Synthetic Simulation Study

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1 Synthetic experiments

In this document, we study the behavior of our ACMMD test when the model and the data disribution are simple, yet non vacuous generative models on sequences. Their specific form allows us to derive closed-form expressions for ACMMD in the goodness-of-fit and calibration settings, which we use to validate the theoretical properties of our tests and estimates, namely (1) unbiasedness of the (unbiased) ACMMD estimate, (2) positivity of the biased ACMMD estimate, (3) type-I error control of the ACMMD test, and (4) power of the ACMMD test.

1.1 Description of the Setting

The distribution on inputs X is given by a uniform categorical distribution over $\{p_1, \ldots, p_m\} \in (0.2, 0.5)$. X is thus a categorical variable with kernel $k_{\mathcal{X}}(x, x')$ For $Y|X$, we consider a finite alphabet with tokens $A = \{A, B\}$ The true conditional distribution on sequences $Y \in \bigcup_{i=0}^{+\infty} A^l$ given the input $x = p$ is given by

$$p(y_n|y_{0:n-1}, x = p) = \begin{cases} A & \text{with probability } p \\ B & \text{with probability } p \\ \text{STOP} & \text{with probability } 1 - 2p \end{cases}$$

In contrast, we define a model of the conditional distribution $p(y|x = p)$ (which we note $q_|$) by perturbing the first entry of the the true conditional distribution using a parameter $\Delta p \in (0, p_1)$

$$q(y_0|x = p) = \begin{cases} A & \text{with probability } p - \Delta p \\ B & \text{with probability } p + \Delta p \\ \text{STOP} & \text{with probability } 1 - 2p \end{cases} \quad q(y_n|y_{0:n-1}, x = p) = p(y_n|y_{0:n-1}, x = p)$$

We set the kernel on Y to the exponentiated Hamming distance kernel $k_{\mathcal{Y}}(y, y) = e^{-\lambda d_H(y, y')}$. This simple setting will allow us to compute the ACMMD in closed form.

1.2 Closed-form ACMMD($\mathbb{P}_|, Q_|$) evaluation

Lemma 1. *In the setting described above, we have:*

$$\text{ACMMD}^2(\mathbb{P}_|, Q_|) = \frac{1}{n^2} \sum_{i,j=1}^{n} k_{\mathcal{X}}(p_i, p_j) 2\Delta p^2 (1 - e^{-\lambda}) \frac{(1 - 2p_i)(1 - 2p_j)}{1 - 4p_i p_j (1 + e^{-\lambda})/2} \left(\frac{2p_j e^{-\lambda}}{1 - 2p_j e^{-\lambda}} + \frac{2p_i e^{-\lambda}}{1 - 2p_i e^{-\lambda}} + 1 \right)$$

The proof is given in `proofs_synthetic_simulation_study.pdf`, present in the same folder. We notice that this expression depends monotonically (and quadratically) on the shift Δp, making smaller shifts increasingly harder to detect. The dependency on the inputs p_i is harder to analyze.

1.3 Closed-form calibration ($\mathrm{ACMMD}(\mathbb{P}_{|Q}, Q_{|})$) evaluation

Assuming the same model, it is also possible to evalute $\mathrm{ACMMD}(\mathbb{P}_{|Q}, Q_{|})$ in closed form. The $\mathrm{ACMMD}^2(\mathbb{P}_{|Q}, Q_{|})$ becomes a special case of the ACMMD formula given above, with the conditionned variable X set to be the models $Q_{|X}$. It is thus possible to show:

Lemma 2. *We have*

$$\mathrm{ACMMD}^2(\mathbb{P}_{|Q}, Q_{|}) = \frac{1}{n^2}\sum_{i,j=1}^{n} k_{\mathcal{P}(\mathcal{Y})}(q_{|p_i}, q_{|p_j}) 2\Delta p^2(1-e^{-\lambda})\frac{(1-2p_i)(1-2p_j)}{1-4p_ip_j(1+e^{-\lambda})/2}\left(\frac{2p_je^{-\lambda}}{1-2p_je^{-\lambda}}+\frac{2p_ie^{-\lambda}}{1-2p_ie^{-\lambda}}+1\right)$$

