Exercises for the tutorials: 5 and 9.
The other exercises are for self-study and exam preparation. All material is examinable unless otherwise mentioned.

## Exercise 1. Maximum likelihood estimation for a Gaussian

The Gaussian pdf parametrised by mean $\mu$ and standard deviation $\sigma$ is given by

$$
p(x ; \boldsymbol{\theta})=\frac{1}{\sqrt{2 \pi \sigma^{2}}} \exp \left[-\frac{(x-\mu)^{2}}{2 \sigma^{2}}\right], \quad \boldsymbol{\theta}=(\mu, \sigma)
$$

(a) Given id data $\mathcal{D}=\left\{x_{1}, \ldots, x_{n}\right\}$, what is the likelihood function $L(\boldsymbol{\theta})$ for the Gaussian model?
(b) What is the log-likelihood function $\ell(\boldsymbol{\theta})$ ?
(c) Show that the maximum likelihood estimates for the mean $\mu$ and standard deviation $\sigma$ are the sample mean

$$
\begin{equation*}
\bar{x}=\frac{1}{n} \sum_{i=1}^{n} x_{i} \tag{1}
\end{equation*}
$$

and the square root of the sample variance

$$
\begin{equation*}
S^{2}=\frac{1}{n} \sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2} \tag{2}
\end{equation*}
$$

## Exercise 2. Posterior of the mean of a Gaussian with known variance

Given iid data $\mathcal{D}=\left\{x_{1}, \ldots, x_{n}\right\}$, compute $p\left(\mu \mid \mathcal{D}, \sigma^{2}\right)$ for the Bayesian model

$$
\begin{equation*}
p(x \mid \mu)=\frac{1}{\sqrt{2 \pi \sigma^{2}}} \exp \left[-\frac{(x-\mu)^{2}}{2 \sigma^{2}}\right] \quad p\left(\mu ; \mu_{0}, \sigma_{0}^{2}\right)=\frac{1}{\sqrt{2 \pi \sigma_{0}^{2}}} \exp \left[-\frac{\left(\mu-\mu_{0}\right)^{2}}{2 \sigma_{0}^{2}}\right] \tag{3}
\end{equation*}
$$

where $\sigma^{2}$ is a fixed known quantity.
Hint: You may use that

$$
\begin{equation*}
\mathcal{N}\left(x ; m_{1}, \sigma_{1}^{2}\right) \mathcal{N}\left(x ; m_{2}, \sigma_{2}^{2}\right) \propto \mathcal{N}\left(x ; m_{3}, \sigma_{3}^{2}\right) \tag{4}
\end{equation*}
$$

where

$$
\begin{align*}
\mathcal{N}\left(x ; \mu, \sigma^{2}\right) & =\frac{1}{\sqrt{2 \pi \sigma^{2}}} \exp \left[-\frac{(x-\mu)^{2}}{2 \sigma^{2}}\right]  \tag{5}\\
\sigma_{3}^{2} & =\left(\frac{1}{\sigma_{1}^{2}}+\frac{1}{\sigma_{2}^{2}}\right)^{-1}=\frac{\sigma_{1}^{2} \sigma_{2}^{2}}{\sigma_{1}^{2}+\sigma_{2}^{2}}  \tag{6}\\
m_{3} & =\sigma_{3}^{2}\left(\frac{m_{1}}{\sigma_{1}^{2}}+\frac{m_{2}}{\sigma_{2}^{2}}\right)=m_{1}+\frac{\sigma_{1}^{2}}{\sigma_{1}^{2}+\sigma_{2}^{2}}\left(m_{2}-m_{1}\right) \tag{7}
\end{align*}
$$

## Exercise 3. Maximum likelihood estimation of probability tables in fully observed directed graphical models of binary variables

We assume that we are given a parametrised directed graphical model for variables $x_{1}, \ldots, x_{d}$,

$$
\begin{equation*}
p(\mathbf{x} ; \boldsymbol{\theta})=\prod_{i=1}^{d} p\left(x_{i} \mid \mathrm{pa}_{i} ; \boldsymbol{\theta}_{i}\right) \quad x_{i} \in\{0,1\} \tag{8}
\end{equation*}
$$

where the conditionals are represented by parametrised probability tables, For example, if pa ${ }_{3}=$ $\left\{x_{1}, x_{2}\right\}, p\left(x_{3} \mid \mathrm{pa}_{3} ; \boldsymbol{\theta}_{3}\right)$ is represented as

