CS480/680: Introduction to Machine Learning

Homework 4

Due: 11:59 pm, December 06, 2022, submit on LEARN.

NAME

student number

Submit your writeup in pdf and all source code in a zip file (with proper documentation). Write a script for each programming exercise so that the TA can easily run and verify your results. Make sure your code runs!

[Text in square brackets are hints that can be ignored.]

Exercise 1: Quantile and push-forward (11 pts)

In this exercise we compute and simulate the push-forward map T that transforms a reference density r into a target density p. Recall that the quantile function of a (univariate) random variable X is defined as the inverse of its cumulative distribution function (cdf) F:

$$F(x) = \Pr(\mathsf{X} \leq x), \qquad Q(u) = F^{-1}(u), \quad u \in (0, 1). \tag{1}$$

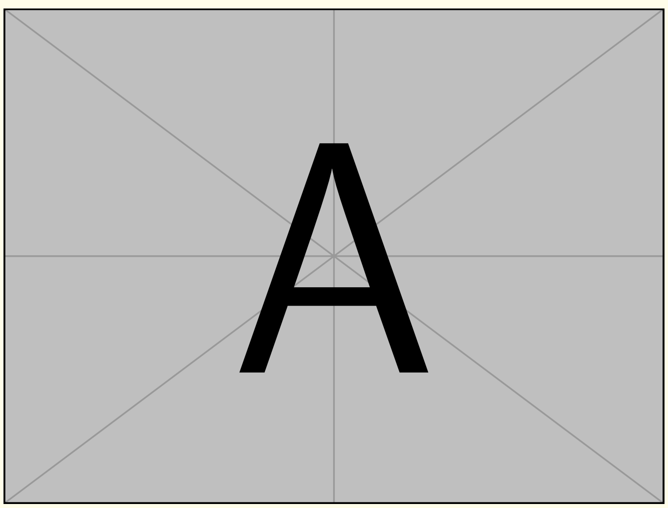
We assume F is continuous and strictly increasing so that $Q^{-1} = F$. A nice property of the quantile function, relevant to sampling, is that if $\mathsf{U} \sim \text{Uniform}(0, 1)$, then $Q(\mathsf{U}) \sim F$.

1. (2 pts) Consider the Gaussian mixture model $p(x) = \frac{\lambda}{\sigma_1}\varphi\left(\frac{x-\mu_1}{\sigma_1}\right) + \frac{1-\lambda}{\sigma_2}\varphi\left(\frac{x-\mu_2}{\sigma_2}\right)$, where φ is the *density* of the standard normal distribution (mean 0 and variance 1). Implement the following to create a dataset of $n = 1000$ samples from the GMM p:

   - Sample $\mathsf{U}_i \sim \text{Uniform}(0, 1)$.
   - If $\mathsf{U}_i < \lambda$, sample $\mathsf{X}_i \sim \mathcal{N}(\mu_1, \sigma_1^2)$; otherwise sample $\mathsf{X}_i \sim \mathcal{N}(\mu_2, \sigma_2^2)$.

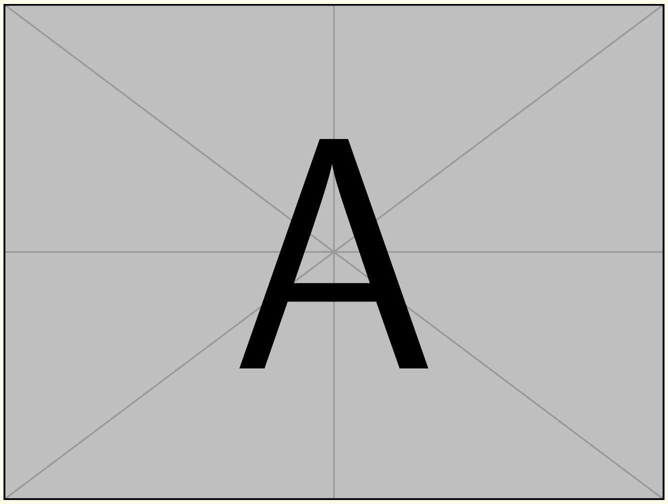
   Plot the histogram of the generated X_i (with $b = 50$ bins) and submit your script as
   `X = GMMsample(gmm, n=1000, b=50), gmm.lambda=0.5, gmm.mu=[1,-1], gmm.sigma=[0.5,0.5]`

   [See here or here for how to plot a histogram in `matplotlib` or `pandas` (or `numpy` if you insist).]

   Ans: 

2. (2 pts) Compute $\mathsf{U}_i = \Phi^{-1}\big(F(\mathsf{X}_i)\big)$, where F is the *cdf* of the GMM in Ex 1.1 and Φ is the *cdf* of standard normal. Plot the histogram of the generated U_i (with b bins). From your inspection, what distribution should U_i follow (approximately)? Submit your script as `GMMinv(X, gmm, b=50)`.

