Clustering applied to Hidden Markov Models

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Abstract

We consider the clustering of observations of a Hidden Markov Model (HMM) comprised of two hidden states and discrete emissions. Clustering amounts to the reconstruction of the hidden states using the observations by minimizing (in average) the number of misclassified observations. Both online and offline clustering are studied.

- We show that the empirical plug-in Bayes classifier using consistent estimators of the model parameters is efficient in the sense that its risk is equivalent to the Bayes risk for large samples.
- We identify the asymptotic Bayes risk using some forgetting properties of Markov Chains.
- We exhibit upper and lower bounds on the asymptotic Bayes risk using the model parameters.

Motivation

- Offline: All observations are used in the classification procedures. Classifiers are of the form: $h(Y_{1:n}) = (h_k(Y_{1:n}))_{1 \leq k \leq n}$.
	- Offline risk: $\mathcal{R}^{\text{Office}}_{\mathbf{n},\text{HMM}}(\mathbf{h}) = \mathbb{E}_{\theta} \left[\frac{1}{\mathbf{n}} \right]$ $\frac{1}{n}\sum_{k=1}^n 1_{\mathbf{X}_k\neq \mathbf{h_k}(\mathbf{Y}_{1:n})}$ $\overline{}$
	- Offline Bayes risk: $\cal R$ ${}^{\star, {\bf Offline}}_{{\bf n}, {\bf HMM}} = \mathbb{E}_\theta[\frac{1}{{\bf n}}$ $\frac{1}{n} \sum_{k=1}^{n} \min_{\mathbf{x} = \mathbf{0}, \mathbf{1}} \mathbb{P}_{\theta} \left(\mathbf{X}_k \neq \mathbf{x} \mid \mathbf{Y}_{1:n} \right)$
- Online: Classification can use only past observations. Classifiers are of the from: $\mathbf{h}(\mathbf{Y_{0:n-1}}) = (\mathbf{h_k}(\mathbf{Y_{0:k-1}}))_{1 \leq k \leq n}$
- Online risk: $\mathcal{R}^{\textbf{Online}}_{\textbf{n},\textbf{HMM}}(\textbf{h}) = \mathbb{E}_{\theta} \left[\frac{1}{\textbf{n}} \right]$ $\frac{1}{n}\sum_{k=1}^n 1_{\mathbf{X}_k\neq(\mathbf{h_k}(\mathbf{Y_{0:k-1}}))}$ $\overline{}$ - Online Bayes risk: $\mathcal R$ ${}^{\star, {\rm Online}}_{{\bf n}, {\rm HMM}} = \mathbb{E}_{\theta}[\frac{1}{{\bf n}}$ $\frac{1}{n} \sum_{k=1}^{n} \min_{\mathbf{x} = 0,1} \mathbb{P}_{\theta} \left(\mathbf{X}_k \neq \mathbf{x} \mid \mathbf{Y}_{0:k-1} \right)$

- Clustering is usually applied to heterogeneous data coming from different populations. These are usually modeled by a **mixture model**. However, without any additional assumption, these models are not identifiable. Inference on parameters and clustering become impossible.
- Assuming in addition that the data is derived from a HMM the model becomes identifiable and inference and clustering algorithms can be used as in [2].

Mathematical setting

- The hidden states $(X_k)_{k \in \mathbb{N}}$ are assumed to form a **Markov chain**.
- The observations $(Y_k)_{k\in\mathbb{N}}$ are independent conditionally on the hidden states and $\mathbf{Y_k} \mid \mathbf{X_k} = \mathbf{j} \sim \mathbf{f_j}.$
- The Markov chain $(X_k)_{k \in \mathbb{N}}$ will be assumed to have two hidden states, initial distribution ν and transition matrix:

Figure 1: A hidden Markov model.