| $\left.p\left(x_{3}=1 \mid x_{1}, x_{2} ; \theta_{3}^{1}, \ldots, \theta_{3}^{4}\right)\right)$ | $x_{1}$ | $x_{2}$ |
| :---: | :--- | :--- |
| $\theta_{3}^{1}$ | 0 | 0 |
| $\theta_{3}^{2}$ | 1 | 0 |
| $\theta_{3}^{3}$ | 0 | 1 |
| $\theta_{3}^{4}$ | 1 | 1 |

with $\boldsymbol{\theta}_{3}=\left(\theta_{3}^{1}, \theta_{3}^{2}, \theta_{3}^{3}, \theta_{3}^{4}\right)$, and where the superscripts $j$ of $\theta_{3}^{j}$ enumerate the different states that the parents can be in.
(a) Assuming that $x_{i}$ has $m_{i}$ parents, verify that the table parametrisation of $p\left(x_{i} \mid \mathrm{pa}_{i} ; \boldsymbol{\theta}_{i}\right)$ is equivalent to writing $p\left(x_{i} \mid \mathrm{pa}_{i} ; \boldsymbol{\theta}_{i}\right)$ as

$$
\begin{equation*}
p\left(x_{i} \mid \mathrm{pa}_{i} ; \boldsymbol{\theta}_{i}\right)=\prod_{s=1}^{S_{i}}\left(\theta_{i}^{s}\right)^{\mathbb{1}\left(x_{i}=1, \mathrm{pa}_{i}=s\right)}\left(1-\theta_{i}^{s}\right)^{\mathbb{1}\left(x_{i}=0, \mathrm{pa}_{i}=s\right)} \tag{9}
\end{equation*}
$$

where $S_{i}=2^{m_{i}}$ is the total number of states/configurations that the parents can be in, and $\mathbb{1}\left(x_{i}=1, \mathrm{pa}_{i}=s\right)$ is one if $x_{i}=1$ and $\mathrm{pa}_{i}=s$, and zero otherwise.
(b) For iid data $\mathcal{D}=\left\{\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(n)}\right\}$ show that the likelihood can be represented as

$$
\begin{equation*}
p(\mathcal{D} ; \boldsymbol{\theta})=\prod_{i=1}^{d} \prod_{s=1}^{S_{i}}\left(\theta_{i}^{s}\right)^{n_{x_{i}}^{s}=1}\left(1-\theta_{i}^{s}\right)^{n_{x_{i}}^{s}=0} \tag{10}
\end{equation*}
$$

where $n_{x_{i}=1}^{s}$ is the number of times the pattern $\left(x_{i}=1, \mathrm{pa}_{i}=s\right)$ occurs in the data $\mathcal{D}$, and equivalently for $n_{x_{i}=0}^{s}$.
(c) Show that the log-likelihood decomposes into sums of terms that can be independently optimised, and that each term corresponds to the log-likelihood for a Bernoulli model.
(d) Referring to the lecture material, conclude that the maximum likelihood estimates are given by

$$
\begin{equation*}
\hat{\theta}_{i}^{s}=\frac{n_{x_{i}=1}^{s}}{n_{x_{i}=1}^{s}+n_{x_{i}=0}^{s}}=\frac{\sum_{j=1}^{n} \mathbb{1}\left(x_{i}^{(j)}=1, \mathrm{pa}_{i}^{(j)}=s\right)}{\sum_{j=1}^{n} \mathbb{1}\left(\mathrm{pa}_{i}^{(j)}=s\right)} \tag{11}
\end{equation*}
$$

## Exercise 4. Cancer-asbestos-smoking example: MLE

Consider the model specified by the DAG


The distribution of $a$ and $s$ are Bernoulli distributions with parameter (success probability) $\theta_{a}$ and $\theta_{s}$, respectively, i.e.

$$
\begin{equation*}
p\left(a ; \theta_{a}\right)=\theta_{a}^{a}\left(1-\theta_{a}\right)^{1-a} \quad p\left(s ; \theta_{s}\right)=\theta_{s}^{s}\left(1-\theta_{s}\right)^{1-s}, \tag{12}
\end{equation*}
$$

and the distribution of $c$ given the parents is parametrised as specified in the following table

| $\left.p\left(c=1 \mid a, s ; \theta_{c}^{1}, \ldots, \theta_{c}^{4}\right)\right)$ | $a$ | $s$ |
| :---: | :---: | :---: |
| $\theta_{c}^{1}$ | 0 | 0 |
| $\theta_{c}^{2}$ | 1 | 0 |
| $\theta_{c}^{3}$ | 0 | 1 |
| $\theta_{c}^{4}$ | 1 | 1 |

