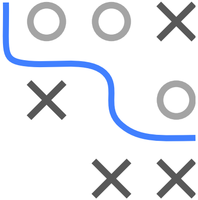
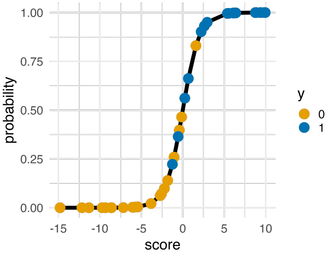
Introduction to Machine Learning



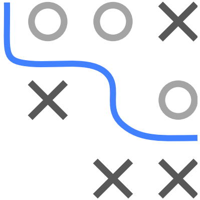
Classification
Logistic Regression



Learning goals

- Hypothesis space of LR
- Log-Loss derivation
- Intuition for loss
- LR as linear classifier

MOTIVATION



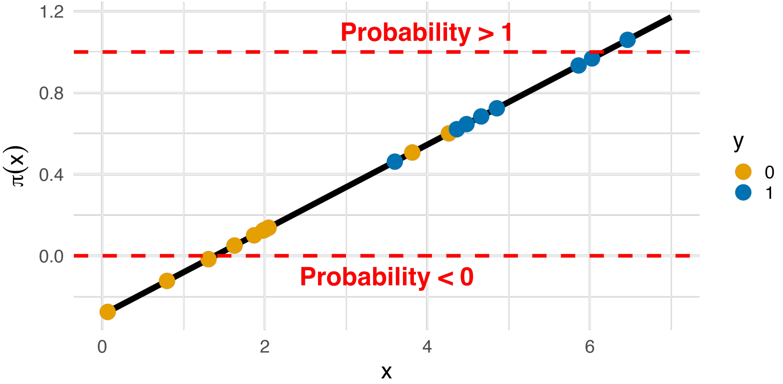
- Let's build a **discriminant** approach, for binary classification, as a probabilistic classifier $\pi(\mathbf{x} \mid \boldsymbol{\theta})$
- We encode $y \in \{0, 1\}$ and use ERM:

$$\underset{\boldsymbol{\theta} \in \Theta}{\arg\min}\, \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = \underset{\boldsymbol{\theta} \in \Theta}{\arg\min} \sum_{i=1}^{n} L\left(y^{(i)}, \pi\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)\right)$$

- We want to "copy" over ideas from linear regression
- In the above, our model structure should be "mainly" linear and we need a loss function

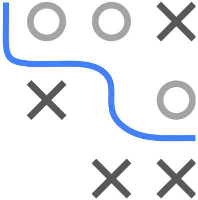
DIRECT LINEAR MODEL FOR PROBABILITIES

We could directly use an LM to model $\pi(\mathbf{x} \mid \boldsymbol{\theta}) = \boldsymbol{\theta}^\top \mathbf{x}$.
And use L2 loss in ERM.



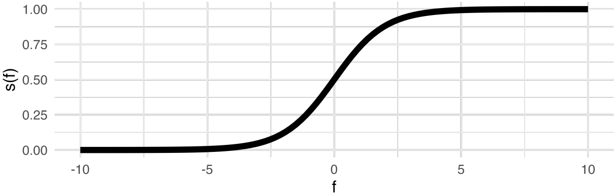
But: This obviously will result in predicted probabilities $\pi(\mathbf{x} \mid \boldsymbol{\theta}) \not\in [0, 1]$!

HYPOTHESIS SPACE OF LR



To avoid this, logistic regression "squashes" the estimated linear scores $\boldsymbol{\theta}^\top \mathbf{x}$ to $[0, 1]$ through the **logistic function** s:

$$\pi(\mathbf{x} \mid \boldsymbol{\theta}) = \frac{\exp\left(\boldsymbol{\theta}^\top \mathbf{x}\right)}{1 + \exp\left(\boldsymbol{\theta}^\top \mathbf{x}\right)} = \frac{1}{1 + \exp\left(-\boldsymbol{\theta}^\top \mathbf{x}\right)} = s\left(\boldsymbol{\theta}^\top \mathbf{x}\right) = s(f(\mathbf{x}))$$