The above lemma leaves the choice of the kernel $k_{\mathcal{P}(\mathcal{Y})}$ open: the tractability of this expression will follow only if such kernel can be tractably computed. In the next lemma, we derive a closed form solution for $k_{\mathcal{P}(\mathcal{Y})}(q, q')$ when $k_{\mathcal{P}(\mathcal{Y})}(q, q') = e^{-\frac{\mathrm{MMD}^2(q,q')}{2\sigma^2}}$, where the MMD is computed with an Exponentiated Hamming kernel on $\mathcal{Y}$.

Lemma 3. *We have*

$$\mathrm{MMD}^2(q_{|p}, q_{|p'}) = T(p,p) + T(p',p') - 2T(p,p')$$

Where

$$\begin{aligned}
T(p,p') &= C(p,p')A(p,p') + T^0(p,p')\\
C(p,p') &= \frac{(1-2p)(1-2p')4pp'}{1-4pp'(1+e^{-\lambda})/2}\left(\frac{2p'e^{-\lambda}}{1-2p'e^{-\lambda}}+\frac{2pe^{-\lambda}}{1-2pe^{-\lambda}}+1\right)\\
A(p,p') &= \frac{2pp'+2\Delta p^2}{4pp'}\times(1-e^{-\lambda})+e^{-\lambda}\\
T^0(p,p') &= (1-2p)(1-2p')\left(\frac{2p'e^{-\lambda}}{1-2p'e^{-\lambda}}+\frac{2pe^{-\lambda}}{1-2pe^{-\lambda}}+1\right)
\end{aligned}$$

Combining the two lemmas allows us to to obtain a computable expression for $\mathrm{ACMMD}(\mathbb{P}_{|Q}, Q_{|})$.

2 Validating the theoretical properties of our ACMMD (test)

Validating $\mathrm{ACMMD}(\mathbb{P}_{|}, Q_{|})$ tests and estimates In this section, we compute two ACMMD estimates: the unbiased ACMMD estimate presented in our paperw, which we note $\mathrm{ACMMD}_u(\mathbb{P}_{|}, Q_{|})$, and a biased, but positive ACMMD estimate of the form:

$$\widehat{\mathrm{ACMMD}}_b^2(\mathbb{P}_{|}, Q_{|})\sum_{i,j=1}^{n} h((x_i, y_i, \tilde{y_j}), ()x_j, y_j, \tilde{y_j})$$

where we used the same notation as in the paper. We compute these estimates using dataset sizes of $\{10, 100, 200, 500, 1000\}$, $m = 5$ $p_1 = 0.3$, $p_2 = 0.45$, $\lambda = 1$, and $\Delta p = 0.3$, and average over 300 runs. In addition, we plot the true value $\mathrm{ACMMD}(\mathbb{P}_{|}, Q_{|})$ using the closed-form expression derived above. To check the behavior of our test, we vary in addition the shift Δp across $\{0, 0.01, 0.03, 0.1, 0.3\}$, and compute the null hypothesis rejection rate. The results are given in Figure 1. We observe:

1. that $\widehat{\mathrm{ACMMD}}_u^2(\mathbb{P}_{|}, Q_{|})$ is indeed unbiased.

2. that $\widehat{\mathrm{ACMMD}}_b^2(\mathbb{P}_{|}, Q_{|})$ remains positive, but exhibit a bias that can be large relative to the true ACMMD value.

3. that our ACMMD tests are well-calibrated, i.e. that the type I error is controlled at the nominal level of 0.05.