Offline vs online frameworks

Denote $\theta = (\nu, \mathbf{Q}, \mathbf{f_0}, \mathbf{f_1})$ and consider the loss function $\mathbf{L}(\mathbf{x_{1:n}}, \mathbf{x'_1})$ $\mathbf{f}_{1:\mathbf{n}}^{\prime })=\frac{1}{\mathbf{n}}% \sum_{i=1}^{n}\left(\mathbf{f}_{i}\right) ^{i}\left(\mathbf{f}_{i}\right) ^{i}$ $\frac{1}{n}\sum_{k=1}^{n}$ We study the risk of clustering observations in two frameworks:

→ Plugging-in consistent estimators of the model parameters is thus an efficient procedure.

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{\mathsf{s}=1}^{\mathsf{h}}\, \mathsf{1}{\mathsf{x}_{\mathsf{k}}\neq \mathsf{x}'_{\mathsf{k}}}.
$$

where $\rho_{\bf 0} = \frac{1-2\delta}{1-\delta}$ $\frac{1-2\delta}{1-\delta}$, ρ ₁ = 1 − 2*δ and δ* = min_{i,j} Q_{i,j} > 0*.* Bounds on the asymptotic Bayes risk

We introduce the following parametrization :

- Assuming in addition that $min(f_0, f_1) \ge c$ *and that* $|\phi_2| \le \frac{c}{12}$ $\frac{\rm c}{12}$ \wedge $\frac{\rm c^2}{4}$ *has:*

Note that the upper bound $\frac{1}{2}$ – $|\phi_1|$ $\frac{\rho_{11}}{2}$ corresponds to the Bayes risk reached by the majority class classifier.

Efficiency of plug-in empirical Bayes classifier

Theorem 1 *Assume:*

• *The initial distribution* $ν$ *is the stationary distribution.* \bullet $\delta = \min_{\mathbf{i},\mathbf{j}} \mathbf{Q}_{\mathbf{i},\mathbf{j}} > \mathbf{0}$ \bullet $(\mathbf{f_0}(\mathbf{y}), \mathbf{f_1}(\mathbf{y})) = (\mathbf{p})$ y $\mathbf{y}_0^{\mathbf{y}}(\mathbf{1}-\mathbf{p_0})^{\mathbf{1}-\mathbf{y}}, \mathbf{p}$ y $\frac{\mathrm{y}}{1} (1 - \mathrm{p}_1)^{1 - \mathrm{y}})$ • $c^* = \min(p_0, p_1, 1 - p_0, 1 - p_1) > 0.$ *Then:* $\mathcal{R}_{\mathbf{n},\mathbf{HMM}}^{\mathbf{Offline}}(\hat{\mathbf{h}})-\mathcal{R}_{\mathbf{n},\mathbf{HMM}}^{\star,\mathbf{Offline}}$ $_{\rm n, HMM}^{*, \rm{on$ ${\bold 4}({\bold 1}-\delta)$ $\frac{1-\sigma)}{\delta^{\mathbf{2}}} \mathbb{E}_{\theta}$ $\begin{bmatrix} 1 \end{bmatrix}$ $\mathbf{n}(\mathbf{1}-\rho)$ $\|\nu - \hat{\nu}\|_2 +$ $\left($ $1/(1-\rho)$

- [1] Kweku Abraham, Ismaël Castillo, and Elisabeth Gassiat. Multiple testing in nonparametric hidden markov models: An empirical bayes approach. *Journal of Machine Learning Research*, 2021.
- [2] Olivier Cappé, Eric Moulines, and Rydén Tobias. Inference in Hidden Markov *Models*. Springer, 2005.

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$$
+1/(1-\hat{\rho})\bigg)\left(\Vert \mathbf{Q}-\hat{\mathbf{Q}}\Vert_{\mathbf{F}}+\frac{2}{c^{\star}}\max\limits_{\mathbf{x}=0,1}\left|\mathbf{p}_{\mathbf{x}}-\hat{\mathbf{p}}_{\mathbf{x}}\right|\right)\right)\\ \mathcal{R}_{n,HMM}^{Online}(\hat{\mathbf{h}})-\mathcal{R}_{n,HMM}^{\star, Online}\leq\frac{8(1-\delta)}{\delta^{2}}\mathbb{E}_{\theta}\Bigg[\frac{1}{n(1-\rho)}\Vert\nu-\hat{\nu}\Vert_{2}+\Big(1/(1-\rho)\frac{1}{\rho^{2}}\Vert\nu-\hat{\mathbf{Q}}\Vert_{2}\Big)\Bigg].
$$

