5SSD0

Bayesian Machine Learning and Information Processing

Exercises

Bert de Vries (Flux 7.101)

Wouter Kouw (Flux 7.060)

• Cheatsheet	3
Machine Learning Overview	3
Probability Theory Review	3
Bayesian Machine Learning	4
• Factor Graphs	5
Continuous Data and the Gaussian Distribution	6
Discrete Data and the Multinomial Distribution	6
• Regression	7
Generative Classification	7
Discriminative Classification	8
Latent Variable Models and Variational Bayes	9
Dynamic Models	9
Intelligent Agents and Active Inference	10

Cheatsheet

- You are not allowed to bring books or notes to the exam. Instead, feel free to make use of the following cheatsheet as we will provide this or a similar cheatsheet in an appendix of the exam papers.
- Some Matrix Calculus, see also Bishop, appendix C.

$$\begin{split} |A^{-1}| &= |A|^{-1} \\ \nabla_A \log |A| &= (A^T)^{-1} = (A^{-1})^T \\ \operatorname{Tr}[ABC] &= \operatorname{Tr}[CAB] = \operatorname{Tr}[BCA] \\ \nabla_A \operatorname{Tr}[AB] &= D^T \\ \nabla_A \operatorname{Tr}[AB] &= D^T \\ \nabla_A \operatorname{Tr}[ABA^T] &= A(B + B^T) \\ \nabla_x x^T Ax &= (A + A^T)x \\ \nabla_X a^T Xb &= \nabla_X \operatorname{Tr}[ba^T X] = ab^T \end{split}$$

• Definition of the Multivariate Gaussian Distribution (MVG)

$$\mathcal{N}(x|\mu,\Sigma) = \left|2\pi\Sigma\right|^{-rac{1}{2}} \exp\left\{-rac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)
ight\}$$

• A linear transformation z = Ax + b of a Gaussian variable $\mathcal{N}(x|\mu, \Sigma)$ is Gaussian distributed as

$$p(z) = \mathcal{N}\left(z \mid A\mu + b, A\Sigma A^T
ight)$$

Multiplication of 2 Gaussian distributions

$$\mathcal{N}(x|\mu_a, \Sigma_a) \cdot \mathcal{N}(x|\mu_b, \Sigma_b) = \alpha \cdot \mathcal{N}(x|\mu_c, \Sigma_c)$$

with

$$\Sigma_c^{-1} = \Sigma_a^{-1} + \Sigma_b^{-1}$$

$$\Sigma_c^{-1} \mu_c = \Sigma_a^{-1} \mu_a + \Sigma_b^{-1} \mu_b$$

$$\alpha = \mathcal{N}(\mu_a | \mu_b, \Sigma_a + \Sigma_b)$$

Conditioning and **marginalization** of Gaussians. Let $z = \begin{bmatrix} x \\ y \end{bmatrix}$ be jointly normal distributed as

$$p(z) = \mathcal{N}(z|\mu, \Sigma) = \mathcal{N}\left(\left[\begin{matrix} x \\ y \end{matrix} \right] \; \middle| \; \left[\begin{matrix} \mu_x \\ \mu_y \end{matrix} \right], \left[\begin{matrix} \Sigma_x & \Sigma_{xy} \\ \Sigma_{yx} & \Sigma_y \end{matrix} \right] \right) \,,$$

then $p(z) = p(y|x) \cdot p(x)$, with

$$\begin{split} p(y|x) &= \mathcal{N}\left(y|\; \mu_y + \Sigma_{yx}\,\Sigma_x^{-1}(x-\mu_x),\; \Sigma_y - \Sigma_{yx}\,\Sigma_x^{-1}\Sigma_{xy}\right) \\ p(x) &= \mathcal{N}\left(x|\; \mu_x,\; \Sigma_x\right) \end{split}$$

For a binary variable $x \in \{0,1\}$, the **Bernoulli** distribution is given by

$$p(x|\mu) = \mu^x (1-\mu)^{1-x}$$

• The conjugate prior for μ is the **Beta** distribution, given by

$$p(\mu) = \mathcal{B}(\mu|\alpha, \beta) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} \mu^{\alpha - 1} (1 - \mu)^{\beta - 1}$$

where α and β are "hyperparameters" that you can set to reflect your prior beliefs about μ .

