Homework 2 – Deep Learning (CS/DS 541, Whitehill, Spring 2020)

You may complete this homework assignment either individually or in teams up to 2 people.

1. **XOR problem** [10 points, on paper]: Show (by deriving the gradient, setting to 0, and solving mathematically, not in Python) that the values for $\mathbf{w} = (w_1, w_2)$ and b that minimize the function $J(\mathbf{w}, b)$ in Equation 6.1 (in the *Deep Learning* textbook) are: $w_1 = 0$, $w_2 = 0$, and $b = 0.5$.

2. **L_2-regularized Linear Regression via Stochastic Gradient Descent** [20 points, in Python]: Train a 2-layer neural network (i.e., linear regression) for age regression using the same data as in homework 1. Your prediction model should be $\hat{y} = \mathbf{x}^\top \mathbf{w} + b$. Note that, in contrast to Homework 1, this model includes a bias term.

   Instead of optimizing the weights of the network with the closed formula, use stochastic gradient descent (SGD). There are several different hyperparameters that you will need to choose:

   - Mini-batch size $\tilde{n}$.
   - Learning rate ϵ.
   - Number of epochs.
   - L_2 Regularization strength α.

   In order not to cheat (in the machine learning sense) – and thus overestimate the performance of the network – it is crucial to optimize the hyperparameters **only** on a *validation set*. (The training set would also be acceptable but typically leads to worse performance.) To create a validation set, simply set aside a fraction (e.g., 20%) of the `age_regression_Xtr.npy` and `age_regression_ytr.npy` to be the validation set; the remainder (80%) of these data files will constitute the "actual" training data. While there are fancier strategies (e.g., Bayesian optimization – another probabilistic method, by the way!) that can be used for hyperparameter optimization, it's common to just use a grid search over a few values for each hyperparameter. In this problem, you are required to explore systematically (e.g., using nested `for` loops) at least 4 different parameters for each hyperparameter.

   Performance evaluation: Once you have tuned the hyperparameters and optimized the weights so as to minimize the cost on the validation set, then: (1) **stop** training the network and (2) evaluate the network on the **test** set. Report the performance in terms of *unregularized* MSE.

3. **Regularization to encourage symmetry** [10 points, on paper]: Faces (and some other kinds of data) tend to be left-right symmetric. How can you use L_2 regularization to discourage the weights from becoming too *a*symmetric? For simplicity, consider the case of a tiny 1×2 "image". Hint: instead of using $\frac{\alpha}{2}\mathbf{w}^\top\mathbf{w} = \frac{\alpha}{2}\mathbf{w}^\top\mathbf{I}\mathbf{w}$ as the L_2 penalty term (where α is the regularization strength), consider a different matrix in the middle. Your answer should consist of a 2×2 matrix $\mathbf{S}$ as well as an explanation of why it works.

4. **Recursive state estimation in Hidden Markov Models** [10 points, on paper]: Teachers try to monitor their student's knowledge of the subject-matter, but teachers cannot directly peer inside students' brains. Hence, they must make *inferences* about what the student knows based on students' *observable behavior*, i.e., how they perform on tests, their facial expressions during class, etc. Let random variable (RV) X_t represent the student's *state*, and let RV Y_t represent the student's observable behavior, at time t. We can model the student as a Hidden Markov Model (HMM):

   (a) X_t depends *only* on the previous state X_{t-1}, *not* on any states prior to that (*Markov* property), i.e.

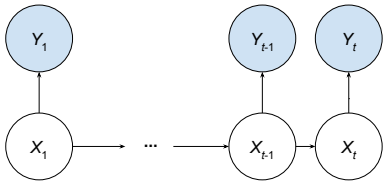
   $$P(x_t \mid x_1, \ldots, x_{t-1}) = P(x_t \mid x_{t-1})$$

   (b) The student's behavior Y_t depends only on his/her current state X_t, i.e.:

   $$P(y_t \mid x_t, y_1, \ldots, y_{t-1}) = P(y_t \mid x_t)$$

(c) X_t cannot be observed directly (it is *hidden*).

A probabilistic graphical model for the HMM is shown below, where only the observed RVs are shaded (the latent ones are transparent):



Suppose that the teacher already knows:

- $P(y_t \mid x_t)$ (*observation likelihood*), i.e., the probability distribution of the student's behaviors given the student's state.
- $P(x_t \mid x_{t-1})$ (*transition dynamics*), i.e., the probability distribution of the student's current state given the student's previous state.

