

The purpose of this additional sheet is to provide more practice and exam preparation material. N.B. The tutors are not required to work through this material in the tutorial.

## Exercise 1. Score matching for the exponential family

In the lecture, we have derived the objective function  $J(\theta)$  for score matching,

$$J(\boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{m} \left[ \partial_j \psi_j(\mathbf{x}_i; \boldsymbol{\theta}) + \frac{1}{2} \psi_j(\mathbf{x}_i; \boldsymbol{\theta})^2 \right], \tag{1}$$

where  $\psi_j$  is the partial derivative of the log model-pdf log  $p(\mathbf{x}; \boldsymbol{\theta})$  with respect to the *j*-th coordinate (slope) and  $\partial_j \psi_j$  its second partial derivative (curvature). The observed data are denoted by  $\mathbf{x}_1, \dots, \mathbf{x}_n$  and  $\mathbf{x} \in \mathbb{R}^m$ .

The goal of this exercise is to show that for statistical models of the form

$$\log p(\mathbf{x}; \boldsymbol{\theta}) = \sum_{k=1}^{K} \theta_k F_k(\mathbf{x}) - \log Z(\boldsymbol{\theta}), \qquad \mathbf{x} \in \mathbb{R}^m,$$
 (2)

the score matching objective function becomes a quadratic form, which can be optimised efficiently (see e.g. Barber Appendix A.5.3).

The set of models above are called the (continuous) exponential family, or also log-linear models because the models are linear in the parameters  $\theta_k$ . Since the exponential family generally includes probability mass functions as well, the qualifier "continuous" may be used to highlight that we are here considering continuous random variables only. The functions  $F_k(\mathbf{x})$  are assumed to be known; they are the sufficient statistics (see e.g. Barber Section 8.5).

(a) Denote by  $\mathbf{K}(\mathbf{x})$  the matrix with elements  $K_{kj}(\mathbf{x})$ ,

$$K_{kj}(\mathbf{x}) = \frac{\partial F_k(\mathbf{x})}{\partial x_j}, \qquad k = 1 \dots K, \quad j = 1 \dots m,$$
 (3)

and by  $\mathbf{H}(\mathbf{x})$  the matrix with elements  $H_{kj}(\mathbf{x})$ ,

$$H_{kj}(\mathbf{x}) = \frac{\partial^2 F_k(\mathbf{x})}{\partial x_j^2}, \qquad k = 1 \dots K, \quad j = 1 \dots m.$$
 (4)

Furthermore, let  $\mathbf{h}_j(\mathbf{x}) = (H_{1j}(\mathbf{x}), \dots, H_{Kj}(\mathbf{x}))^{\top}$  be the j-th column vector of  $\mathbf{H}(\mathbf{x})$ .

Show that for the continuous exponential family, the score matching objective in Equation (1) becomes

$$J(\boldsymbol{\theta}) = \boldsymbol{\theta}^{\top} \mathbf{r} + \frac{1}{2} \boldsymbol{\theta}^{\top} \mathbf{M} \boldsymbol{\theta}, \tag{5}$$

where

$$\mathbf{r} = \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{m} \mathbf{h}_{j}(\mathbf{x}_{i}), \qquad \mathbf{M} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{K}(\mathbf{x}_{i}) \mathbf{K}(\mathbf{x}_{i})^{\top}.$$
 (6)

(b) The pdf of a zero mean Gaussian parametrised by the variance  $\sigma^2$  is

$$p(x; \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2}{2\sigma^2}\right), \qquad x \in \mathbb{R}.$$
 (7)

The (multivariate) Gaussian is a member of the exponential family. By comparison with Equation (2), we can re-parametrise the statistical model  $\{p(x; \sigma^2)\}_{\sigma^2}$  and work with

$$p(x;\theta) = \frac{1}{Z(\theta)} \exp(\theta x^2), \qquad \theta < 0, \qquad x \in \mathbb{R},$$
 (8)

instead. The two parametrisations are related by  $\theta = -1/(2\sigma^2)$ . Using the previous result on the (continuous) exponential family, determine the score matching estimate  $\hat{\theta}$ , and show that the corresponding  $\hat{\sigma}^2$  is the same as the maximum likelihood estimate. This result is noteworthy because unlike in maximum likelihood estimation, score matching does not need the partition function  $Z(\theta)$  for the estimation.