CSCI567 Machine Learning (Spring 2021)

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Outline

1. Logistics
2. Review of last lecture
3. Linear Discriminant Analysis and Quadratic Discriminant Analysis
4. Relationship between Logistic Regression and LDA

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Logistics

- HW 2 was assigned. Solutions for HW 1 will be delayed, stay tuned!
- Please form the groups by Friday, let us know if cannot find a group.

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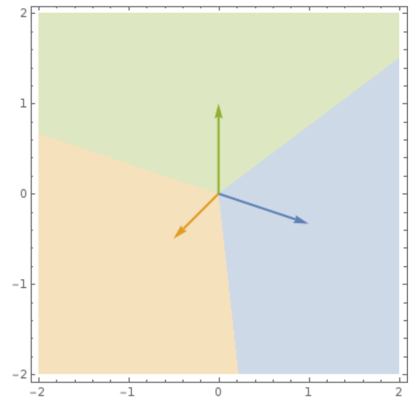
Linear models: from binary to multiclass



$\boldsymbol{w}_1 = (1, -\frac{1}{3})$
$\boldsymbol{w}_2 = (-\frac{1}{2}, -\frac{1}{2})$
$\boldsymbol{w}_3 = (0, 1)$

- Blue class: $\{\boldsymbol{x} : 1 = \operatorname{argmax}_k \boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x}\}$
- Orange class: $\{\boldsymbol{x} : 2 = \operatorname{argmax}_k \boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x}\}$
- Green class: $\{\boldsymbol{x} : 3 = \operatorname{argmax}_k \boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x}\}$

$$\mathcal{F} = \left\{ f(\boldsymbol{x}) = \operatorname*{argmax}_{k \in [\mathsf{C}]} \; \boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x} \mid \boldsymbol{w}_1, \ldots, \boldsymbol{w}_{\mathsf{C}} \in \mathbb{R}^{\mathsf{D}} \right\}$$

Softmax + MLE = minimizing cross-entropy loss

Maximize probability of see labels $y_1, \ldots, y_{\mathsf{N}}$ given $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{\mathsf{N}}$

$$P(\boldsymbol{W}) = \prod_{n=1}^{\mathsf{N}} \mathbb{P}(y_n \mid \boldsymbol{x}_n; \boldsymbol{W}) = \prod_{n=1}^{\mathsf{N}} \frac{e^{\boldsymbol{w}_{y_n}^{\mathrm{T}}\boldsymbol{x}_n}}{\sum_{k \in [\mathsf{C}]} e^{\boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x}_n}}$$

By taking **negative log**, this is equivalent to minimizing

$$F(\boldsymbol{W}) = \sum_{n=1}^{\mathsf{N}} \ln \left(\frac{\sum_{k \in [\mathsf{C}]} e^{\boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x}_n}}{e^{\boldsymbol{w}_{y_n}^{\mathrm{T}}\boldsymbol{x}_n}} \right) = \sum_{n=1}^{\mathsf{N}} \ln \left(1 + \sum_{k \neq y_n} e^{(\boldsymbol{w}_k - \boldsymbol{w}_{y_n})^{\mathrm{T}}\boldsymbol{x}_n} \right)$$

This is the *multiclass logistic loss*, a.k.a *cross-entropy loss*.

Comparisons of multiclass-to-binary reductions

In big O notation,

Reduction	**#training points**	**test time**	**Idea**
OvA	CN	C	is class k or not?
OvO	CN	C^2	is class k or class k'?
ECOC	LN	L	is bit b on or off?
Tree	$(\log_2 \mathsf{C})\mathsf{N}$	$\log_2 \mathsf{C}$	belong to which half of the label set?

Outline

Revisiting Bayes optimal classifier

Tells us what to predict for $\boldsymbol{x}$, *knowing $\mathcal{P}(y|\boldsymbol{x})$*

Bayes optimal classifier: $f^*(\boldsymbol{x}) = \text{argmax}_{c \in [C]} \mathcal{P}(c|\boldsymbol{x})$.

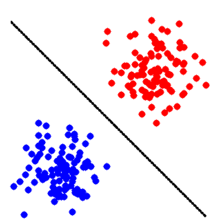
But the main issue was that in practice we don't know what $\mathcal{P}(y|\boldsymbol{x})$ is!

What do we know?