The goal of the teacher is to estimate the student's current state X_t given the *entire* history of observations $Y_1, \ldots, Y_t$ he/she has made so far. Show that the teacher can, at each time t, update his/her belief *recursively*:

$$P(x_t \mid y_1, \ldots, y_t) \propto P(y_t \mid x_t) \sum_{x_{t-1}} P(x_t \mid x_{t-1}) P(x_{t-1} \mid y_1, \ldots, y_{t-1})$$

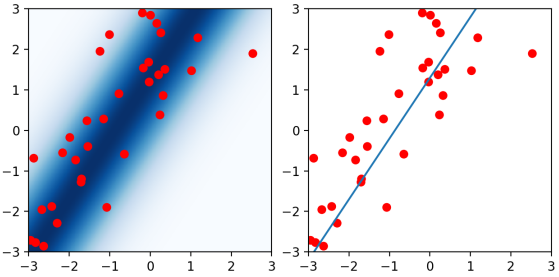
where $P(x_{t-1} \mid y_1, \ldots, y_{t-1})$ is the teacher's belief of the student's state from time $t-1$, and the summation is over every possible value of the previous state x_{t-1}. **Hint**: You will need to use Bayes' rule, i.e., for any RVs A, B, and C:

$$P(a \mid b, c) = \frac{P(b \mid a, c) P(a \mid c)}{P(b \mid c)}$$

However, since the denominator in the right-hand side does not depend on a, this can also be rewritten as:

$$P(a \mid b, c) \propto P(b \mid a, c) P(a \mid c)$$

5. **Linear-Gaussian prediction model** [15 points, on paper]:



Probabilistic prediction models enable us to estimate not just the "most likely" or "expected" value of the target y (see figure above, right), but rather an entire *probability distribution* about which target values are more likely than others, given input $\mathbf{x}$ (see figure above, left). In particular, a linear-Gaussian model is a Gaussian distribution whose expected value (mean μ) is a linear function of the input features $\mathbf{x}$, and whose variance is σ^2:

$$P(y \mid \mathbf{x}) = \mathcal{N}(\mu = \mathbf{x}^\top \mathbf{w}, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y - \mathbf{x}^\top \mathbf{w})^2}{2\sigma^2}\right)$$

Note that, in general, σ^2 can also be a function of $\mathbf{x}$ (heteroscedastic case). Moreover, *non*-linear Gaussian models are also completely possible, e.g., the mean (and possibly the variance) of the Gaussian distribution is output by a deep neural network. However, in this problem, we will assume that μ is linear in $\mathbf{x}$, and that σ^2 is the same for all $\mathbf{x}$ (homoscedastic case).

MLE: The parameters of probabilistic models are commonly optimized by *maximum likelihood estimation* (MLE). (Another common approach is *maximum a posteriori* estimation, which allows the practitioner to incorporate a "prior belief" about the parameters' values.) Suppose the training dataset $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^n$. Let the parameters/weights of the linear-Gaussian model be $\mathbf{w}$, such that the mean $\mu = \mathbf{x}^\top \mathbf{w}$. Prove that the MLE of $\mathbf{w}$ and σ^2 given $\mathcal{D}$ is:

$$\mathbf{w} = \left(\sum_{i=1}^{n} \mathbf{x}^{(i)} {\mathbf{x}^{(i)}}^\top \right)^{-1} \left(\sum_{i=1}^{n} \mathbf{x}^{(i)} y^{(i)} \right)$$

$$\sigma^2 = \frac{1}{n} \sum_{i=1}^{n} ({\mathbf{x}^{(i)}}^\top \mathbf{w} - y^{(i)})^2$$

Note that this solution – derived based on *maximizing* probability – is exactly the same as the optimal weights of a 2-layer neural network optimized to *minimize* MSE.

Hint: Follow the same strategy as the MLE derivation for a biased coin in `Class2.pdf`. For a linear-Gaussian model, the argmax of the likelihood equals the argmax of the log-likelihood. The log of the Gaussian likelihood simplifies beautifully.

Put your code in a Python file called `homework2_WPIUSERNAME1.py`
(or `homework2_WPIUSERNAME1_WPIUSERNAME2.py` for teams). For the proofs, please create a PDF called `homework2_WPIUSERNAME1.pdf`
(or `homework2_WPIUSERNAME1_WPIUSERNAME2.pdf` for teams). Create a Zip file containing both your Python and PDF files, and then submit on Canvas.