Machine Learning Overview

• [1] (##) Pick three applications from the "Some Machine Learning Applications"-slide and (shortly) describe for each application how (a combination of) clustering, dimensionality reduction, regression classification or reinforcement learning could accomplish the task.

Probability Theory Review

• [1] (a) (#) Proof that the "elementary" sum rule p(A) + p(A) = 1 follows from the (general) sum rule

$$p(A+B) = p(A) + p(B) - p(A, B).$$

(b) (###) Conversely, derive the general sum rule p(A+B) = p(A) + p(B) - p(A,B) from the elementary sum rule p(A) + p(A) = 1 and the product rule. Here, you may make use of the (Boolean logic) fact that $A + B = \overline{AB}$.

- [2] Box 1 contains 8 apples and 4 oranges. Box 2 contains 10 apples and 2 oranges. Boxes are chosen with equal probability.
 - (a) (#) What is the probability of choosing an apple?
 - (b) (##) If an apple is chosen, what is the probability that it came from box 1?

- [3] (###) The inhabitants of an island tell the truth one third of the time. They lie with probability 2/3. On an occasion, after one of them made a statement, you ask another "was that statement true?" and he says "yes". What is the probability that the statement was indeed true?
- [4] (##) A bag contains one ball, known to be either white or black. A white ball is put in, the bag is shaken, and a ball is drawn out, which proves to be white. What is now the chance of drawing a white ball? (Note that the state of the bag, after the operations, is exactly identical to its state before.)
- [5] A dark bag contains five red balls and seven green ones.
 - (a) (#) What is the probability of drawing a red ball on the first draw?
 - (b) (##) Balls are not returned to the bag after each draw. If you know that on the second draw the ball was a green one, what is now the probability of drawing a red ball on the first draw?
- [6] (#) Is it more correct to speak about the likelihood of a model (or model parameters) than about the likelihood of an observed data set. And why?
- [7] (##) Is a speech signal a 'probabilistic' (random) or a deterministic signal?
- [8] (##) Proof that, for any distribution of x and y and z = x + y

$$egin{aligned} \mathbb{E}[z] &= \mathbb{E}[x] + \mathbb{E}[y] \\ \mathbb{V}[z] &= \mathbb{V}[x] + \mathbb{V}[y] + 2\mathbb{V}[x,y] \end{aligned}$$

where $\mathbb{E}[\cdot]$, $\mathbb{V}[\cdot]$ and $\mathbb{V}[\cdot,\cdot]$ refer to the expectation (mean), variance and covariance operators respectively. You may make use of the more general theorem that the mean and variance of any distribution p(x) is processed by a linear tranformation as

$$\mathbb{E}[Ax + b] = A\mathbb{E}[x] + b$$

$$\mathbb{V}[Ax + b] = A\mathbb{V}[x]A^{T}$$

Bayesian Machine Learning

- [1] (#) (a) Explain shortly the relation between machine learning and Bayes rule.
 (b) How are Maximum a Posteriori (MAP) and Maximum Likelihood (ML) estimation related to Bayes rule and machine learning?
- [2] (#) What are the four stages of the Bayesian design approach?
- [3] (##) The Bayes estimate is a summary of a posterior distribution by a delta distribution on its mean, i.e.,

$$\theta_{bayes} = \int \theta p \left(\theta | D \right) d\theta$$

Proof that the Bayes estimate minimizes the expected mean-squared error, i.e., proof that

$$\hat{\theta}_{bayes} = \arg\min_{\hat{\theta}} \int_{\theta} (\hat{\theta} - \theta)^2 p(\theta|D) d\theta$$

- [4] (##) We consider the coin toss example from the notebook and use a conjugate prior for a Bernoulli likelihood function.
 - (a) Derive the Maximum Likelihood estimate.
 - (b) Derive the MAP estimate.
 - (c) Do these two estimates ever coincide (if so under what circumstances)?
- [5] (##) A model m_1 is described by a single parameter θ , with $0 \le \theta \le 1$. The system can produce data $x \in \{0, 1\}$. The sampling distribution and prior are given by

$$p(x|\theta, m_1) = \theta^x (1-\theta)^{(1-x)}$$
$$p(\theta|m_1) = 6\theta(1-\theta)$$

- (a) Work out the probability $p(x=1|m_1)$.
- (b) Determine the posterior $p(\theta|x=1,m_1)$.

