE(y, \sigma(z)) = -y \log \sigma(z) - (1 - y) \log(1 - \sigma(z))$$

$$\frac{\partial \log(p)}{\partial w_j} = \frac{1}{p} \cdot \frac{\partial p}{\partial w_j} = \frac{1}{p} \cdot p(1-p) \cdot \frac{\partial}{\partial w_j} (\mathbf{w}^\top \mathbf{x}) = (1-p)x_j$$

Annotations: Chain Rule (blue arrow), $p = \sigma(\mathbf{w}^\top \mathbf{x})$ (red arrow), $\frac{\partial p}{\partial(\mathbf{w}^\top \mathbf{x})}$ (red arrow), $\mathbf{w}^\top \mathbf{x} = \mathbf{w} \cdot \mathbf{x} = \sum w_j x_j$ (green arrow), $\frac{\partial \log(p)}{\partial p}$ (blue arrow), Chain Rule (red arrow), $\frac{\partial}{\partial w_j} (\mathbf{w}^\top \mathbf{x}) = x_j$ (green arrow).

$$\frac{\partial \log(1-p)}{\partial w_j} = \frac{-1}{1-p} \cdot \frac{\partial p}{\partial w_j} = \frac{-1}{1-p} \cdot p(1-p) \cdot \frac{\partial}{\partial w_j} (\mathbf{w}^\top \mathbf{x}) = -px_j$$

Annotations: $\frac{\partial \log(1-p)}{\partial p}$ (blue arrow), $\frac{\partial}{\partial w_j} (\mathbf{w}^\top \mathbf{x}) = x_j$ (green arrow).

Q2. Loss Function of Logistic Regression

(b) Show that $\frac{\partial}{\partial w_j} BCE(y, \sigma(z)) = (\sigma(z) - y)x_j$, where

$$BCE(y, \sigma(z)) = -y \log \sigma(z) - (1 - y) \log(1 - \sigma(z))$$

$$\begin{aligned} \frac{\partial}{\partial w_j} BCE(y, p) &= -y \frac{\partial \log(p)}{\partial w_j} - (1 - y) \frac{\partial \log(1 - p)}{\partial w_j} \\ &= -y(1 - p)x_j - (1 - y)(-px_j) \\ &= -yx_j + ypx_j + px_j - ypx_j \\ &= (p - y)x_j \end{aligned}$$

Q2. Loss Function of Logistic Regression

Logistic Regression:

$$z = \mathbf{w}^\top \mathbf{x} \Rightarrow p = \frac{1}{1 + e^{-z}}$$

(Intuition: z predicts $\ln\left(\frac{p}{1-p}\right)$.)

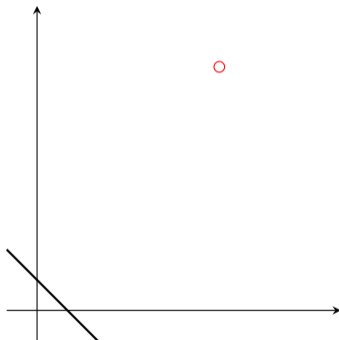
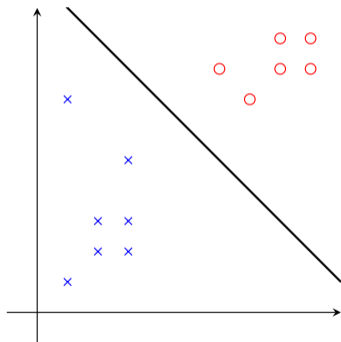
Softmax function (for multi-class classification with k classes):

$$z_1, z_2, \dots, z_k \Rightarrow p_i = \frac{e^{z_i}}{e^{z_1} + e^{z_2} + \dots + e^{z_k}}$$

(Intuition: z_j predicts $\ln\left(\frac{p_j}{p_k}\right)$.)

Discussion Question

Are probabilities outputted by logistic regression models trustable? In other words, does the p outputted by the model resemble $p(y = 1 \mid \mathbf{x}, \text{training data})$ correctly (or match our intuitions of $p(y = 1)$)?