   [This page may be helpful.]

Ans: 

3. (3 pts) Let $\mathsf{Z} \sim \mathcal{N}(0,1)$. We now compute the push-forward map T so that $T(\mathsf{Z}) = \mathsf{X} \sim p$ (the GMM in Ex 1.1). We use the formula:

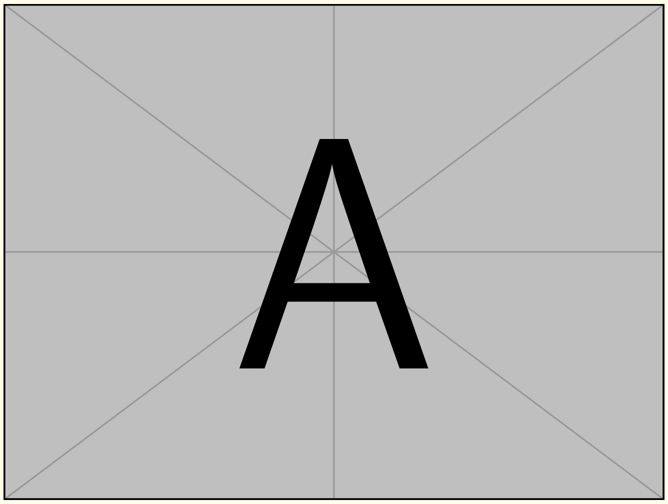
$$T(z) = Q(\Phi(z)), \tag{2}$$

where Φ is the *cdf* of the standard normal distribution and $Q = F^{-1}$ is the quantile function of X, namely the GMM p in Ex 1.1. Implement the following binary search Algorithm 1 to numerically compute T. Plot the function T with input $z \in [-5,5]$ (increment 0.1). Submit your main script as `BinarySearch(F, u, lb=-100, ub=100, maxiter=100, tol=1e-5)`, where `F` is a function. You may need to write another script to compute and plot T (based on `BinarySearch`).

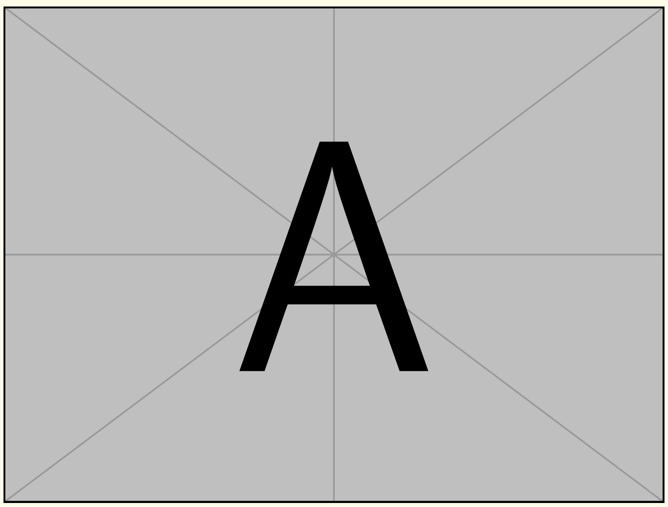
Algorithm 1: Binary search for solving a monotonic nonlinear equation $F(x) = u$.

Input: $u \in (0,1)$, $\mathtt{lb} < 0 < \mathtt{ub}$, $\mathtt{maxiter}, \mathtt{tol}$
Output: x such that $|F(x) - u| \leq \mathtt{tol}$

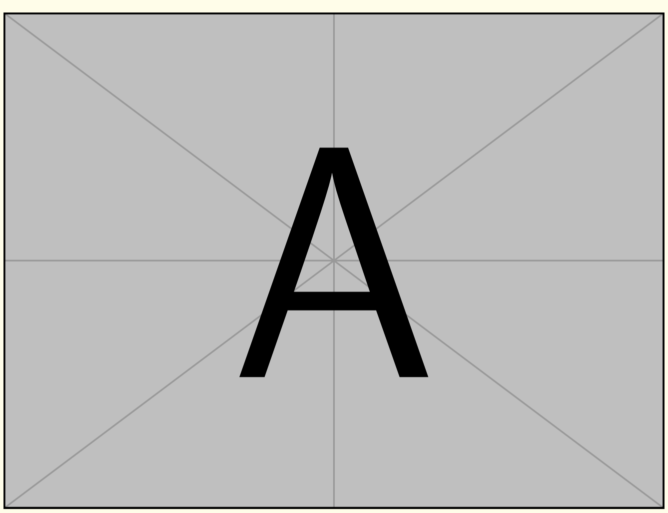
while $F(\mathtt{lb}) > u$ **do** // lower bound too large
  $\mathtt{ub} \leftarrow \mathtt{lb}$
  $\mathtt{lb} \leftarrow 2 * \mathtt{lb}$
while $F(\mathtt{ub}) < u$ **do** // upper bound too small
  $\mathtt{lb} \leftarrow \mathtt{ub}$
  $\mathtt{ub} \leftarrow 2 * \mathtt{ub}$
for $i = 1, \ldots, \mathtt{maxiter}$ **do**
  $x \leftarrow \frac{\mathtt{lb}+\mathtt{ub}}{2}$ // try middle point
  $t \leftarrow F(x)$
  if $t > u$ **then**
    $\mathtt{ub} \leftarrow x$
  else
    $\mathtt{lb} \leftarrow x$
  if $|t - u| \leq \mathtt{tol}$ **then**
    break