Now consider a second model m_2 with the following sampling distribution and prior on $0 \le \theta \le 1$:

$$p(x|\theta, m_2) = (1- heta)^x heta^{\left(1-x
ight)} \ p(heta|m_2) = 2 heta$$

(c) Determine the probability $p(x=1|m_2)$.

Now assume that the model priors are given by

$$\begin{array}{l} p(m_1)=1/3 \\ p(m_2)=2/3 \end{array}$$

- (d) Compute the probability p(x=1) by "Bayesian model averaging", i.e., by weighing the predictions of both models appropriately.
- (e) Compute the fraction of posterior model probabilities $\frac{p(m_1|x=1)}{x}$
- (f) Which model do you prefer after observation x = 1?

1) Which model do you prefer after observation x=1

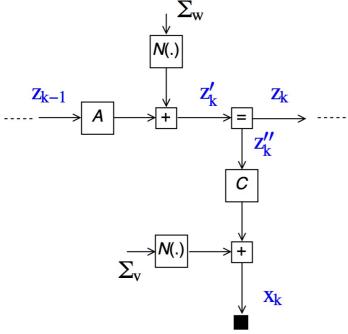
- [6] (###) Given a single observation x_0 from a uniform distribution Unif $[0, 1/\theta]$, where $\theta > 0$.
 - (a) Show that $\mathbb{E}[g(x_0)] = \theta$ if and only if $\int_0^{1/\theta} g(u) du = 1$.
 - (b) Show that there is no function g that satisfies the condition for all $\theta > 0$.

Factor Graphs

• [1] Consider the following state-space model:

$$\begin{aligned} z_k &= A z_{k-1} + w_k \\ x_k &= C z_k + v_k \end{aligned}$$

where k = 1, 2, ..., n is the time step counter; z_k is an *unobserved* state sequence; x_k is an *observed* sequence; $x_k \sim \mathcal{N}(0, \Sigma_w)$ and $x_k \sim \mathcal{N}(0, \Sigma_w)$ are (unobserved) state and observation noise sequences respectively; $x_0 \sim \mathcal{N}(0, \Sigma_0)$ is the initial state and $x_0 \sim \mathcal{N}(0, \Sigma_w)$ and $x_0 \sim \mathcal{N}(0, \Sigma_w)$ are known parameters. The Forney-style factor graph (FFG) for one time step is depicted here:



(a) Rewrite the state-space equations as a set of conditional probability distributions.

$$p(z_k|z_{k-1}, A, \Sigma_w) = \dots$$

 $p(x_k|z_k, C, \Sigma_v) = \dots$
 $p(z_0|\Sigma_0) = \dots$

- (b) Define $z^n \triangleq (z_0, z_1, \dots, z_n)$, $x^n \triangleq (x_1, \dots, x_n)$ and $\theta = \{A, C, \Sigma_w, \Sigma_v\}$. Now write out the generative model $p(x^n, z^n | \theta)$ as a product of factors.
- (c) We are interested in estimating z_k from a given estimate for z_{k-1} and the current observation x_{kt} i.e., we are interested in computing $p(z_k|z_{k-1},x_k,\theta)$. Can $p(z_k|z_{k-1},x_k,\theta)$ be expressed as a Gaussian distribution? Explain why or why not in one sentence.
- (d) Copy the graph onto your exam paper and draw the message passing schedule for computing $p(z_k|z_{k-1},x_k,\theta)$ by drawing arrows in the factor graph. Indicate the order of the messages by assigning numbers to the arrows.
- (e) Now assume that our belief about parameter Σ_v is instead given by a distribution $p(\Sigma_v)$ (rather than a known value). Adapt the factor graph drawing of the previous answer to reflects our belief about Σ_v .
- [2] Consider an addition node

$$\begin{array}{c|c}
 & X \\
 & \downarrow \\
 & Y \\
 & Z
\end{array}$$

 $f_+(x, y, z) = \delta(z - x - y)$

- (a) Derive an expression for the outgoing message $\vec{\mu}_{Z^{(z)}}$ in terms of the incoming messages $\vec{\mu}_{X^{(\cdot)}}$ and $\vec{\mu}_{Y^{(\cdot)}}$.
- (b) Now assume that both incoming messages are Gaussian, namely $\vec{\mu}_X(x) \sim \mathcal{N}(\vec{m}_X, \vec{V}_X)$ and $\vec{\mu}_Y(y) \sim \mathcal{N}(\vec{m}_Y, \vec{V}_Y)$. Evaluate the outgoing message $\vec{\mu}_Z(z)$. You will need the multiplication rule for Gaussians.