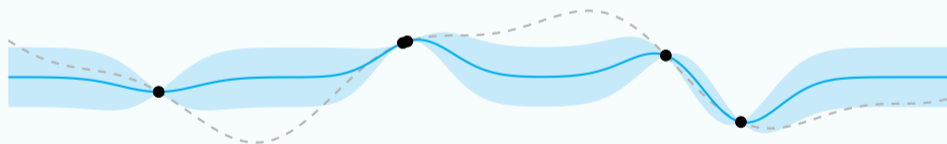
Discussion Question

Bayesian approaches: Models uncertainty by injecting a **prior**.

$$p(\text{belief} \mid \text{data}) \propto p(\text{data} \mid \text{belief}) \times p(\text{belief})$$

posterior likelihood prior

--- Ground Truth — Gaussian Process Mean



Example: Bayesian (Gaussian Process) Regression

Discussion Question

Demo (if we have time) – See the HTML version.

Q3. Logistic Regression for Multi-Class Classification

- (a) Compute the probability of an animal belonging to a certain class and classify them accordingly.

First animal: $\mathbf{x} = [1 \quad 4.2 \quad 0.4]^T$

$$\blacktriangleright \mathbf{w}_{cat} \cdot \mathbf{x} = 1 \cdot 4.2 + 4.2 \cdot (-0.01) + 0.4 \cdot (-0.12) = 4.11$$

$$p_{cat} = \frac{1}{1 + e^{-4.11}} = 0.984$$

$$\blacktriangleright \mathbf{w}_{horse} \cdot \mathbf{x} = -6.336$$

$$p_{horse} = \frac{1}{1 + e^{6.336}} = 0.00177$$

$$\blacktriangleright \mathbf{w}_{elephant} \cdot \mathbf{x} = -1246.196$$

$$p_{elephant} = \frac{1}{1 + e^{1246.196}} \approx 0$$

$$\mathbf{w}_{cat} = [4.2 \quad -0.01 \quad -0.12]^T$$

$$\mathbf{w}_{horse} = [-20 \quad -0.08 \quad 35]^T$$

$$\mathbf{w}_{elephant} = [-1250 \quad 0.82 \quad 0.9]^T$$

Weight (kg)	Length (m)
4.2	0.4
720	2.4
2350	5.5

Q3. Logistic Regression for Multi-Class Classification

- (a) Compute the probability of an animal belonging to a certain class and classify them accordingly.

Second animal: $\mathbf{x} = [1 \quad 720 \quad 2.4]^\top$

▶ $\mathbf{w}_{cat} \cdot \mathbf{x} = -3.288$

$$p_{cat} = \frac{1}{1 + e^{3.288}} = 0.0360$$

▶ $\mathbf{w}_{horse} \cdot \mathbf{x} = 6.4$

$$p_{horse} = \frac{1}{1 + e^{-6.4}} = 0.998$$

▶ $\mathbf{w}_{elephant} \cdot \mathbf{x} = -657.44$

$$p_{elephant} = \frac{1}{1 + e^{657.44}} \approx 0$$

$$\mathbf{w}_{cat} = [4.2 \quad -0.01 \quad -0.12]^\top$$

$$\mathbf{w}_{horse} = [-20 \quad -0.08 \quad 35]^\top$$

$$\mathbf{w}_{elephant} = [-1250 \quad 0.82 \quad 0.9]^\top$$

Weight (kg)	Length (m)
4.2	0.4
720	2.4
2350	5.5

Q3. Logistic Regression for Multi-Class Classification

- (a) Compute the probability of an animal belonging to a certain class and classify them accordingly.