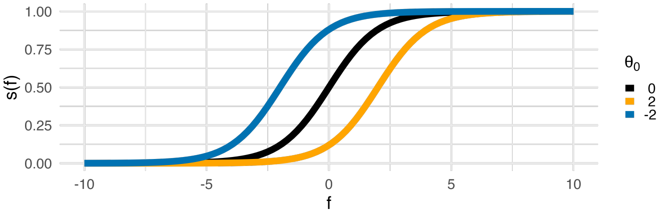


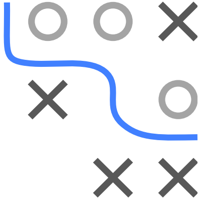
$\Rightarrow$ **Hypothesis space** of LR:

$$\mathcal{H} = \left\{\pi : \mathcal{X} \to [0, 1] \mid \pi(\mathbf{x} \mid \boldsymbol{\theta}) = s(\boldsymbol{\theta}^\top \mathbf{x}) \mid \boldsymbol{\theta} \in \mathbb{R}^{p+1}\right\}$$

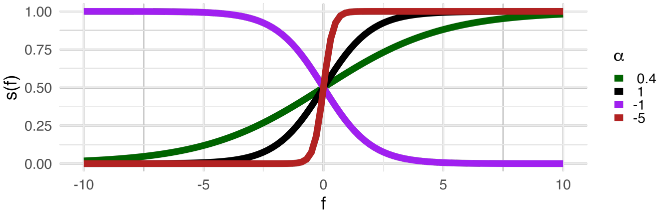
LOGISTIC FUNCTION

Intercept θ_0 shifts $\pi = s(\theta_0 + f) = \frac{\exp(\theta_0+f)}{1+\exp(\theta_0+f)}$ horizontally



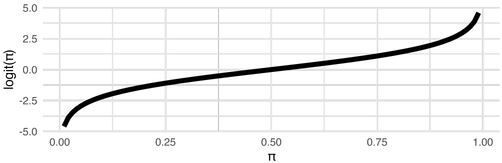


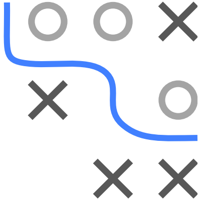
Scaling f like $s(\alpha f) = \frac{\exp(\alpha f)}{1+\exp(\alpha f)}$ controls slope and direction



THE LOGIT

The inverse $s^{-1}(\pi) = \log\left(\frac{\pi}{1-\pi}\right)$ where π is a probability is called **logit** (also called **log odds** since it is equal to the logarithm of the odds $\frac{\pi}{1-\pi}$)

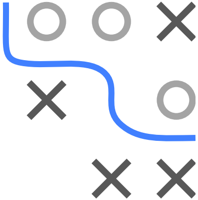




- Positive logits indicate probabilities > 0.5 and vice versa
- E.g.: if $p = 0.75$, odds are $3:1$ and logit is $log(3) \approx 1.1$
- Features $\mathbf{x}$ act linearly on logits, controlled by coefficients $\boldsymbol{\theta}$:

$$s^{-1}(\pi(\mathbf{x})) = \log\left(\frac{\pi(\mathbf{x})}{1-\pi(\mathbf{x})}\right) = \boldsymbol{\theta}^T x$$

DERIVING LOG-LOSS



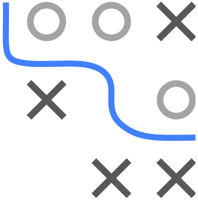
We need to find a suitable loss function for **ERM**. We look at likelihood which multiplies up $\pi\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)$ for positive examples, and $1 - \pi\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)$ for negative.

$$\mathcal{L}(\boldsymbol{\theta}) = \prod_{i \text{ with } y^{(i)}=1} \pi\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right) \prod_{i \text{ with } y^{(i)}=0} \left(1 - \pi\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)\right)$$

We can now cleverly combine the 2 cases by using exponents (note that only one of the 2 factors is not 1 and “active”):

$$\mathcal{L}(\boldsymbol{\theta}) = \prod_{i=1}^{n} \pi\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)^{y^{(i)}} \left(1 - \pi\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)\right)^{1-y^{(i)}}$$