(c) For the same summation node, work out the SP update rule for the backward message $\stackrel{\leftarrow}{\iota}_X(x)$ as a function of $\stackrel{\leftarrow}{\iota}_Z(z)$. And further refine the answer for Gaussian messages.

Continuous Data and the Gaussian Distribution

• [1] (##) We are given an IID data set $D = \{x_1, x_2, ..., x_N\}$, where $x_n \in \mathbb{R}^M$. Let's assume that the data were drawn from a multivariate Gaussian (MVG),

$$p(x_n|\theta) = \mathcal{N}(x_n|\mu, \Sigma) = |2\pi\Sigma|^{-\frac{1}{2}} \exp\left\{-\frac{1}{2}(x_n - \mu)^T \Sigma^{-1}(x_n - \mu)\right\}$$

- (a) Derive the log-likelihood of the parameters for these data.
- (b) Derive the maximum likelihood estimates for the mean μ and variance Σ by setting the derivative of the log-likelihood to zero.
- [2] (#) Shortly explain why the Gaussian distribution is often preferred as a prior distribution over other distributions with the same support?
- [3] (###) We make N IID observations $D = \{x_1 ... x_N\}$ and assume the following model

$$\begin{split} x_k &= A + \epsilon_k \\ A &\sim \mathcal{N}(m_A^{}, v_A^{}) \\ \epsilon_k &\sim \mathcal{N}(0, \sigma^2) \; . \end{split}$$

We assume that σ has a known value and are interested in deriving an estimator for A.

- (a) Derive the Bayesian (posterior) estimate p(A|D).
- (b) (##) Derive the Maximum Likelihood estimate for A.
- (c) Derive the MAP estimates for A.
- (d) Now assume that we do not know the variance of the noise term? Describe the procedure for Bayesian estimation of both A and σ^2 (No need to fully work out to closed-form estimates).
- [4] (##) Proof that a linear transformation z = Ax + b of a Gaussian variable $\mathcal{N}(x|\mu,\Sigma)$ is Gaussian distributed as

$$p(z) = \mathcal{N}\left(z | A\mu + b, A\Sigma A^T\right)$$

- [5] (#) Given independent variables $x \sim \mathcal{N}(\mu_x, \sigma_x^2)$ and $y \sim \mathcal{N}(\mu_y, \sigma_y^2)$, what is the PDF for $z = A \cdot (x y) + b$?
- [6] (###) Compute

$$\int_{-\infty}^{\infty} \exp(-x^2) \, \mathrm{d}x.$$

Discrete Data and the Multinomial Distribution

• [1] (##) We consider IID data $D = \{x_1, x_2, ..., x_N\}$ obtained from tossing a K-sided die. We use a binary selection variable

$$x_{nk} \equiv \left\{ egin{array}{ll} 1 & ext{if } x_n ext{ lands on } k ext{th face} \\ 0 & ext{otherwise} \end{array}
ight.$$

with probabilities $p(x_{nk} = 1) = \theta_k$.

- (a) Write down the probability for the nth observation $p(x_n|\theta)$ and derive the log-likelihood $\log p(D|\theta)$.
- (b) Derive the maximum likelihood estimate for θ .
- [2] (#) In the notebook, Laplace's generalized rule of succession (the probability that we throw the kth face at the next toss) was derived as

$$p(x_{\bullet,k} = 1|D) = \frac{m_k + \alpha_k}{N + \sum_k \alpha_k}$$

Provide an interpretation of the variables m_k , N, α_k , $\sum_k \alpha_k$.

