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 μ and standard deviation σ 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 iid data $\mathcal{D} = \{x_1, \dots, x_n\}$, 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 μ and standard deviation σ are the sample mean

$$\bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i \tag{1}$$

and the square root of the sample variance

$$S^{2} = \frac{1}{n} \sum_{i=1}^{n} (x_{i} - \bar{x})^{2}.$$
 (2)

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

Given iid data $\mathcal{D} = \{x_1, \dots, x_n\}$, compute $p(\mu|\mathcal{D}, \sigma^2)$ for the Bayesian model

$$p(x|\mu) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right] \qquad p(\mu;\mu_0,\sigma_0^2) = \frac{1}{\sqrt{2\pi\sigma_0^2}} \exp\left[-\frac{(\mu-\mu_0)^2}{2\sigma_0^2}\right]$$
(3)

where σ^2 is a fixed known quantity.

Hint: You may use that

$$\mathcal{N}(x; m_1, \sigma_1^2) \mathcal{N}(x; m_2, \sigma_2^2) \propto \mathcal{N}(x; m_3, \sigma_3^2)$$
(4)

where

$$\mathcal{N}(x;\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right]$$
 (5)

$$\sigma_3^2 = \left(\frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2}\right)^{-1} = \frac{\sigma_1^2 \sigma_2^2}{\sigma_1^2 + \sigma_2^2} \tag{6}$$

$$m_3 = \sigma_3^2 \left(\frac{m_1}{\sigma_1^2} + \frac{m_2}{\sigma_2^2}\right) = m_1 + \frac{\sigma_1^2}{\sigma_1^2 + \sigma_2^2} (m_2 - m_1)$$
 (7)

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 ,

$$p(\mathbf{x}; \boldsymbol{\theta}) = \prod_{i=1}^{d} p(x_i | \text{pa}_i; \boldsymbol{\theta}_i) \qquad x_i \in \{0, 1\}$$
(8)

where the conditionals are represented by parametrised probability tables, For example, if $pa_3 = \{x_1, x_2\}, p(x_3|pa_3; \theta_3)$ is represented as

$\overline{p(x_3 = 1 x_1, x_2; \theta_3^1, \dots, \theta_3^4))}$	x_1	x_2
θ_3^1	0	0
$egin{array}{c} heta_3^3 \ heta_3^3 \end{array}$	1	0
$ heta_3^{ ilde{3}}$	0	1
$ heta_3^4$	1	1

with $\theta_3 = (\theta_3^1, \theta_3^2, \theta_3^3, \theta_3^4)$, and where the superscripts j of θ_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 $p(x_i|pa_i; \boldsymbol{\theta}_i)$ is equivalent to writing $p(x_i|pa_i; \boldsymbol{\theta}_i)$ as

$$p(x_i|pa_i; \boldsymbol{\theta}_i) = \prod_{s=1}^{S_i} (\theta_i^s)^{\mathbb{1}(x_i=1, pa_i=s)} (1 - \theta_i^s)^{\mathbb{1}(x_i=0, pa_i=s)}$$
(9)

where $S_i = 2^{m_i}$ is the total number of states/configurations that the parents can be in, and $\mathbb{1}(x_i = 1, pa_i = s)$ is one if $x_i = 1$ and $pa_i = s$, and zero otherwise.

(b) For iid data $\mathcal{D} = \{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}\}$ show that the likelihood can be represented as

$$p(\mathcal{D}; \boldsymbol{\theta}) = \prod_{i=1}^{d} \prod_{s=1}^{S_i} (\theta_i^s)^{n_{x_i=1}^s} (1 - \theta_i^s)^{n_{x_i=0}^s}$$
(10)

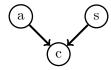
where $n_{x_i=1}^s$ is the number of times the pattern $(x_i=1, pa_i=s)$ occurs in the data \mathcal{D} , and equivalently for $n_{x_i=0}^s$.