DERIVING LOG-LOSS / 2



Taking the log to convert products into sums:

$$\ell(\boldsymbol{\theta}) = \log \mathcal{L}(\boldsymbol{\theta}) = \sum_{i=1}^{n} \log \left(\pi \left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta} \right)^{y^{(i)}} \left(1 - \pi \left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta} \right) \right)^{1 - y^{(i)}} \right)$$

$$= \sum_{i=1}^{n} y^{(i)} \log \left(\pi \left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta} \right) \right) + \left(1 - y^{(i)} \right) \log \left(1 - \pi \left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta} \right) \right)$$

Since we want to minimize the risk, we work with the negative $\ell(\boldsymbol{\theta})$:

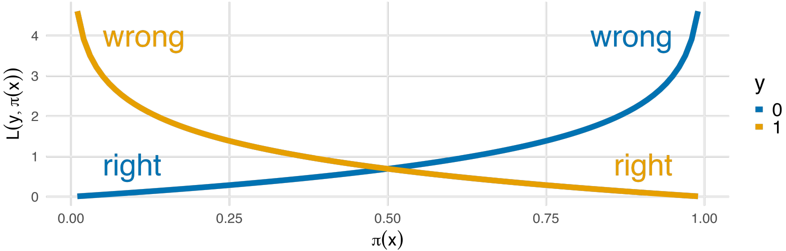
$$-\ell(\boldsymbol{\theta}) = \sum_{i=1}^{n} -y^{(i)} \log \left(\pi \left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta} \right) \right) - \left(1 - y^{(i)} \right) \log \left(1 - \pi \left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta} \right) \right)$$

BERNOULLI / LOG LOSS

The resulting loss

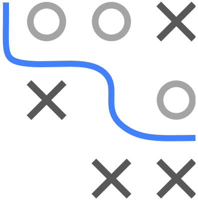
$$L(y, \pi) = -y \log(\pi) - (1 - y) \log(1 - \pi)$$

is called **Bernoulli, binomial, log** or **cross-entropy** loss

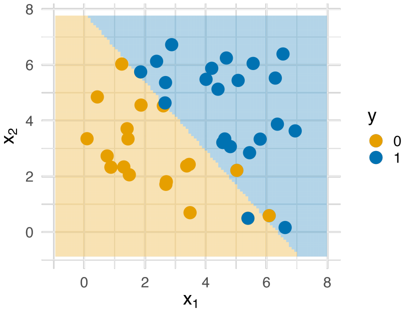


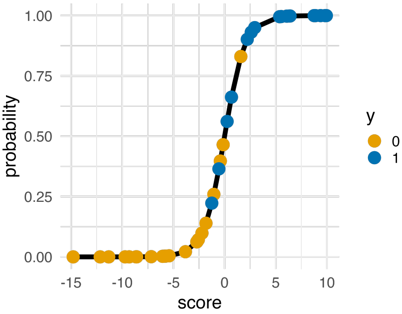
- Penalizes confidently wrong predictions heavily
- Is used for many other classifiers, e.g., in NNs or boosting

LOGISTIC REGRESSION IN 2D

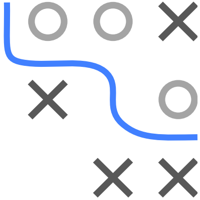


LR is a linear classifier, as $\pi(\mathbf{x} \mid \boldsymbol{\theta}) = s\left(\boldsymbol{\theta}^\top \mathbf{x}\right)$ and s is isotonic.





OPTIMIZATION



- Log-Loss is convex, under regularity conditions LR has a unique solution (because of its linear structure), but not an analytical one
- To fit LR we use numerical optimization, e.g., Newton-Raphson
- If data is linearly separable, the optimization problem is unbounded and we would not find a solution; way out is regularization
- Why not use least squares on $\pi(\mathbf{x}) = s(f(\mathbf{x}))$?
  Answer: ERM problem is not convex anymore :(
- We can also write the ERM as

$$\underset{\boldsymbol{\theta} \in \Theta}{\arg\min}\, \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = \underset{\boldsymbol{\theta} \in \Theta}{\arg\min} \sum_{i=1}^{n} L\left(y^{(i)}, f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)\right)$$

With $f(\mathbf{x} \mid \boldsymbol{\theta}) = \boldsymbol{\theta}^T \mathbf{x}$ and $L\left(y, f\right) = -yf + \log(1 + \exp(f))$

This combines the sigmoid with the loss and shows a convex loss directly on a linear function