

Calculation of the cost matrix

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1 Problem statement and definitions

Let y_{nj} be the data value at position (genomic coordinate) $n = 1, \dots, N$ for replicate array $j = 1, \dots, J$. Hence we have J arrays and sequences of length N . The goal of this note is to describe an $O(NJ)$ algorithm to calculate the cost matrix of a piecewise linear model for the segmentation of the $(1, \dots, N)$ axis. It is implemented in the function `costMatrix` in the package `tilingArray`. The cost matrix is the input for a dynamic programming algorithm that finds the optimal (least squares) segmentation.

The cost matrix G_{km} is the sum of squared residuals for a segment from m to $m+k-1$ (i. e. including $m+k-1$ but excluding $m+k$),

$$G_{km} := \sum_{j=1}^J \sum_{n=m}^{m+k-1} (y_{nj} - \hat{\mu}_{km})^2 \quad (1)$$

where $1 \leq m \leq m+k-1 \leq N$ and $\hat{\mu}_{km}$ is the mean of that segment,

$$\hat{\mu}_{km} = \frac{1}{Jk} \sum_{j=1}^J \sum_{n=m}^{m+k-1} y_{nj}. \quad (2)$$

Sidenote: a perhaps more straightforward definition of a cost matrix would be $\tilde{G}_{m'm} = G_{(m'-m)m}$, the sum of squared residuals for a segment from m to $m'-1$. I use version (1) because it makes it easier to use the condition of maximum segment length ($k \leq k_{\max}$), which I need to get the algorithm from complexity $O(N^2)$ to $O(N)$.

2 Algebra

$$G_{km} = \sum_{j=1}^J \sum_{n=m}^{m+k-1} (y_{nj} - \hat{\mu}_{km})^2 \quad (3)$$

$$= \sum_{n,j} y_{nj}^2 - \frac{1}{Jk} \left(\sum_{n',j'} y_{n'j'} \right)^2 \quad (4)$$

$$= \sum_n q_n - \frac{1}{Jk} \left(\sum_{n'} r_{n'} \right)^2 \quad (5)$$

with

$$q_n := \sum_j y_{nj}^2 \quad (6)$$

$$r_n := \sum_j y_{nj} \quad (7)$$

If y is an $N \times J$ matrix, then the N -vectors \mathbf{q} and \mathbf{r} can be obtained by

$$\mathbf{q} = \text{rowSums}(y*y)$$

$$\mathbf{r} = \text{rowSums}(y)$$

Now define

$$c_\nu = \sum_{n=1}^{\nu} r_n \quad (8)$$

$$d_\nu = \sum_{n=1}^{\nu} q_n \quad (9)$$

which be obtained from

$$\mathbf{c} = \text{cumsum}(\mathbf{r})$$

$$\mathbf{d} = \text{cumsum}(\mathbf{q})$$

then (5) becomes

$$(d_{m+k-1} - d_{m-1}) - \frac{1}{Jk} (c_{m+k-1} - c_{m-1})^2 \quad (10)$$