The free parameters of the model are $\left(\theta_{a}, \theta_{s}, \theta_{c}^{1}, \ldots, \theta_{c}^{4}\right)$.
Assume we observe the following iid data (each row is a data point).

| a | s | c |
| :---: | :---: | :---: |
| 0 | 1 | 1 |
| 0 | 0 | 0 |
| 1 | 0 | 1 |
| 0 | 0 | 0 |
| 0 | 1 | 0 |

(a) Determine the maximum-likelihood estimates of $\theta_{a}$ and $\theta_{s}$
(b) Determine the maximum-likelihood estimates of $\theta_{c}^{1}, \ldots, \theta_{c}^{4}$.

## Exercise 5. Bayesian inference for the Bernoulli model

Consider the Bayesian model

$$
p(x \mid \theta)=\theta^{x}(1-\theta)^{1-x} \quad p\left(\theta ; \boldsymbol{\alpha}_{0}\right)=\mathcal{B}\left(\theta ; \alpha_{0}, \beta_{0}\right)
$$

where $x \in\{0,1\}, \theta \in[0,1], \boldsymbol{\alpha}_{0}=\left(\alpha_{0}, \beta_{0}\right)$, and

$$
\begin{equation*}
\mathcal{B}(\theta ; \alpha, \beta) \propto \theta^{\alpha-1}(1-\theta)^{\beta-1} \quad \theta \in[0,1] \tag{13}
\end{equation*}
$$

(a) Given iid data $\mathcal{D}=\left\{x_{1}, \ldots, x_{n}\right\}$ show that the posterior of $\theta$ given $\mathcal{D}$ is

$$
\begin{array}{rlr}
p(\theta \mid \mathcal{D}) & =\mathcal{B}\left(\theta ; \alpha_{n}, \beta_{n}\right) & \\
\alpha_{n} & =\alpha_{0}+n_{x=1} \quad \beta_{n}=\beta_{0}+n_{x=0}
\end{array}
$$

where $n_{x=1}$ denotes the number of ones and $n_{x=0}$ the number of zeros in the data.
(b) Compute the mean of a Beta random variable $f$,

$$
\begin{equation*}
p(f ; \alpha, \beta)=\mathcal{B}(f ; \alpha, \beta) \quad f \in[0,1], \tag{14}
\end{equation*}
$$

using that

$$
\begin{equation*}
\int_{0}^{1} f^{\alpha-1}(1-f)^{\beta-1} \mathrm{~d} f=B(\alpha, \beta)=\frac{\Gamma(\alpha) \Gamma(\beta)}{\Gamma(\alpha+\beta)} \tag{15}
\end{equation*}
$$

where $B(\alpha, \beta)$ denotes the Beta function and where the Gamma function $\Gamma(t)$ is defined as

$$
\begin{equation*}
\Gamma(t)=\int_{o}^{\infty} f^{t-1} \exp (-f) \mathrm{d} f \tag{16}
\end{equation*}
$$

and satisfies $\Gamma(t+1)=t \Gamma(t)$.
Hint: It will be useful to represent the partition function in terms of the Beta function.
(c) Show that the predictive posterior probability $p(x=1 \mid \mathcal{D})$ for a new independently observed data point $x$ equals the posterior mean of $p(\theta \mid \mathcal{D})$, which in turn is given by

$$
\begin{equation*}
\mathbb{E}(\theta \mid \mathcal{D})=\frac{\alpha_{0}+n_{x=1}}{\alpha_{0}+\beta_{0}+n} \tag{17}
\end{equation*}
$$

