MOTIVATION

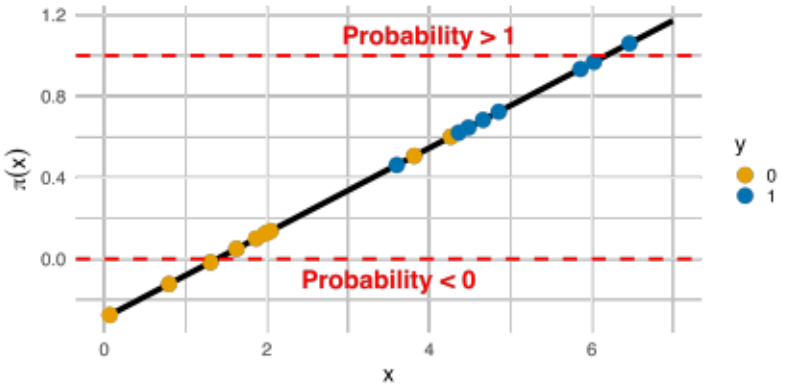
- Let's build a **discriminant** approach, for binary classification, as a probabilistic classifier $\pi(\mathbf{x} \mid \boldsymbol{\theta})$
- We encode $y \in \{0, 1\}$ and use ERM:

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

- 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 $\pi(\mathbf{x} \mid \theta) = \theta^\top \mathbf{x}$.
And use L2 loss in ERM.

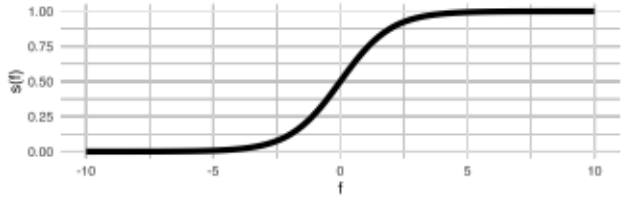


But: This obviously will result in predicted probabilities $\pi(\mathbf{x} \mid \theta) \notin [0, 1]$!

HYPOTHESIS SPACE OF LR

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

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

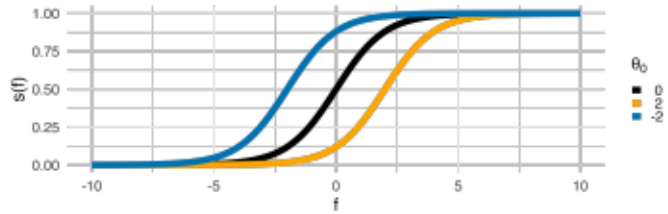


$\Rightarrow$ **Hypothesis space** of LR:

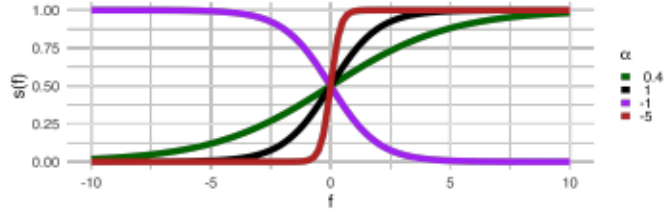
$$\mathcal{H} = \left\{ \pi : \mathcal{X} \to [0, 1] \mid \pi(\mathbf{x} \mid \theta) = s(\theta^\top \mathbf{x}) \mid \theta \in \mathbb{R}^{p+1} \right\}$$

LOGISTIC FUNCTION

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

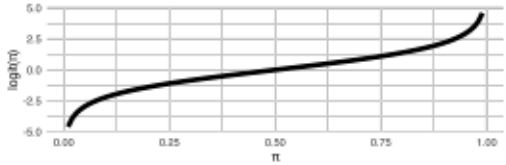


Scaling f like $s(\alpha f) = \frac{\exp(\alpha f)}{1+\exp(\alpha f)}$ controls slope and direction



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 θ:

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

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"):

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

BERNOULLI LOG LOSS

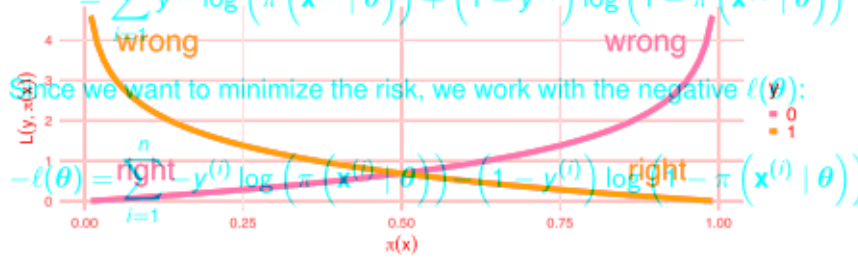
The resulting loss

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

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

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

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



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

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

- 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 $\pi(\mathbf{x} \mid \theta) = s\left(\theta^\top \mathbf{x}\right)$ and s is isotonic.

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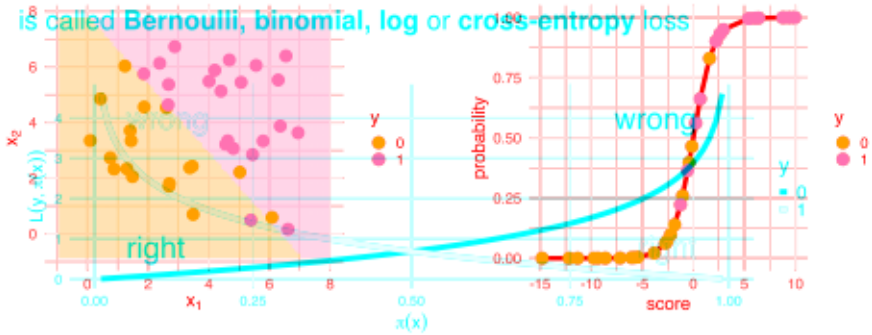

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OPTIMIZATION

LOGISTIC REGRESSION IN 2D

LR is a linear classifier as $\pi(\mathbf{x} \mid \theta) = s(\theta^T \mathbf{x})$ and sigmoid is monotonic.

- 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

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

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

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

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