4. that our ACMMD tests can detect shifts in the model distribution of order $\delta = 0.1$

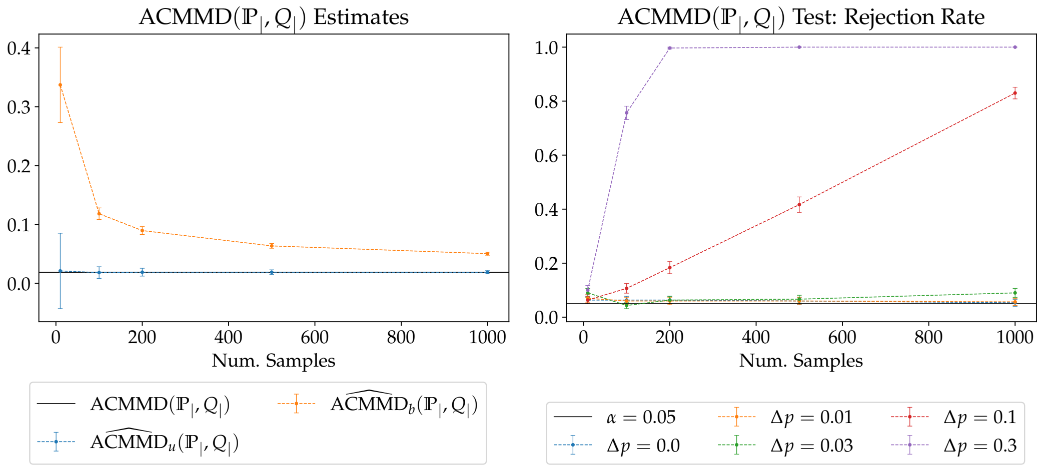

Figure 1: ACMMD estimates (left panel) and ACMMD average rejection rate for various number of samples, and shifts (right panel).

Validating $\mathrm{ACMMD}(\mathbb{P}_{|Q}, Q_{|})$ **tests and estimates** To validate our calibration estimates, we repeat the same experiment as above, but with $\mathrm{ACMMD}(\mathbb{P}_{|Q}, Q_{|})$ instead of $\mathrm{ACMMD}(\mathbb{P}_{|}, Q_{|})$. We make the same observations as above.

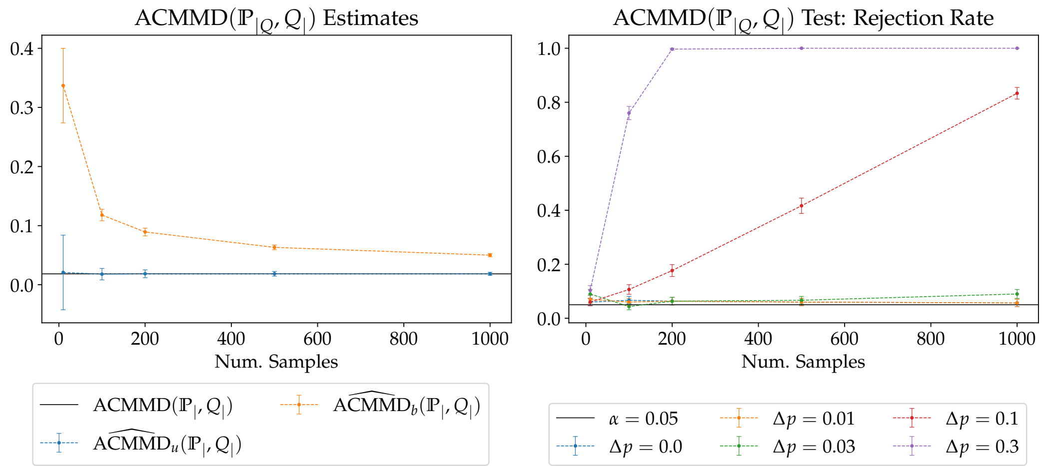

Figure 2: ACMMD estimates (left panel) and ACMMD average rejection rate for various number of samples, and shifts (right panel) in the calibration case.