- (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

$$\hat{\theta}_i^s = \frac{n_{x_i=1}^s}{n_{x_i=1}^s + n_{x_i=0}^s} = \frac{\sum_{j=1}^n \mathbb{1}(x_i^{(j)} = 1, pa_i^{(j)} = s)}{\sum_{j=1}^n \mathbb{1}(pa_i^{(j)} = s)}$$
(11)

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) θ_a and θ_s , respectively, i.e.

$$p(a; \theta_a) = \theta_a^a (1 - \theta_a)^{1-a}$$
 $p(s; \theta_s) = \theta_s^s (1 - \theta_s)^{1-s},$ (12)

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

$p(c=1 a,s;\theta_c^1,\ldots,\theta_c^4))$	a	s
$ heta_c^1$	0	0
$ heta_c^1 \ heta_c^2$	1	0
$ heta_c^c$	0	1
$ heta_c^4$	1	1

The free parameters of the model are $(\theta_a, \theta_s, \theta_c^1, \dots, \theta_c^4)$.

Assume we observe the following iid data (each row is a data point).

a	\mathbf{s}	c
0	1	1
0	0	0
1	0	1
0	0	0
0	1	0

- (a) Determine the maximum-likelihood estimates of θ_a and θ_s
- (b) Determine the maximum-likelihood estimates of $\theta_c^1, \dots, \theta_c^4$.

Exercise 5. Bayesian inference for the Bernoulli model

Consider the Bayesian model

$$p(x|\theta) = \theta^x (1-\theta)^{1-x}$$
 $p(\theta; \alpha_0) = \mathcal{B}(\theta; \alpha_0, \beta_0)$

where $x \in \{0, 1\}, \ \theta \in [0, 1], \alpha_0 = (\alpha_0, \beta_0), \text{ and }$

$$\mathcal{B}(\theta; \alpha, \beta) \propto \theta^{\alpha - 1} (1 - \theta)^{\beta - 1} \qquad \theta \in [0, 1]$$
 (13)

(a) Given iid data $\mathcal{D} = \{x_1, \dots, x_n\}$ show that the posterior of θ given \mathcal{D} is

$$p(\theta|\mathcal{D}) = \mathcal{B}(\theta; \alpha_n, \beta_n)$$

$$\alpha_n = \alpha_0 + n_{x=1}$$

$$\beta_n = \beta_0 + n_{x=0}$$

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,

$$p(f;\alpha,\beta) = \mathcal{B}(f;\alpha,\beta) \qquad f \in [0,1], \tag{14}$$

using that

$$\int_0^1 f^{\alpha - 1} (1 - f)^{\beta - 1} df = B(\alpha, \beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha + \beta)}$$
(15)

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

$$\Gamma(t) = \int_{0}^{\infty} f^{t-1} \exp(-f) df$$
 (16)

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 $p(x=1|\mathcal{D})$ for a new independently observed data point x equals the posterior mean of $p(\theta|\mathcal{D})$, which in turn is given by

$$\mathbb{E}(\theta|\mathcal{D}) = \frac{\alpha_0 + n_{x=1}}{\alpha_0 + \beta_0 + n}.$$
 (17)

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

$$p(\mathbf{x}|\boldsymbol{\theta}) = \prod_{i=1}^{d} p(x_i|\mathrm{pa}_i, \boldsymbol{\theta}_i) \qquad x_i \in \{0, 1\}$$

$$p(\boldsymbol{\theta}; \boldsymbol{\alpha}_0, \boldsymbol{\beta}_0) = \prod_{i=1}^{d} \prod_{j=1}^{S_i} \mathcal{B}(\theta_i^s; \alpha_{i,0}^s, \beta_{i,0}^s)$$
(18)

$$p(\boldsymbol{\theta}; \boldsymbol{\alpha}_0, \boldsymbol{\beta}_0) = \prod_{i=1}^d \prod_{s=1}^{S_i} \mathcal{B}(\theta_i^s; \alpha_{i,0}^s, \beta_{i,0}^s)$$
(19)

where $p(x_i|pa_i, \boldsymbol{\theta}_i)$ 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 $\mathcal{D} = \{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}\}$ show that

$$p(\boldsymbol{\theta}|\mathcal{D}) = \prod_{i=1}^{d} \prod_{s=1}^{S_i} \mathcal{B}(\theta_i^s, \alpha_{i,n}^s, \beta_{i,n}^s)$$
 (20)

where

$$\alpha_{i,n}^s = \alpha_{i,0}^s + n_{x_i=1}^s \qquad \beta_{i,n}^s = \beta_{i,0}^s + n_{x_i=0}^s \qquad (21)$$

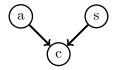
and that the parameters are also independent under the posterior.