Third animal: $\mathbf{x} = [1 \quad 2350 \quad 5.5]^\top$

▶ $\mathbf{w}_{cat} \cdot \mathbf{x} = -19.96$

$$p_{cat} = \frac{1}{1 + e^{19.96}} \approx 0$$

▶ $\mathbf{w}_{horse} \cdot \mathbf{x} = -15.5$

$$p_{horse} = \frac{1}{1 + e^{15.5}} \approx 0$$

▶ $\mathbf{w}_{elephant} \cdot \mathbf{x} = 681.95$

$$p_{elephant} = \frac{1}{1 + e^{-681.95}} \approx 1$$

$$\mathbf{w}_{cat} = [4.2 \quad -0.01 \quad -0.12]^\top$$

$$\mathbf{w}_{horse} = [-20 \quad -0.08 \quad 35]^\top$$

$$\mathbf{w}_{elephant} = [-1250 \quad 0.82 \quad 0.9]^\top$$

Weight (kg)	Length (m)
4.2	0.4
720	2.4
2350	5.5

Q3. Logistic Regression for Multi-Class Classification

- (b) What if we want to extend the classification task to classify other animals? Can we train a new model while keeping the weights of the previous models?
- ▶ For an animal that are very distinct with the three animals, we can create a new logistic regression model without changing the previous weights.
 - ▶ For classifying a new animal that is similar with one of the classes (e.g, classifying a dog), we need to retrain the old models.

Q3. Logistic Regression for Multi-Class Classification

(c) Derive the pairwise decision boundaries (lines) between each pair of classes in the (weight, length) plane using the given \mathbf{w} 's.

► cat vs horse:

$$\begin{aligned}\mathbf{w}_{cat} \cdot \mathbf{x} &= \mathbf{w}_{horse} \cdot \mathbf{x} \\ 24.2 + 0.07W - 35.12L &= 0\end{aligned}$$

► cat vs elephant:

$$\begin{aligned}\mathbf{w}_{cat} \cdot \mathbf{x} &= \mathbf{w}_{elephant} \cdot \mathbf{x} \\ 1254.2 - 0.83W - 1.02L &= 0\end{aligned}$$

$$\mathbf{w}_{cat} = [4.2 \quad -0.01 \quad -0.12]^T$$

$$\mathbf{w}_{horse} = [-20 \quad -0.08 \quad 35]^T$$

$$\mathbf{w}_{elephant} = [-1250 \quad 0.82 \quad 0.9]^T$$

► horse vs elephant:

$$\begin{aligned}\mathbf{w}_{horse} \cdot \mathbf{x} &= \mathbf{w}_{elephant} \cdot \mathbf{x} \\ 1230 - 0.90W + 34.1L &= 0\end{aligned}$$

Recap: Performance measures

Evaluation Metric:

- ▶ Judges the performance, doesn't care about the process.

[MRQ] Which of the following link(s) are pruned? Shade all that is/are true.

<input type="radio"/> a	<input type="radio"/> b	<input type="radio"/> c	<input type="radio"/> d	<input type="radio"/> e
<input type="radio"/> f	<input type="radio"/> g	<input type="radio"/> h	<input type="radio"/> i	<input type="radio"/> j
<input type="radio"/> k	<input type="radio"/> l	<input checked="" type="radio"/> m	<input type="radio"/> n	<input type="radio"/> o
<input type="radio"/> p	<input type="radio"/> q	<input checked="" type="radio"/> r	<input type="radio"/> s	<input checked="" type="radio"/> t
<input type="radio"/> u	<input type="radio"/> v	<input type="radio"/> w	<input type="radio"/> x	<input type="radio"/> y
<input type="radio"/> z				

0 / 4

Loss Function:

- ▶ Helps with model training.
Minimized by the optimizer.

[MRQ] Which of the following link(s) are pruned? Shade all that is/are true.

<input type="radio"/> a	<input type="radio"/> b	<input type="radio"/> c	<input type="radio"/> d	<input type="radio"/> e
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<input type="radio"/> k	<input type="radio"/> l	<input checked="" type="radio"/> m	<input type="radio"/> n	<input type="radio"/> o
<input type="radio"/> p	<input type="radio"/> q	<input checked="" type="radio"/> r	<input type="radio"/> s	<input checked="" type="radio"/> t
<input type="radio"/> u	<input type="radio"/> v	<input type="radio"/> w	<input type="radio"/> x	<input type="radio"/> y
<input type="radio"/> z				

25/26 items right 👍 Try again!

Recap: Performance measures

📌 Which of the following are more likely used as evaluation metrics (rather than loss functions)?

- A. Binary cross-entropy loss
- B. Accuracy
- C. Mean-squared error
- D. F1 Score