- [3] (##) Show that Laplace's generalized rule of succession can be worked out to a prediction that is composed of a prior prediction and data-based correction term.
- [4] (#) Verify that
 - (a) the categorial distribution is a special case of the multinomial for N=1.
 - (b) the Bernoulli is a special case of the categorial distribution for K=2.
 - (c) the binomial is a special case of the multinomial for K = 2.
- [5] (###) Consider a data set of binary variables $D = \{x_1, x_2, ..., x_N\}$ with a Bernoulli distribution $Ber(x_k|\mu)$ as data generating distribution and a Beta prior for μ . Assume that you make n observations with x = 1 and N n observations with x = 0. Now consider a new draw x_* . We are interested in computing $p(x_*|D)$. Show that the mean value for $p(x_*|D)$ lies in between the prior mean and Maximum Likelihood estimate.
- **[6]** Consider a data set $D = \{(x_1, y_1), (x_2, y_2), ..., (x_N, y_N)\}$ with one-hot encoding for the K discrete classes, i.e., $y_{nk} = 1$ if and only if $y_n \in \mathcal{C}_{kr}$ else $y_{nk} = 0$. Also given are the class-conditional distribution $p(x_n|y_{nk} = 1, \theta) = \mathcal{N}(x_n|\mu_k, \Sigma)$ and multinomial prior $p(y_{nk} = 1) = \pi_k$.

 (a) Proof that the joint log-likelihood is given by

$$\log p(D|\theta) = \sum_{n,k} y_{nk} \log \mathcal{N}(x_n|\mu_k, \Sigma) + \sum_{n,k} y_{nk} \log \pi_k$$

(b) Show now that the MLE of the class-conditional mean is given by

$$\hat{\mu}_k = \frac{\sum_n y_{nk} x_n}{\sum_n y_{nk}}$$

Regression

- [1] (#) (a) Write down the generative model for Bayesian linear ordinary regression (i.e., write the likelihood and prior).
 - (b) State the inference task for the weight parameter in the model.
 - (c) Why do we call this problem linear?
- [2] (##) Consider a linear regression problem

$$\begin{split} p(y|\;\mathbf{X}, w, \beta) &= \mathcal{N}(y\,|\;\mathbf{X}w, \beta^{-1}\mathbf{I}) \\ &= \prod \mathcal{N}(yn\,|\,w^T\,x_n, \,\beta^{-1}) \end{split}$$

with y, X and w as defined in the notebook.

(a) Work out the maximum likelihood solution for linear regression by solving

$$\nabla w \log p(y|X, w) = 0.$$

- (b) Work out the MAP solution. How does it relate to the ML solution?
- [3] (###) Show that the variance of the predictive distribution for linear regression decreases as more data becomes available.
- [4] (#) Assume a given data set $D = \{(x_1, y_1), (x_2, y_2), ..., (x_N, y_N)\}$ with $x \in \mathbb{R}^M$ and $y \in \mathbb{R}$. We propose a model given by the following data generating distribution and weight prior functions:

$$p(y_n|x_n, w) \cdot p(w)$$
.

- (a) Write down Bayes rule for generating the posterior p(w|D) from a prior and likelihood.
- (b) Work out how to compute a distribution for the predicted value y_0 , given a new input x_0 .
- [5] (#) In the class we use the following prior for the weights:

$$p(w|\alpha) = \mathcal{N}\left(w|0, \alpha^{-1}I\right)$$

- (a) Give some considerations for choosing a Gaussian prior for the weights.
- (b) We could have chosen a prior with full (not diagonal) covariance matrix $p(w|\alpha) = \mathcal{N}(w|0,\Sigma)$. Would that be better? Give your thoughts on that issue.
- (c) Generally we choose α as a small positive number. Give your thoughts on that choice as opposed to choosing a large positive value. How about choosing a negative value for α ?
- [6] Consider an IID data set $D = \{(x_1, y_1), ..., (x_N, y_N)\}$. We will model this data set by a model

$$y_n = \theta^T f(x_n) + e_n$$

where $f(x_n)$ is an *M*-dimensional feature vector of input $x_{n'}$ y_n is a scalar output and $e_n \sim \mathcal{N}(0, \sigma^2)$.