(b) For a variable x_i with parents pa_i , compute the posterior predictive probability $p(x_i = 1|pa_i, \mathcal{D})$

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) θ_a and θ_s , respectively, i.e.

$$p(a|\theta_a) = \theta_a^a (1 - \theta_a)^{1-a}$$
 $p(s|\theta_s) = \theta_s^s (1 - \theta_s)^{1-s},$ (22)

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

$p(c=1 a,s,\theta_c^1,\ldots,\theta_c^4))$	a	\overline{s}
	0	
θ_c^2	1	0
$ heta_c^3$	0	1
$ heta_c^4$	1	1

We assume that the prior over the parameters of the model, $(\theta_a, \theta_s, \theta_c^1, \dots, \theta_c^4)$, factorises and is given by beta distributions with hyperparameters $\alpha_0 = 1$ and $\beta_0 = 1$ (same for all parameters).

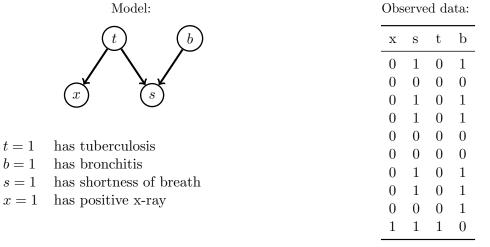
Assume we observe the following iid data (each row is a data point).

a	\mathbf{s}	\mathbf{c}
0	1	1
0	0	0
1	0	1
0	0	0
0	1	0

- (a) Determine the posterior predictive probabilities $p(a=1|\mathcal{D})$ and $p(s=1|\mathcal{D})$.
- (b) Determine the posterior predictive probabilities p(c = 1|pa, 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.



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

$\overline{p(s=1 t,b;\theta_s^1,\ldots,\theta_s^4))}$	t	b
$ heta_s^1$	0	0
$egin{array}{c} heta_s^1 \ heta_s^2 \ heta_s^3 \end{array}$	1	0
$ heta_s^3$	0	1
$ heta_s^4$	1	1

- (a) What are the maximum likelihood estimates for p(s=1|b=0,t=0) and p(s=1|b=0,t=1), i.e. the parameters θ_s^1 and θ_s^3 ?
- (b) Assume each parameter in the table for p(s|t,b) has a uniform prior on (0,1). Compute the posterior mean of the parameters of p(s=1|b=0,t=0) and p(s=1|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

$$p(\mathbf{h}; \mathbf{C}) = \mathcal{N}(\mathbf{h}; \mathbf{0}, \mathbf{C}) \qquad p(\mathbf{v}|\mathbf{h}; \mathbf{F}, \mathbf{\Psi}, \mathbf{c}) = \mathcal{N}(\mathbf{v}; \mathbf{F}\mathbf{h} + \mathbf{c}, \mathbf{\Psi})$$
(23)

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 C is given by

$$\mathbf{C} = \mathbf{E} \mathbf{\Lambda} \mathbf{E}^{\top} \tag{24}$$

where $\mathbf{\Lambda} = \operatorname{diag}(\lambda_1, \dots, \lambda_H)$ 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

$$\mathbf{MM} = \mathbf{C},\tag{25}$$

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

$$\mathbf{C}^{1/2} = \mathbf{E} \operatorname{diag}(\sqrt{\lambda_1}, \dots, \sqrt{\lambda_D}) \mathbf{E}^{\top}.$$
 (26)

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

$$p(\mathbf{h}; \mathbf{I}) = \mathcal{N}(\mathbf{h}; \mathbf{0}, \mathbf{I})$$
 $p(\mathbf{v}|\mathbf{h}; \tilde{\mathbf{F}}, \mathbf{\Psi}, \mathbf{c}) = \mathcal{N}(\mathbf{v}; \tilde{\mathbf{F}}\mathbf{h} + \mathbf{c}, \mathbf{\Psi})$ (27)

with $\tilde{\mathbf{F}} = \mathbf{F}\mathbf{C}^{1/2}$, 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.

$$z = Vx$$
 with $V[x] = C$ and $V[z] = I$.