## Exercise 6. Bayesian inference of probability tables in fully observed directed graphical models of binary variables

This is the Bayesian analogue of Exercise 3 and the notation follows that exercise. We consider the Bayesian model

$$
\begin{align*}
p(\mathbf{x} \mid \boldsymbol{\theta}) & =\prod_{i=1}^{d} p\left(x_{i} \mid \mathrm{pa}_{i}, \boldsymbol{\theta}_{i}\right) \quad x_{i} \in\{0,1\}  \tag{18}\\
p\left(\boldsymbol{\theta} ; \boldsymbol{\alpha}_{0}, \boldsymbol{\beta}_{0}\right) & =\prod_{i=1}^{d} \prod_{s=1}^{S_{i}} \mathcal{B}\left(\theta_{i}^{s} ; \alpha_{i, 0}^{s}, \beta_{i, 0}^{s}\right) \tag{19}
\end{align*}
$$

where $p\left(x_{i} \mid \mathrm{pa}_{i}, \boldsymbol{\theta}_{i}\right)$ is defined via (9), $\boldsymbol{\alpha}_{0}$ is a vector of hyperparameters containing all $\alpha_{i, 0}^{s}, \boldsymbol{\beta}_{0}$ the vector containing all $\beta_{i, 0}^{s}$, and as before $\mathcal{B}$ denotes the Beta distribution. Under the prior, all parameters are independent.
(a) For iid data $\mathcal{D}=\left\{\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(n)}\right\}$ show that

$$
\begin{equation*}
p(\boldsymbol{\theta} \mid \mathcal{D})=\prod_{i=1}^{d} \prod_{s=1}^{S_{i}} \mathcal{B}\left(\theta_{i}^{s}, \alpha_{i, n}^{s}, \beta_{i, n}^{s}\right) \tag{20}
\end{equation*}
$$

where

$$
\begin{equation*}
\alpha_{i, n}^{s}=\alpha_{i, 0}^{s}+n_{x_{i}=1}^{s} \quad \beta_{i, n}^{s}=\beta_{i, 0}^{s}+n_{x_{i}=0}^{s} \tag{21}
\end{equation*}
$$

and that the parameters are also independent under the posterior.
(b) For a variable $x_{i}$ with parents $\mathrm{pa}_{i}$, compute the posterior predictive probability $p\left(x_{i}=\right.$ $\left.1 \mid \mathrm{pa}_{i}, \mathcal{D}\right)$
where $n^{s}=n_{x_{i}=0}^{s}+n_{x_{i}=1}^{s}$ denotes the number of times the parent configuration $s$ occurs in the observed data $\mathcal{D}$.

## Exercise 7. Cancer-asbestos-smoking example: Bayesian inference

Consider the model specified by the DAG


The distribution of $a$ and $s$ are Bernoulli distributions with parameter (success probability) $\theta_{a}$ and $\theta_{s}$, respectively, i.e.

$$
\begin{equation*}
p\left(a \mid \theta_{a}\right)=\theta_{a}^{a}\left(1-\theta_{a}\right)^{1-a} \quad p\left(s \mid \theta_{s}\right)=\theta_{s}^{s}\left(1-\theta_{s}\right)^{1-s} \tag{22}
\end{equation*}
$$

and the distribution of $c$ given the parents is parametrised as specified in the following table

| $\left.p\left(c=1 \mid a, s, \theta_{c}^{1}, \ldots, \theta_{c}^{4}\right)\right)$ | $a$ | $s$ |
| ---: | ---: | ---: |
| $\theta_{c}^{1}$ | 0 | 0 |
| $\theta_{c}^{2}$ | 1 | 0 |
| $\theta_{c}^{3}$ | 0 | 1 |
| $\theta_{c}^{4}$ | 1 | 1 |

We assume that the prior over the parameters of the model, $\left(\theta_{a}, \theta_{s}, \theta_{c}^{1}, \ldots, \theta_{c}^{4}\right)$, factorises and is given by beta distributions with hyperparameters $\alpha_{0}=1$ and $\beta_{0}=1$ (same for all parameters). Assume we observe the following iid data (each row is a data point).

| a | s | c |
| :--- | :--- | :--- |
| 0 | 1 | 1 |
| 0 | 0 | 0 |
| 1 | 0 | 1 |
| 0 | 0 | 0 |
| 0 | 1 | 0 |

(a) Determine the posterior predictive probabilities $p(a=1 \mid \mathcal{D})$ and $p(s=1 \mid \mathcal{D})$.
(b) Determine the posterior predictive probabilities $p(c=1 \mid \mathrm{pa}, \mathcal{D})$ for all possible parent configurations.

## Exercise 8. Learning parameters of a directed graphical model

We consider the directed graphical model shown below on the left for the four binary variables $t, b, s, x$, each being either zero or one. Assume that we have observed the data shown in the table on the right.