Ok, so we know that by **Bayes theorem** for a C class classification task

$$\mathcal{P}(y = c|X = \boldsymbol{x}) = \frac{\mathcal{P}(X = \boldsymbol{x}|y = c)\mathcal{P}(y = c)}{\mathcal{P}(X = \boldsymbol{x})}$$

Let's consider a Binary Classification task, $C = \{0, 1\}$. *What is the decision boundary?*



$$\mathcal{P}(y = 0|X = \boldsymbol{x}) = \mathcal{P}(y = 1|X = \boldsymbol{x})$$

The main bottleneck is *not knowing $\mathcal{P}(X = \boldsymbol{x}|y = c)$*

$$\mathcal{P}(y = c|X = \boldsymbol{x}) = \frac{\mathcal{P}(X = \boldsymbol{x}|y = c)\mathcal{P}(y = c)}{\mathcal{P}(X = \boldsymbol{x})}.$$

LDA makes **two simplifying assumptions**:

- Let $\mathcal{P}(X = \boldsymbol{x}|y = c) \sim \mathcal{N}(\boldsymbol{\mu}_c, \Sigma_c)$, and
- Let all class covariances be the same i.e. $\Sigma_c = \Sigma$ for all $c \in [C]$

If so, the *decision boundary* (for binary classification) is given by

$$\mathcal{P}(y = 0|X = \boldsymbol{x}) = \mathcal{P}(y = 1|X = \boldsymbol{x})$$

$$\frac{\mathcal{P}(X = \boldsymbol{x}|y = 0)\mathcal{P}(y = 0)}{\mathcal{P}(X = \boldsymbol{x})} = \frac{\mathcal{P}(X = \boldsymbol{x}|y = 1)\mathcal{P}(y = 1)}{\mathcal{P}(X = \boldsymbol{x})}$$

The main bottleneck is *not knowing* $\mathcal{P}(X = \boldsymbol{x}|y = c)$

$$\mathcal{P}(y = c|X = \boldsymbol{x}) = \frac{\mathcal{P}(X = \boldsymbol{x}|y = c)\mathcal{P}(y = c)}{\mathcal{P}(X = \boldsymbol{x})}.$$

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If so, the *decision boundary* (for binary classification) is given by

$$\mathcal{P}(y = 0|X = \boldsymbol{x}) = \mathcal{P}(y = 1|X = \boldsymbol{x})$$

$$\mathcal{P}(X = \boldsymbol{x}|y = 0)\mathcal{P}(y = 0) = \mathcal{P}(X = \boldsymbol{x}|y = 1)\mathcal{P}(y = 1)$$

Now, $\mathcal{P}(X = \boldsymbol{x}|y = 0) \sim \mathcal{N}(\boldsymbol{\mu}_0, \Sigma_0)$ **and** $\mathcal{P}(X = \boldsymbol{x}|y = 1) \sim \mathcal{N}(\boldsymbol{\mu}_1, \Sigma_1)$**.**

For $\boldsymbol{\mu}_c \in \mathbb{R}^d$ and $\Sigma_c^{-1} \in \mathbb{R}^{d \times d}$, we have

$$\mathcal{P}(X = \boldsymbol{x}|y = c) = \frac{1}{(2\pi)^{d/2}|\Sigma_c|^{1/2}} \exp\left(-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu}_c)^\top \Sigma_c^{-1}(\boldsymbol{x} - \boldsymbol{\mu}_c)\right)$$

The *decision boundary* is given by

$$\mathcal{P}(X = \boldsymbol{x}|y = 0)\mathcal{P}(y = 0) = \mathcal{P}(X = \boldsymbol{x}|y = 1)\mathcal{P}(y = 1).$$

Substituting for $\mathcal{P}(X = \boldsymbol{x}|y = c)$, and taking $\log(\cdot)$ and simplifying[1]

$$\log\left(\frac{\mathcal{P}(y = 0)}{\mathcal{P}(y = 1)}\right) - \frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu}_0)^\top \Sigma_0^{-1}(\boldsymbol{x} - \boldsymbol{\mu}_0) = -\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu}_1)^\top \Sigma_1^{-1}(\boldsymbol{x} - \boldsymbol{\mu}_1)$$

For simplicity of this exposition we have ignored the $1/(2\pi)^{d/2}|\Sigma_c|^{1/2}$ terms since these will just add to the constants.