The matrix V is called the whitening matrix. We do not make a distributional assumption on x, in particular x may or may not be Gaussian.

Given the eigenvalue decomposition $\mathbf{C} = \mathbf{E} \mathbf{\Lambda} \mathbf{E}^{\top}$, show that

$$\mathbf{V} = \operatorname{diag}(\lambda_1^{-1/2}, \dots, \lambda_d^{-1/2}) \mathbf{E}^{\top}$$
(28)

is a whitening matrix.

(b) Consider the ICA model

$$\mathbf{v} = \mathbf{Ah}, \qquad \mathbf{h} \sim p_{\mathbf{h}}(\mathbf{h}), \qquad p_{\mathbf{h}}(\mathbf{h}) = \prod_{i=1}^{D} p_{h}(h_{i}), \qquad (29)$$

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

$$\mathbf{z} = \tilde{\mathbf{A}}\mathbf{h}, \qquad \mathbf{h} \sim p_{\mathbf{h}}(\mathbf{h}), \qquad p_{\mathbf{h}}(\mathbf{h}) = \prod_{i=1}^{D} p_{h}(h_{i}), \qquad (30)$$

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

$$J(\boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{m} \left[\partial_j \psi_j(\mathbf{x}_i; \boldsymbol{\theta}) + \frac{1}{2} \psi_j(\mathbf{x}_i; \boldsymbol{\theta})^2 \right], \tag{31}$$

where ψ_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

$$\log p(\mathbf{x}; \boldsymbol{\theta}) = \sum_{k=1}^{K} \theta_k F_k(\mathbf{x}) - \log Z(\boldsymbol{\theta}), \qquad \mathbf{x} \in \mathbb{R}^m,$$
 (32)

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 θ_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 $K_{kj}(\mathbf{x})$,

$$K_{kj}(\mathbf{x}) = \frac{\partial F_k(\mathbf{x})}{\partial x_j}, \qquad k = 1 \dots K, \quad j = 1 \dots m,$$
 (33)

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

$$H_{kj}(\mathbf{x}) = \frac{\partial^2 F_k(\mathbf{x})}{\partial x_i^2}, \qquad k = 1 \dots K, \quad j = 1 \dots m.$$
 (34)

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 (31) becomes

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

where

$$\mathbf{r} = \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{m} \mathbf{h}_{j}(\mathbf{x}_{i}), \qquad \mathbf{M} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{K}(\mathbf{x}_{i}) \mathbf{K}(\mathbf{x}_{i})^{\top}.$$
(36)

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

$$p(x; \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2}{2\sigma^2}\right), \qquad x \in \mathbb{R}.$$
 (37)

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

$$p(x;\theta) = \frac{1}{Z(\theta)} \exp(\theta x^2), \qquad \theta < 0, \qquad x \in \mathbb{R},$$
 (38)

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.

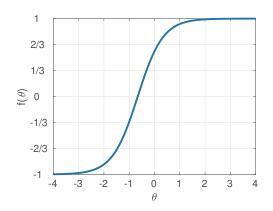
Exercise 12. Maximum likelihood estimation and unnormalised models

Consider the Ising model for two binary random variables (x_1, x_2) ,

$$p(x_1, x_2; \theta) \propto \exp(\theta x_1 x_2 + x_1 + x_2), \quad x_i \in \{-1, 1\},$$

- (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 (x_1, x_2) equal to (-1, -1), (-1, 1), and (1, -1). Using the figure, what is the maximum likelihood estimate of θ ? Justify your answer.



Exercise 13. Parameter estimation for unnormalised models

Let $p(\mathbf{x}; \mathbf{A}) \propto \exp(-\mathbf{x}^{\top} \mathbf{A} \mathbf{x})$ be a parametric statistical model for $\mathbf{x} = (x_1, \dots, x_{100})$, 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 $\mathbf{x}_1, \dots, \mathbf{x}_n$, a friend proposes to estimate **A** by maximising $J(\mathbf{A})$,

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

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 $\bf A$ if the x are binary?