Ans: 

4. (2 pts) Sample (independently) $\mathsf{Z}_i \sim \mathcal{N}(0,1), i = 1, \ldots, n = 1000$ and let $\tilde{\mathsf{X}}_i = T(\mathsf{Z}_i)$, where T is computed by your `BinarySearch`. Plot the histogram of the generated $\tilde{\mathsf{X}}_i$ (with b bins) and submit your script as `PushForward(Z, gmm)`. Is the histogram similar to the one in Ex 1.1?

Ans: 

5. (2 pts) Now let us compute $\tilde{\mathsf{U}}_i = \Phi^{-1}\big(F(\tilde{\mathsf{X}}_i)\big)$ as in Ex 1.2, with $\tilde{\mathsf{X}}_i$'s being generated in Ex 1.4. Plot the histogram of the resulting $\tilde{\mathsf{U}}_i$ (with b bins). From your inspection what distribution should $\tilde{\mathsf{U}}_i$ follow (approximately)? [No need to submit any script, as you can recycle `GMMinv`.]

Ans: 

Exercise 2: Understanding attention (9 pts)

Let $X_0 \in \mathbb{R}^{n\times d}$ represent n input representations in $\mathbb{R}^d$. Applying self-attention we obtain

$$S_t \leftarrow \exp(+X_t X_t^\top/\lambda) \tag{3}$$

$$P_t \leftarrow [\operatorname{diag}(S_t\mathbf{1})]^{-1}\cdot S_t \tag{4}$$

$$X_{t+1} \leftarrow P_t X_t, \tag{5}$$

where $\mathbf{1}$ is the vector of all 1s and diag turns the input vector into a diagonal matrix.

1. (3 pts) Each row of P can be determined as follows:

$$\operatorname*{argmin}_{\mathbf{p}\in\mathbb{R}^n_+,\sum_i p_i=1} \sum_{i=1}^n \left[p_i\cdot -\mathbf{x}^\top\mathbf{x}_i + \lambda\cdot p_i\log p_i\right], \tag{6}$$

where the second term $p_i \log p_i$ is the so-called entropic regularizer. Prove that the solution of (6) is given as:

$$p_i = \frac{\exp(+\mathbf{x}^\top\mathbf{x}_i/\lambda)}{\sum_{j=1}^n \exp(+\mathbf{x}^\top\mathbf{x}_j/\lambda)}, \quad \textit{i.e.}, \quad \mathbf{p} = \mathsf{softmax}(+\mathbf{x}^\top X/\lambda). \tag{7}$$

[Hint: use the fact that $\mathsf{KL}(\mathbf{p}\|\mathbf{q}) := \sum_i p_i \log\frac{p_i}{q_i} \geq 0$, with equality attained iff $\mathbf{p}=\mathbf{q}$.]

Ans:

2. (2 pts) Now, with the above $\mathbf{p}$, we solve a weighted linear regression problem to retrieve the query value:

$$\operatorname*{argmin}_{\mathbf{z}\in\mathbb{R}^d} \sum_{i=1}^n p_i\cdot\|\mathbf{z}-\mathbf{x}_i\|_2^2. \tag{8}$$

Prove that the solution is given as:

$$\mathbf{z} = \sum_{i=1}^n p_i\mathbf{x}_i. \tag{9}$$

Ans:

3. (4 pts) W.l.o.g., let $n = 3$, $d = 2$, $\lambda = 1$ and $t = 1, \ldots, 100$. Repeat the self-attention in (3)-(5), and plot the trajectory of each row of X_t w.r.t. t, with $X_0 = \texttt{randn}(n, d)$, i.e., each entry is an iid sample from the standard Gaussian. For ease of understanding, include all rows of X_0 in each plot (namely, 3 initial points). What do you think the trajectories converge to, if at all?

Ans: