Formal statement of the pseudotime reconstruction problem

Guilherme de Sena Brandine

September 28, 2016

1 Problem statement

Let $X = \{x_1 \dots x_N\} \subset R^D$ be a set of N points in the D-dimensional space. Let also $K \in \mathbb{N}$ be a fixed, small integer and $T = \{t_0 = 0, t_1 \dots t_k, t_{k+1} = 1\} \subset [0, 1]$ a knot time set. Finally, define $\mathbb{I}_A(x)$ as the indicator function:

$$\mathbb{I}_A(x) = \begin{cases} 1, & \text{if } x \in A, \\ 0, & \text{otherwise} \end{cases}$$

A k-piecewise linear function with knot time set T is a function $f_T : [0, 1] \to \mathbb{R}^D$ defined as:

$$f_T(t) = \sum_{i=1}^{k} f_i(t)\mathbb{I}_{[t_{i-1},t_i]}(t)$$

Where $f_j : [0, 1] \to \mathbb{R}^D$ is given by:

$$f_j(t) = (\alpha_{j1} + \beta_{j1}t, \dots, \alpha_{jD} + \beta_{jD}t)$$

And the family of functions $f_1(t) \dots f_k(t)$ satisfy the continuity constraint, that is, $\forall 1 \le j < k$:

$$f_j(t_j) = f_{j+1}(t_j) \tag{1}$$

Equation [1] implies the following constraint, which automatically defines t_j as a function of the other parameters:

$$t_j = \frac{\alpha_{j1} - \alpha_{j+1,1}}{\beta_{j+1,1} - \beta_{j1}} = \dots = \frac{\alpha_{jD} - \alpha_{j+1,D}}{\beta_{j+1,D} - \beta_{jD}} \tag{2}$$

Finally, let $P = \{p_1 \dots p_N\} \subset [0, 1]$ be an assignment of pseudotimes for each element in X.

The problem to optimize is: *Find the sets $P_{opt} = \{p_1 \dots p_N\}$, $A_{opt} = \{\alpha_{ij}, 1 \le i \le k, 1 \le j \le D\}$ and $B_{opt} = \{\beta_{ij}, 1 \le i \le k, 1 \le j \le D\}$ that satisfy [2] and mimimizes the error function*:

$$E(P, A, B) = \sum_{i=1}^{N} ||X_i - f_T(p_i)||^2$$