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Clustering of Multidimensional Random Variables to Improve HMM Sequence Alignment Accuracy

Project proposal

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1 Introduction

1.1 Clustering

Given $X = \{x_i | x_i \in \mathbb{R}^d, i \in (1 \dots n)\}$ and $m \in \mathbb{N}$, where n is the number of points, m - number of clusters.

Clustering algorithm takes X and m and outputs $C = \{c_i | c_i \in (1 \dots m), i \in (1 \dots n)\}$.



Figure 1: Example of clustering for $d = 2$, $m = 2$, color represents class.

1.2 Strings

Definition 1.1. String of length l over alphabet $A = \{1 \dots m\}$ is a map $s : \{1 \dots l\} \rightarrow A$. Usually elements of A are denoted as characters for convenience.

Definition 1.2. Alignment of strings s_1 and s_2 of lengths l_1 and l_2 respectively, over alphabet A is a pair of strings \hat{s}_1 and \hat{s}_2 of length l over alphabet $A \sqcup \{-\}$, such that there exists increasing functions $f_i : \{1 \dots l_i\} \rightarrow \{1 \dots l\}$ such that $\hat{s}_i|_{\hat{s}_i^{-1}(A)} \circ f_i = s_i$.

Remark. $\text{Im}(f_i) = \hat{s}_i^{-1}(A)$

Example 1.1. Alignment of strings $s_1 = CABC AABA$ and $s_2 = ABADBBAD$ over alphabet $\{A, B, C, D\}$.

$$\left\| \begin{array}{c|cccccccc} s_1 & C & A & B & C & A & A & B & A \\ s_2 & A & B & A & D & B & B & A & \\ \hline \hat{s}_1 & C & A & B & C & - & A & A & B & A \\ \hat{s}_2 & - & A & B & - & A & D & B & B & A \end{array} \right\|$$

Definition 1.3. For given matrix $G \in \mathbb{R}^{|A| \times |A|}$ and $p \in \mathbb{R}$ score of alignment \hat{s}_1, \hat{s}_2 is

$$S(\hat{s}_1, \hat{s}_2) = \sum_{i=1}^l \delta_i, \text{ where } \delta_i = \begin{cases} g_{\hat{s}_1(i)\hat{s}_2(i)}, & \hat{s}_1(i) \neq - \text{ and } \hat{s}_2(i) \neq - \\ p, & \end{cases}$$

Theorem 1. If G is symmetric and $g_{ij} = \begin{cases} 0, & i = j \\ > 0, & \end{cases}$ and $p > 0$, then we can define metric for strings over alphabet A as

$$d(s_1, s_2) = \min\{S(\hat{s}_1, \hat{s}_2)\}$$

Proof.

□

Definition 1.4. For a string s of length l , substring s_s is a string of length l_s , such that there exists an function

$$\begin{aligned} f : \{1 \dots l_s\} &\rightarrow \{1 \dots l\} \\ f(i) &= i + d \\ s \circ f &= s_s \end{aligned}$$

Definition 1.5. For a string s_1 and s_2 define string-substring score as

$$S_s(s_1, s_2) = \min\{S(s_s, s_2) | s_s \text{ is a substring of } s\}$$

Definition 1.6. Set of reads R for string s of length l and rate r is

$$R = \{s_s | s_s \text{ is a substring of } s, \}$$