Model:

$t=1$ has tuberculosis
$b=1$ has bronchitis
$s=1$ has shortness of breath
$x=1$ has positive x-ray

Observed data:

| x | s | t | b |
| :---: | :---: | :---: | :---: |
| 0 | 1 | 0 | 1 |
| 0 | 0 | 0 | 0 |
| 0 | 1 | 0 | 1 |
| 0 | 1 | 0 | 1 |
| 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 |
| 0 | 1 | 0 | 1 |
| 0 | 1 | 0 | 1 |
| 0 | 0 | 0 | 1 |
| 1 | 1 | 1 | 0 |

We assume the (conditional) pmf of $s \mid t, b$ is specified by the following parametrised probability table:

| $\left.p\left(s=1 \mid t, b ; \theta_{s}^{1}, \ldots, \theta_{s}^{4}\right)\right)$ | $t$ | $b$ |
| :---: | :---: | :---: |
| $\theta_{s}^{1}$ | 0 | 0 |
| $\theta_{s}^{2}$ | 1 | 0 |
| $\theta_{s}^{3}$ | 0 | 1 |
| $\theta_{s}^{4}$ | 1 | 1 |

(a) What are the maximum likelihood estimates for $p(s=1 \mid b=0, t=0)$ and $p(s=1 \mid b=$ $0, t=1$ ), i.e. the parameters $\theta_{s}^{1}$ and $\theta_{s}^{3}$ ?
(b) Assume each parameter in the table for $p(s \mid t, b)$ has a uniform prior on $(0,1)$. Compute the posterior mean of the parameters of $p(s=1 \mid b=0, t=0)$ and $p(s=1 \mid b=0, t=1)$ and explain the difference to the maximum likelihood estimates.

## Exercise 9. Factor analysis

A friend proposes to improve the factor analysis model by working with correlated latent variables. The proposed model is

$$
\begin{equation*}
p(\mathbf{h} ; \mathbf{C})=\mathcal{N}(\mathbf{h} ; \mathbf{0}, \mathbf{C}) \quad p(\mathbf{v} \mid \mathbf{h} ; \mathbf{F}, \boldsymbol{\Psi}, \mathbf{c})=\mathcal{N}(\mathbf{v} ; \mathbf{F h}+\mathbf{c}, \mathbf{\Psi}) \tag{23}
\end{equation*}
$$

where $\mathbf{C}$ is some covariance matrix, and the other variables are defined as in the lecture slides. $\mathcal{N}(\mathbf{x} ; \boldsymbol{\mu}, \boldsymbol{\Sigma})$ denotes the pdf of a Gaussian with mean $\boldsymbol{\mu}$ and covariance matrix $\boldsymbol{\Sigma}$.
(a) What is marginal distribution of the visibles $p(\mathbf{v} ; \boldsymbol{\theta})$ where $\boldsymbol{\theta}$ stands for the parameters $\mathbf{C}, \mathbf{F}, \mathbf{c}, \boldsymbol{\Psi}$ ?
(b) Assume that the singular value decomposition of $\mathbf{C}$ is given by

$$
\begin{equation*}
\mathbf{C}=\mathbf{E} \boldsymbol{\Lambda} \mathbf{E}^{\top} \tag{24}
\end{equation*}
$$

where $\boldsymbol{\Lambda}=\operatorname{diag}\left(\lambda_{1}, \ldots, \lambda_{H}\right)$ is a diagonal matrix containing the eigenvalues, and $\mathbf{E}$ is a orthonormal matrix containing the corresponding eigenvectors. The matrix square root of $\mathbf{C}$ is the matrix $\mathbf{M}$ such that

$$
\begin{equation*}
\mathbf{M M}=\mathbf{C} \tag{25}
\end{equation*}
$$

and we denote it by $\mathbf{C}^{1 / 2}$. Show that the matrix square root of $\mathbf{C}$ equals

$$
\begin{equation*}
\mathbf{C}^{1 / 2}=\mathbf{E} \operatorname{diag}\left(\sqrt{\lambda_{1}}, \ldots, \sqrt{\lambda_{D}}\right) \mathbf{E}^{\top} \tag{26}
\end{equation*}
$$

(c) Show that the proposed factor analysis model is equivalent to the original factor analysis model

$$
\begin{equation*}
p(\mathbf{h} ; \mathbf{I})=\mathcal{N}(\mathbf{h} ; \mathbf{0}, \mathbf{I}) \quad p(\mathbf{v} \mid \mathbf{h} ; \tilde{\mathbf{F}}, \boldsymbol{\Psi}, \mathbf{c})=\mathcal{N}(\mathbf{v} ; \tilde{\mathbf{F}} \mathbf{h}+\mathbf{c}, \boldsymbol{\Psi}) \tag{27}
\end{equation*}
$$

with $\tilde{\mathbf{F}}=\mathbf{F C}^{1 / 2}$, so that the extra parameters given by the covariance matrix $\mathbf{C}$ are actually redundant and nothing is gained with the richer parametrisation.