Let's simplify this

$$\log \frac{\mathcal{P}(y=0)}{\mathcal{P}(y=1)} - \frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu}_0)^\top \Sigma_0^{-1}(\boldsymbol{x} - \boldsymbol{\mu}_0) = -\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu}_1)^\top \Sigma_1^{-1}(\boldsymbol{x} - \boldsymbol{\mu}_1)$$

$$\log \frac{\mathcal{P}(y = 0)}{\mathcal{P}(y = 1)} - \frac{1}{2}\boldsymbol{x}^\top \Sigma_0^{-1}\boldsymbol{x} + \boldsymbol{\mu}_0^\top \Sigma_0^{-1}\boldsymbol{x} - \frac{1}{2}\boldsymbol{\mu}_0^\top \Sigma_0^{-1}\boldsymbol{\mu}_0 = -\frac{1}{2}\boldsymbol{x}^\top \Sigma_1^{-1}\boldsymbol{x} + \boldsymbol{\mu}_1^\top \Sigma_1^{-1}\boldsymbol{x} - \frac{1}{2}\boldsymbol{\mu}_1^\top \Sigma_1^{-1}\boldsymbol{\mu}_1$$

Setting $\Sigma_0 = \Sigma_1 = \Sigma$,

$$\boldsymbol{w}^\top \boldsymbol{x} + w_0 = 0$$

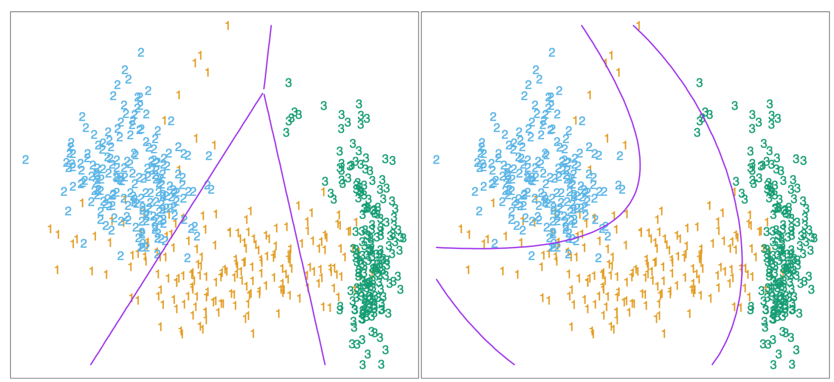
Here,

$$\boldsymbol{w}^\top = \boldsymbol{\mu}_0^\top \Sigma^{-1} - \boldsymbol{\mu}_1^\top \Sigma^{-1}$$

and

$$w_0 = \log \frac{\mathcal{P}(y = 0)}{\mathcal{P}(y = 1)} - \frac{1}{2}\boldsymbol{\mu}_0^\top \Sigma^{-1}\boldsymbol{\mu}_0 + \frac{1}{2}\boldsymbol{\mu}_1^\top \Sigma^{-1}\boldsymbol{\mu}_1$$

What do the decision boundaries look like?



The decision boundaries are a quadratic when Σ's are not the same, this is known as *Quadratic Discriminant Analysis*!

Outline

For **Logistic Regression** we assumed:

$$\mathcal{P}(y=1|X=\boldsymbol{x}) = \sigma(\boldsymbol{w}^\top \boldsymbol{x}) = \frac{1}{1+e^{-\boldsymbol{w}^\top \boldsymbol{x}}}$$

This can be written as follows, in terms of *log-odds*

$$\log \frac{\mathcal{P}(y=1|X=\boldsymbol{x})}{\mathcal{P}(y=0|X=\boldsymbol{x})} = \boldsymbol{w}^\top \boldsymbol{x}$$

The log-odds can be modeled as a linear function of x.

For **LDA** we can write the *log-odds* as

$$\begin{aligned}
\log \frac{\mathcal{P}(y=1|X=\boldsymbol{x})}{\mathcal{P}(y=0|X=\boldsymbol{x})} &= \log \frac{\mathcal{P}(X=\boldsymbol{x}|y=1)\mathcal{P}(y=1)}{\mathcal{P}(X=\boldsymbol{x}|y=0)\mathcal{P}(y=0)} \\
&= \log \frac{\mathcal{P}(y=1)}{\mathcal{P}(y=0)} + (\boldsymbol{\mu}_1^\top \Sigma^{-1} - \boldsymbol{\mu}_0^\top \Sigma^{-1})\boldsymbol{x} - \frac{1}{2}\boldsymbol{\mu}_1^\top \Sigma^{-1} \boldsymbol{\mu}_1 + \frac{1}{2}\boldsymbol{\mu}_0^\top \Sigma^{-1} \boldsymbol{\mu}_0 \\
&= \boldsymbol{w}^\top \boldsymbol{x}
\end{aligned}$$

LDA satisfies the assumptions of the Logistics Regression model!

LDA imposes additional assumptions on the data, i.e., it **assumes that the class conditional densities are Gaussian**.