## LOGISTIC REGRESSION

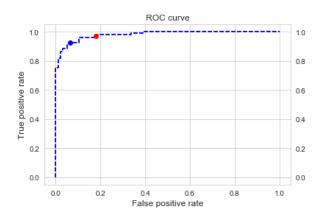
## 1 Warm-up

The logistic model assumes that the random variables  $(X,Y) \in \mathbb{R}^d \times \{0,1\}$  are such that

$$\mathbb{P}(Y=1|X) = \frac{\exp\left(\langle \beta^*, X \rangle\right)}{1 + \exp\left(\langle \beta^*, X \rangle\right)},$$

with  $\beta^* \in \mathbb{R}^d$ . In this case,  $\mathbb{P}(Y = 1|X) > 1/2$  if and only if  $\langle \beta^*, X \rangle > 0$ , so the frontier between  $\{x : h_*(x) = 1\}$  and  $\{x : h_*(x) = 0\}$  is an hyperplane, with orthogonal direction  $\beta^*$ .

- 1. In this question only,  $\beta^* = (\beta_0, \beta_1) \in \mathbb{R}^2$  and  $X_i = (1, x_i)$  for all  $1 \leq i \leq n$ .
  - (a) Provide the value  $x_*$  of  $x_i$  such that  $\mathbb{P}(Y_i = 1|X_i) = 1/2$ . The logistic Bayes classifier is therefore defined by  $h_*(X_i) = 1$  if and only if  $x_i > x_*$ .
  - (b) Another classifier could be defined by choosing a threshold  $\tilde{p} \in (0,1)$  and defining  $\tilde{h}(X_i) = 1$  if and only if  $\mathbb{P}(Y_i = 1 | X_i) > \tilde{p}$ . Provide  $\tilde{x}$  such that  $\tilde{h}(X_i) = 1$  if and only if  $x_i > \tilde{x}$ . Explain a practical interest to choose  $\tilde{p} < 1/2$ .
- 2. The usual logistic regression classifier is defined by  $h_n: x \mapsto 1$  is  $x^{\top} \hat{\beta}_n > 0$  and 0 otherwise, where  $\hat{\beta}_n$  is an estimator of  $\beta$ . Therefore  $h_n(X) = 1$  if and only if  $\mathbb{P}(Y = 1|X) > 1/2$ . Other classifiers can be defined by setting  $h_n(X) = 1$  if and only if  $\mathbb{P}(Y = 1|X) > p_*$  for a chosen  $p_* \in (0,1)$ . Two classifiers were built with  $p_* = 0.5$  and  $p_* = 0.2$ , associate each classifier with its point on ROC curve displayed above.



## 2 Softmax regression

Assume that the observation Y takes values in  $\{1, ..., M\}$  and that  $X \in \mathbb{R}^d$ . The negative loglikelihood to be minimized to estimate the parameters of the model is given by:

$$\theta \mapsto \ell_n^{\text{multi}}(\theta) = -\frac{1}{n} \sum_{i=1}^n \sum_{k=1}^M \mathbb{1}_{Y_i = k} \log \mathbb{P}_{\theta}(Y_i = k | X_i),$$

where  $\{(X_i, Y_i)\}_{1 \le i \le n}$  are i.i.d. observations with the same law as (X, Y).

- 1. Explain the construction of  $\mathbb{P}_{\theta}(Y_i = k|X_i)$ ,  $1 \leq i \leq n$  for a softmax regression model with parameters  $\omega_m \in \mathbb{R}^d$  for  $1 \leq m \leq M$ .
- 2. In the setting of the softmax regression function, compute  $\theta \mapsto \nabla_{\theta} \ell_n^{\text{multi}}(\theta)$ .

## 3 Maximum likelihood estimation

The unknown parameter  $\beta^*$  may be estimated by maximizing the conditional likelihood of Y given X

$$\widehat{\beta}_n \in \operatorname{argmax}_{\beta \in \mathbb{R}^d} \prod_{i=1}^n \left[ \left( \frac{\exp\left( \langle \beta, x_i \rangle \right)}{1 + \exp\left( \langle \beta, x_i \rangle \right)} \right)^{Y_i} \left( \frac{1}{1 + \exp\left( \langle \beta, x_i \rangle \right)} \right)^{1 - Y_i} \right],$$

to define the empirical classifier

$$\widehat{h}_n: x \mapsto \mathbb{1}_{\langle \widehat{\beta}_n, x \rangle > 0}.$$

In the following,  $\{(x_i, Y_i)\}_{1 \leqslant i \leqslant n}$  are assumed to be i.i.d. with the same distribution as (X, Y).

1. Compute the gradient and the Hessian  $H_n$  of

$$\ell_n: \beta \mapsto -\sum_{i=1}^n \left[ Y_i \langle x_i, \beta \rangle - \log(1 + \exp(\langle x_i, \beta \rangle)) \right].$$

What can be said about the function  $\ell_n$  when for all  $\beta \in \mathbb{R}^d$ ,  $H_n(\beta)$  is nonsingular? This assumption is supposed to hold in the following questions.

2. Prove that there exists  $\widetilde{\beta}_n \in \mathbb{R}^d$  such that  $\|\widetilde{\beta}_n - \beta^*\| \le \|\widehat{\beta}_n - \beta^*\|$  and

$$\widehat{\beta}_n - \beta^* = -H_n(\widetilde{\beta}_n)^{-1} \nabla \ell_n(\beta^*).$$

In the following it is assumed that the  $(x_i)_{1 \leq i \leq n}$  are uniformly bounded,  $\widehat{\beta}_n \to \beta^*$  a.s. and that there exists a continuous and nonsingular function H such that  $n^{-1}H_n(\beta)$  converges to  $H(\beta)$ , uniformly in a ball around  $\beta^*$ .

3. Define for all  $1 \leq i \leq n$ ,  $p_i(\beta) = e^{\langle x_i, \beta \rangle} / (1 + e^{\langle x_i, \beta \rangle})$ . Check that

$$\mathbb{E}\left[e^{-n^{-1/2}\langle t, \nabla \ell_n(\beta^*)\rangle}\right] = \prod_{i=1}^n \left(1 - p_i(\beta^*) + p_i(\beta^*)e^{\langle t, x_i \rangle / \sqrt{n}}\right) e^{-p_i(\beta^*)\langle t, x_i \rangle / \sqrt{n}},$$

$$= \exp\left(\frac{1}{2}t^T \left(n^{-1}H_n(\beta^*)\right)t + O(n^{-1/2})\right).$$

- 4. What is the asymptotic distribution of  $-n^{-1/2}\nabla \ell_n(\beta^*)$  and of  $\sqrt{n}(\widehat{\beta}_n \beta^*)$ ?
- 5. For all  $1 \leq j \leq d$  and all  $\alpha \in (0,1)$ , propose a confidence interval  $\mathcal{I}_{n,\alpha}$  such that  $\beta_j^* \in \mathcal{I}_{n,\alpha}$  with asymptotic probability  $1 \alpha$ .