- (a) Rewrite the model in matrix form by lumping input features in a matrix $F = [f(x_1), \dots, f(x_N)]^T$, outputs and noise in the vectors $y = [y_1, \dots, y_N]^T$ and $e = [e_1, \dots, e_N]^T$, respectively.
- (b) Now derive an expression for the log-likelihood $\log p(y|F,\theta,\sigma^2)$.
- (c) Proof that the maximum likelihood estimate for the parameters is given by

$$\theta_{\text{ml}} = (F^T F)^{-1} F^T y$$

- (d) What is the predicted output value y_{\bullet} , given an observation x_{\bullet} and the maximum likelihood parameters $\theta_{\rm ml}$. Work this expression out in terms of F_{\bullet} , Y_{\bullet} and Y_{\bullet}
- (e) Suppose that, before the data set D was observed, we had reason to assume a prior distribution $p(\theta) = \mathcal{N}(0, \sigma_0^2)$. Derive the Maximum a posteriori (MAP) estimate θ_{map} (hint: work this out in the \log domain.)

Generative Classification

• [1] You have a machine that measures property x_t , the "orangeness" of liquids. You wish to discriminate between $C_1 = Fanta$ and $C_2 = Ganta$. It is known that

$$\begin{split} p(x|C_1) &= \begin{cases} 10 & 1.0 \leq x \leq 1.1 \\ 0 & \text{otherwise} \end{cases} \\ p(x|C_2) &= \begin{cases} 200(x-1) & 1.0 \leq x \leq 1.1 \\ 0 & \text{otherwise} \end{cases} \end{split}$$

The prior probabilities $p(C_1) = 0.6$ and $p(C_2) = 0.4$ are also known from experience.

(a) (##) A "Bayes Classifier" is given by

$$ext{Decision} = \left\{ egin{aligned} C_1 & ext{if } p(C_1|x) > p(C_2|x) \ C_2 & ext{otherwise} \end{aligned}
ight.$$

Derive the optimal Bayes classifier.

(b) (###) The probability of making the wrong decision, given x_i is

$$p(\text{error}|x) = p(C_1|x, \text{we-decide-}C_2) + p(C_2|x, \text{we-decide-}C_1)$$

Compute the **total** error probability p(error) for the Bayes classifier in this example.

- [2] (#) (see Bishop exercise 4.8): Using (4.57) and (4.58) (from Bishop's book), derive the result (4.65) for the posterior class probability in the two-class generative model with Gaussian densities, and verify the results (4.66) and (4.67) for the parameters w and wo.
- [3] (##) (see Bishop exercise 4.10).

Discriminative Classification

• [1] Given a data set $D = \{(x_1, y_1), \dots, (x_N, y_N)\}$, where $x_n \in \mathbb{R}^M$ and $y_n \in \{0, 1\}$. The probabilistic classification method known as *logistic regression* attempts to model these data as

$$p(y_n = 1 | x_n) = \sigma(\theta^T x_n + b)$$

where $\sigma(x) = 1/(1 + e^{-x})$ is the *logistic function*. Let's introduce shorthand notation $\mu_n = \sigma(\theta^T x_n + b)$. So, for every input x_n , we have a model output μ_n and an actual data output y_n .

- (a) Express $p(y_n|x_n)$ as a Bernoulli distribution in terms of μ_n and y_n .
- (b) If furthermore is given that the data set is IID, show that the log-likelihood is given by

$$L(heta) riangleq \log p(D| heta) = \sum_n \left\{ y_n \log \mu_n + (1-y_n) \log (1-\mu_n)
ight\}$$

(c) Prove that the derivative of the logistic function is given by

$$\sigma'(\xi) = \sigma(\xi) \cdot (1 - \sigma(\xi))$$

(d) Show that the derivative of the log-likelihood is

$$\nabla_{\theta} L(\theta) = \sum_{n=1}^{N} (y_n - \sigma(\theta^T x_n + b)) x_n$$

- (e) Design a gradient-ascent algorithm for maximizing $L(\theta)$ with respect to θ .
- [2] Describe shortly the similarities and differences between the discriminative and generative approach to classification.
- [3] (Bishop ex.4.7) (#) Show that the logistic sigmoid function $\sigma(a) = \frac{1}{1 + \exp(-a)}$ satisfies the property $\sigma(-a) = 1 \sigma(a)$ and that its inverse is given by $\sigma^{-1}(y) = \log\{y/(1-y)\}$.
- [4] (###) Let x be a real valued random variable with probability density

$$p_X(x) = \frac{e^{-x^2/2}}{\sqrt{2\pi}}, \quad \text{for all } x.$$

Also y is a real valued random variable with conditional density

$$p_{Y|X}(y|x) = \frac{e^{-(y-x)^2/2}}{\sqrt{2\pi}}$$
, for all x and y .