## Exercise 10. Independent component analysis

(a) Whitening corresponds to linearly transforming a random variable $\mathbf{x}$ (or the corresponding data) so that the resulting random variable $\mathbf{z}$ has an identity covariance matrix, i.e.

$$
\mathbf{z}=\mathbf{V} \mathbf{x} \quad \text { with } \quad \mathbb{V}[\mathbf{x}]=\mathbf{C} \quad \text { and } \quad \mathbb{V}[\mathbf{z}]=\mathbf{I}
$$

The matrix $\mathbf{V}$ is called the whitening matrix. We do not make a distributional assumption on $\mathbf{x}$, in particular $\mathbf{x}$ may or may not be Gaussian.
Given the eigenvalue decomposition $\mathbf{C}=\mathbf{E} \boldsymbol{\Lambda} \mathbf{E}^{\top}$, show that

$$
\begin{equation*}
\mathbf{V}=\operatorname{diag}\left(\lambda_{1}^{-1 / 2}, \ldots, \lambda_{d}^{-1 / 2}\right) \mathbf{E}^{\top} \tag{28}
\end{equation*}
$$

is a whitening matrix.
(b) Consider the ICA model

$$
\begin{equation*}
\mathbf{v}=\mathbf{A h}, \quad \quad \mathbf{h} \sim p_{\mathbf{h}}(\mathbf{h}), \quad p_{\mathbf{h}}(\mathbf{h})=\prod_{i=1}^{D} p_{h}\left(h_{i}\right) \tag{29}
\end{equation*}
$$

where the matrix $\mathbf{A}$ is invertible and the $h_{i}$ are independent random variables of mean zero and variance one. Let $\mathbf{V}$ be a whitening matrix for $\mathbf{v}$. Show that $\mathbf{z}=\mathbf{V} \mathbf{v}$ follows the ICA model

$$
\begin{equation*}
\mathbf{z}=\tilde{\mathbf{A}} \mathbf{h}, \quad \quad \mathbf{h} \sim p_{\mathbf{h}}(\mathbf{h}), \quad p_{\mathbf{h}}(\mathbf{h})=\prod_{i=1}^{D} p_{h}\left(h_{i}\right) \tag{30}
\end{equation*}
$$

where $\tilde{\mathbf{A}}$ is an orthonormal matrix.

## Exercise 11. Score matching for the exponential family

The objective function $J(\boldsymbol{\theta})$ that is minimised in score matching is

$$
\begin{equation*}
J(\boldsymbol{\theta})=\frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{m}\left[\partial_{j} \psi_{j}\left(\mathbf{x}_{i} ; \boldsymbol{\theta}\right)+\frac{1}{2} \psi_{j}\left(\mathbf{x}_{i} ; \boldsymbol{\theta}\right)^{2}\right], \tag{31}
\end{equation*}
$$

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 $\mathbf{x}_{1}, \ldots, \mathbf{x}_{n}$ and $\mathbf{x} \in \mathbb{R}^{m}$.

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

$$
\begin{equation*}
\log p(\mathbf{x} ; \boldsymbol{\theta})=\sum_{k=1}^{K} \theta_{k} F_{k}(\mathbf{x})-\log Z(\boldsymbol{\theta}), \quad \mathbf{x} \in \mathbb{R}^{m} \tag{32}
\end{equation*}
$$

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 called the sufficient statistics).
(a) Denote by $\mathbf{K}(\mathbf{x})$ the matrix with elements $K_{k j}(\mathbf{x})$,

$$
\begin{equation*}
K_{k j}(\mathbf{x})=\frac{\partial F_{k}(\mathbf{x})}{\partial x_{j}}, \quad k=1 \ldots K, \quad j=1 \ldots m, \tag{33}
\end{equation*}
$$

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

$$
\begin{equation*}
H_{k j}(\mathbf{x})=\frac{\partial^{2} F_{k}(\mathbf{x})}{\partial x_{j}^{2}}, \quad k=1 \ldots K, \quad j=1 \ldots m \tag{34}
\end{equation*}
$$