$$
+1/(1-\hat{\rho})\Big)\left(\|\mathbf{Q}-\hat{\mathbf{Q}}\|_{\mathbf{F}}+\frac{1}{\mathbf{c}^{\star}}\max_{\mathbf{x}=\mathbf{0},\mathbf{1}}|\mathbf{p}_{\mathbf{x}}-\hat{\mathbf{p}}_{\mathbf{x}}|\right)\Bigg]+2\mathbb{E}_{\theta}\left[\|\mathbf{Q}-\hat{\mathbf{Q}}\|_{\mathbf{F}}\right.
$$

where $\rho = \frac{1-2\delta}{1-\delta}$ $1{-}\delta$, $\hat{\rho} =$ $\underline{1-2}\hat{\delta}$ $\overline{1\!-\!\hat{\delta}}$ $\hat{\delta}$ = $\min_{\mathbf{i},\mathbf{j}} \hat{\mathbf{Q}}_{\mathbf{i},\mathbf{j}} > 0$ *and* $\hat{\mathbf{h}}$ *is the empirical Bayes classifier using estimates of the model parameters* $\hat{\theta} = (\hat{\nu}, \hat{\mathbf{Q}}, \hat{\mathbf{p}}_0, \hat{\mathbf{p}}_1)$.

• Note that there is no need for consistent estimators of the initial distribution.

• Existence of consistent estimators of (Q, f_0, f_1) is ensured (cf. [1]).

Define the following two quantities:

$$
\mathcal{R}_{\infty,\text{HMM}}^{\star,\text{Offline}} = \mathbb{E}_{\theta}[\min(\mathbb{P}_{\theta}(\mathbf{X_0} = 1 \mid \mathbf{Y}_{-\infty;+\infty}), \mathbb{P}_{\theta}(\mathbf{X_0} = 0 \mid \mathbf{Y}_{-\infty;+\infty})]
$$

$$
\mathcal{R}_{\infty,\text{HMM}}^{\star,\text{Online}} = \mathbb{E}_{\theta}[\min(\mathbb{P}_{\theta}(\mathbf{X_1} = 1 \mid \mathbf{Y}_{-\infty:0}), \mathbb{P}_{\theta}(\mathbf{X_1} = 0 \mid \mathbf{Y}_{-\infty:0}))]
$$

Theorem 2 *Under the same assumptions:*

$$
\left| \mathcal{R}_{n, HMM}^{\star, Offline} - \mathcal{R}_{\infty, HMM}^{\star, Offline} \right| \leq \frac{2}{n(1 - \rho_0)} \\\left| \mathcal{R}_{n, HMM}^{\star, Online} - \mathcal{R}_{\infty, HMM}^{\star, Online} \right| \leq \frac{\rho_1}{2n} \frac{1}{1 - \rho_0}
$$

$$
\phi(\theta)=\left(\frac{q-p}{q+p},\quad 1-p-q,\quad \|f_0-f_1\|_\infty\right)
$$

Theorem 3 *- The asymptotic Bayes risk for online clustering verifies:*

$$
\mathcal{R}_{\infty,\mathrm{HMM}}^{\star,\mathrm{Online}} \leq \frac{1}{2} - \frac{|\phi_1|}{2}
$$

$$
\mathcal{R}_{\infty,\mathrm{HMM}}^{\star,\mathrm{Online}} \geq \frac{1}{2} - \frac{|\phi_1|}{2} - \frac{(1-\phi_1^2)\phi_2^2\phi_3}{2c}
$$

Conclusion and future directions

This work clarifies some features of the asymptotic behavior of the Bayes risk and empirical estimation procedures. However, some aspects still need to be studied:

- Extension of the results to the nonparametric setting.
- Bounds on the asymptotic Bayes risk in the offline framework.
- Matching the upper and lower bounds in order to understand how much better is the HMM Bayes classifier compared to majority class classifier.

References