- (a) Give an (integral) expression for $p_Y(y)$. Do not try to evaluate the integral.
- (b) Approximate $p_{Y}(y)$ using the Laplace approximation. Give the detailed derivation, not just the answer. Hint: You may use the following results. Let

$$g(x) = \frac{e^{-x^2/2}}{\sqrt{2\pi}}$$

and

$$h(x) = \frac{e^{-(y-x)^2/2}}{\sqrt{2\pi}}$$

for some real value y. Then:

$$\begin{split} \frac{\partial}{\partial x}g(x) &= -xg(x) \\ \frac{\partial^2}{\partial x^2}g(x) &= (x^2-1)g(x) \\ \frac{\partial}{\partial x}h(x) &= (y-x)h(x) \\ \frac{\partial^2}{\partial x}h(x) &= ((y-x)^2-1)h(x) \end{split}$$

Latent Variable Models and Variational Bayes

• [1] (##) For a Gaussian mixture model, given by generative equations

$$p(x, z) = \prod_{k=1}^{K} (\underbrace{\pi_k \cdot \mathcal{N} \left(x | \mu_k, \Sigma_k \right)}_{p(x, z_k = 1)})^{z_k}$$

proof that the marginal distribution for observations x_n evaluates to

$$p(x) = \sum_{j=1}^{K} \pi_k \cdot \mathcal{N}\left(x|\mu_j, \Sigma_j
ight)$$

- [2] (#) Given the free energy functional $F[q] = \sum_z q(z) \log \frac{q(z)}{p(x,z)}$, proof the EE, DE and AC decompositions.
- [3] (#) The Free energy functional $F[q] = -\sum_z q(z) \log p(x,z) \sum_z q(z) \log \frac{1}{q(z)}$ decomposes into "Energy minus Entropy". So apparently the entropy of the posterior q(z) is maximized. This entropy maximization may seem puzzling at first because inference should intuitively lead to *more* informed posteriors, i.e., posterior distributions whose entropy is smaller than the entropy of the prior. Explain why entropy maximization is still a reasonable objective.
- [4] (#) Explain the following update rule for the mean of the Gaussian cluster-conditional data distribution (from the example about mean-field updating of a Gaussian mixture model):

$$m_k = \frac{1}{\beta_k} (\beta_0 m_0 + N_k \bar{x}_k) \tag{B-10.61}$$

• [5] (##) Consider a model $p(x, z|\theta)$, where $D = \{x_1, x_2, \dots, x_N\}$ is observed, z are unobserved variables and θ are parameters. The EM algorithm estimates the parameters by iterating over the following two equations (i is the iteration index):

$$\begin{split} q^{(i)}(z) &= p(z|D, \theta^{(i-1)}) \\ \theta^{(i)} &= \arg\max_{\theta} \sum_{} q^{(i)}(z) \cdot \log p(D, z|\theta) \end{split}$$

Proof that this algorithm minimizes the Free Energy functional

$$F[q, heta] = \sum_{z} q(z) \log rac{q(z)}{p(D, z| heta)}$$

- [6] (###) Consult the internet on what overfitting and underfitting is and then explain how FE minimization finds a balance between these two (unwanted) extremes.
- [7] (##) Consider a model $p(x, z|\theta) = p(x|z, \theta)p(z|\theta)$ where x and z relate to observed and unobserved variables, respectively. Also available is an observed data set $D = \{x_1, x_2, ..., x_N\}$. One iteration of the EM-algorithm for estimating the parameters θ is described by (m is the iteration counter)

$$heta^{ig(m+1ig)} := rg \max_{ heta} \left(\sum_{z} p(z|x=D, heta^{ig(m)}) \log p(x=D, z| heta)
ight).$$

- (a) Apparently, in order to execute EM, we need to work out an expression for the 'responsibility' $p(z|x=D,\theta^{(m)})$. Use Bayes rule to show how we can compute the responsibility that allows us to execute an EM step.
- (b) Why do we need multiple iterations in the EM algorithm?
- (c) Why can't we just use simple maximum log-likelihood to estimate parameters, as described by

$$\hat{\theta} := \arg \max_{\theta} \log p(x = D, z | \theta)$$
?