Furthermore, let $\mathbf{h}_{j}(\mathbf{x})=\left(H_{1 j}(\mathbf{x}), \ldots, H_{K j}(\mathbf{x})\right)^{\top}$ be the $j$-th column vector of $\mathbf{H}(\mathbf{x})$.
Show that for the continuous exponential family, the score matching objective in Equation (31) becomes

$$
\begin{equation*}
J(\boldsymbol{\theta})=\boldsymbol{\theta}^{\top} \mathbf{r}+\frac{1}{2} \boldsymbol{\theta}^{\top} \mathbf{M} \boldsymbol{\theta}, \tag{35}
\end{equation*}
$$

where

$$
\begin{equation*}
\mathbf{r}=\frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{m} \mathbf{h}_{j}\left(\mathbf{x}_{i}\right), \quad \mathbf{M}=\frac{1}{n} \sum_{i=1}^{n} \mathbf{K}\left(\mathbf{x}_{i}\right) \mathbf{K}\left(\mathbf{x}_{i}\right)^{\top} . \tag{36}
\end{equation*}
$$

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

$$
\begin{equation*}
p\left(x ; \sigma^{2}\right)=\frac{1}{\sqrt{2 \pi \sigma^{2}}} \exp \left(-\frac{x^{2}}{2 \sigma^{2}}\right), \quad x \in \mathbb{R} . \tag{37}
\end{equation*}
$$

The (multivariate) Gaussian is a member of the exponential family. By comparison with Equation (32), we can re-parametrise the statistical model $\left\{p\left(x ; \sigma^{2}\right)\right\}_{\sigma^{2}}$ and work with

$$
\begin{equation*}
p(x ; \theta)=\frac{1}{Z(\theta)} \exp \left(\theta x^{2}\right), \quad \theta<0, \quad x \in \mathbb{R} \tag{38}
\end{equation*}
$$

instead. The two parametrisations are related by $\theta=-1 /\left(2 \sigma^{2}\right)$. 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.

## Exercise 12. Maximum likelihood estimation and unnormalised models

Consider the Ising model for two binary random variables $\left(x_{1}, x_{2}\right)$,

$$
p\left(x_{1}, x_{2} ; \theta\right) \propto \exp \left(\theta x_{1} x_{2}+x_{1}+x_{2}\right), \quad x_{i} \in\{-1,1\}
$$

(a) Compute the partition function $Z(\theta)$.
(b) The figure below shows the graph of $f(\theta)=\frac{\partial \log Z(\theta)}{\partial \theta}$.

Assume you observe three data points $\left(x_{1}, x_{2}\right)$ equal to $(-1,-1),(-1,1)$, and $(1,-1)$. Using the figure, what is the maximum likelihood estimate of $\theta$ ? Justify your answer.


## Exercise 13. Parameter estimation for unnormalised models

Let $p(\mathbf{x} ; \mathbf{A}) \propto \exp \left(-\mathbf{x}^{\top} \mathbf{A} \mathbf{x}\right)$ be a parametric statistical model for $\mathbf{x}=\left(x_{1}, \ldots, x_{100}\right)$, where the parameters are the elements of the matrix $\mathbf{A}$. Assume that $\mathbf{A}$ is symmetric and positive semi-definite, i.e. $\mathbf{A}$ satisfies $\mathbf{x}^{\top} \mathbf{A} \mathbf{x} \geq 0$ for all values of $\mathbf{x}$.
(a) For $n$ iid data points $\mathbf{x}_{1}, \ldots, \mathbf{x}_{n}$, a friend proposes to estimate $\mathbf{A}$ by maximising $J(\mathbf{A})$,

$$
\begin{equation*}
J(\mathbf{A})=\prod_{k=1}^{n} \exp \left(-\mathbf{x}_{k}^{\top} \mathbf{A} \mathbf{x}_{k}\right) \tag{39}
\end{equation*}
$$

Explain why this procedure cannot give reasonable parameter estimates.
(b) Explain why maximum likelihood estimation is easy when the $x_{i}$ are real numbers, i.e. $x_{i} \in \mathbb{R}$, while typically very difficult when the $x_{i}$ are binary, i.e. $x_{i} \in\{0,1\}$.
(c) Can we use score matching instead of maximum likelihood estimation to learn $\mathbf{A}$ if the $x_{i}$ are binary?