• [8] In a particular model with hidden variables, the log-likelihood can be worked out to the following expression:

$$L(heta) = \sum_n \log \left(\sum_k \pi_k \, \mathcal{N}(x_n \, | \, \mu_k, \, \Sigma_k)
ight)$$

Do you prefer a gradient descent or EM algorithm to estimate maximum likelihood values for the parameters? Explain your answer. (No need to work out the equations.)

Dynamic Models

• [1] (##) Given the Markov property

$$p(x_n|x_{n-1},x_{n-2},\ldots,x_1) = p(x_n|x_{n-1}) \tag{A1}$$

proof that, for any n,

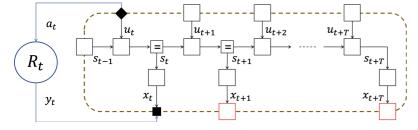
$$\begin{array}{l} p(x_n,x_{n-1},\ldots,x_{k+1},x_{k-1},\ldots,x_1|x_k) = \\ p(x_n,x_{n-1},\ldots,x_{k+1}|x_k) \cdot p(x_{k-1},x_{k-2},\ldots,x_1|x_k) \,. \end{array} \tag{A2}$$

In other words, proof that, if the Markov property A1 holds, then, given the "present" (x_k) , the "future" $(x_n, x_{n-1}, \dots, x_{k+1})$ is *independent* of the "past" $(x_{k-1}, x_{k-2}, \dots, x_1)$.

- [2] (#)
 - (a) What's the difference between a hidden Markov model and a linear Dynamical system?
 - (b) For the same number of state variables, which of these two models has a larger memory capacity, and why?
- [3] (#) (a) What is the 1st-order Markov assumption?
 - (b) Derive the joint probability distribution $p(x_{1:T}, z_{0:T})$ (where x_t and z_t are observed and latent variables respectively) for the state-space model with transition and observation models $p(z_t|z_{t-1})$ and $p(x_t|z_t)$.
 - (c) What is a Hidden Markov Model (HMM)?
 - (d) What is a Linear Dynamical System (LDS)?
 - (e) What is a Kalman Filter?
 - (f) How does the Kalman Filter relate to the LDS?
 - (g) Explain the popularity of Kalman filtering and HMMs?
 - (h) How relates a HMM to a GMM?

Intelligent Agents and Active Inference

- [1] (##) I asked you to watch a video segment (https://youtu.be/L0pVHbEg4Yw) where Karl Friston talks about two main approaches to goal-directed acting by agents: (1) choosing actions that maximize (the expectation of) a value function V(s) of the state (s) of the environment; or (2) choosing actions that minimize a functional (F[q(s)]) of beliefs (q(s)) over environmental states (s). Discuss the advantage of the latter appraach.
- [2] (#) The good regulator theorem states that a "successful and efficient" controller of the world must contain a model of the world. But it's hard to imagine how just learning a model of the world leads to goal-directed behavior, like learning how to read or drive a car. Which other ingredient do we need to get learning agents to behave as goal-directed agents?
- [3] (##) The figure below reflects the state of a factor graph realization of an active inference agent after having pushed action a_t onto the environment and having received observation x_t . In this graph, the variables x_0 , u_0 and u_1 and u_2 correspond to observations, and unobserved control and internal states respectively. Copy the figure onto your sheet and draw a message passing schedule to infer a posterior belief (i.e. after observing u_1) over the next control state u_1 .



- [4] (##) The Free Energy Principle (FEP) is a theory about biological self-organization, in particular about how brains develop through interactions with their environment. Which of the following statements is not consistent with FEP (and explain your answer):
 - (a) We act to fullfil our predictions about future sensory inputs.
 - (b) Perception is inference about the environmental causes of our sensations.
 - (c) Our actions aim to reduce the complexity of our model of the environment.