Hidden Markov model segmentation of hydrological and environmental time series

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Abstract

Motivated by Hubert’s segmentation procedure [16, 17], we discuss the application of hidden Markov models (HMM) to the segmentation of hydrological and environmental time series. We use a HMM algorithm which segments time series of several hundred terms in a few seconds and is computationally feasible for even longer time series. The segmentation algorithm computes the Maximum Likelihood segmentation by use of an expectation / maximization iteration. We rigorously prove algorithm convergence and use numerical experiments, involving temperature and river discharge time series, to show that the algorithm usually converges to the globally optimal segmentation. The relation of the proposed algorithm to Hubert’s segmentation procedure is also discussed.

1 Introduction

In this paper we discuss the following problem of time series segmentation: given a time series, divide it into two or more segments (i.e. blocks of contiguous data) such that each segment is homogeneous, but contiguous segments are heterogeneous. Homogeneity / heterogeneity is described in terms of some appropriate statistics of the segments. The term change point detection is also used to describe the problem.

Examples of this problem arise in a wide range of fields, including engineering, computer science, biology and econometrics. The segmentation problem is also relevant to hydrology and environmetrics. For instance, in climate change studies it is often desirable to test a time series (such as river flow, rainfall or temperature records) for one or more sudden changes of its mean value.

The time series segmentation problem has been studied in the hydrological literature. The reported approaches can be divided into two categories: sequential and nonsequential. Sequential approaches often involve intervention models; see for example [14] and, for a critique of intervention models, [32].

Most of the nonsequential time segmentation work appearing in the hydrological literature involves two segments. In other words, the goal is to detect the existence and estimate the location of a single change point. A classical early study of changes in the flow of Nile appears in [8]. Buishand’s work [6, 7] is also often cited. For some case studies see [15, 21, 34]. Bayesian approaches have recently generated considerable interest [27, 28, 29, 30, 32].

It appears that the multiple change point problem has not been studied as extensively. Hubert’s segmentation procedure [16, 17] is an important step in this direction. The goodness of a segmentation is evaluated by the sum squared deviation of the data from the means of their respective segments; in what follows we will use the term segmentation cost for this quantity. Given a time series, Hubert’s procedure computes the minimal cost segmentation with $K = 2, 3, \ldots$ change points. The procedure gradually increases $K$; for every value of $K$ the best segmentation is computed; the procedure is terminated when differences in the means of the obtained segments are no longer statistically significant (as measured
by Scheffe’s contrast criterion [33]). Hubert mentions that this procedure can segment time series with several tens of terms but is "... unable at the present state to tackle series of much more than a hundred terms ..." because of the combinatorial increase of computational burden [17].

The work reported in this paper has been inspired by Hubert’s procedure. Our goal is to develop an algorithm which can locate multiple change points in hydrological and/or environmental time series with several hundred terms or more. To achieve this goal, we adapt some hidden Markov models (HMM) algorithms which have originally appeared in the speech recognition literature. (A survey of the relevant literature is postponed to Section 3.3.) We introduce a HMM of hydrological and/or environmental time series with change points and describe an approximate Expectation / Maximization (EM) algorithm which produces a converging sequence of segmentations. The algorithm also produces a sequence of estimates for the HMM parameters. Time series of several hundred points can be segmented in a few seconds (see Section 4), hence the algorithm can be used in an interactive manner as an exploratory tool. Even for time series of several thousand points the segmentation time is in the order of seconds.

This paper is organized as follows. In Section 2 we review Hubert’s formulation of the time series segmentation problem. In Section 3 we formulate the segmentation problem in terms of hidden Markov models and present a segmentation algorithm; also we compare the hidden Markov model approach with that of Hubert. We present some segmentation experiments in Section 4. In Section 5 we summarize our results. Finally, in the Appendix we present an alternative, non-HMM segmentation method, which is more accurate but also slower.

2 Time Series Segmentation as an Optimization Problem

In this section we formulate time series segmentation as an optimization problem. We follow Hubert’s presentation, but we modify his notation.

Given a time series \( x = (x_1, x_2, \ldots, x_T) \) and a number \( K \), a segmentation is a sequence of times \( t = (t_0, t_1, \ldots, t_K) \) which satisfy

\[
0 = t_0 < t_1 < \ldots < t_{K-1} < t_K = T.
\]  

(1)

The intervals of integers \( [t_0 + 1, t_1], [t_1 + 1, \ldots, t_2], \ldots, [t_{K-1} + 1, t_K] \) are the segments; the times \( t_0, t_1, \ldots, t_K \) are the change points. \( K \), the number of segments, is the order of the segmentation. The length of the \( k \)-th segment (for \( k = 1, 2, \ldots, K \)) is denoted by \( T_k = t_k - t_{k-1} \). The following notation is used for a given segmentation \( t = (t_0, t_1, \ldots, t_K) \). For \( k = 1, 2, \ldots, K \), define

\[
\hat{\mu}_k = \frac{\sum_{t=0}^{t_k-1} x_t}{T_k}, \quad d_k = \sum_{t=t_{k-1}+1}^{t_k} (x_t - \hat{\mu}_k)^2.
\]  

(2)

Define the cost of segmentation \( t = (t_0, \ldots, t_K) \) by

\[
D_K(t) = \sum_{k=1}^{K} d_k = \sum_{k=1}^{K} \sum_{t=t_{k-1}+1}^{t_k} (x_t - \hat{\mu}_k)^2.
\]  

(3)

If \( D_K \) has a small value, then the segments are homogeneous, i.e. the \( x_t \)'s are close to \( \hat{\mu}_k \) for \( k = 1, 2, \ldots, K \) and for \( t = t_{k-1} + 1, \ldots, t_k \). Now we can define the best \( K \)-th order segmentation \( \hat{t} \) to be the one minimizing \( D_K(t) \) and denote the minimal cost by \( \hat{D}_K = \hat{D}_K(\hat{t}) \). Note that for every \( K \) we have \( \hat{D}_K \geq \hat{D}_{K+1} \) [16]. Also, there is only one segmentation \( t \) of order \( T \); in this case every time instant \( t \) is a segment by itself and \( D_T(t) = 0 \).
It can be seen [16] that the number of possible segmentations grows exponentially with $T$. To efficiently search the set of all possible segmentations, Hubert uses a *branch-and-bound* approach. Even so, the computational load increases excessively with $T$ and this approach is not able currently (in 2000) to segment series of much more than a hundred terms [17].

Minimization of $D_K$ can be achieved by several alternative (and faster than branch-and-bound) algorithms. A *dynamic programming* approach is presented in the Appendix to obtain the globally minimum cost; this is feasible for $T$ in the order of several hundreds and will be reported in greater length in a future publication [20]. In this paper a different approach is followed, which is based on HMM’s.

3 Hidden Markov Models

We now present a HMM formulation of the time series segmentation problem. HMM’s have been used for runoff modeling [25] and the possibility of using them for hydrological time series segmentation has been mentioned in [30] but, as far as the author knows, an actual implementation has not been presented yet. On the other hand, we have already mentioned that HMM’s are used for segmentation of time series in several other fields (see the discussion in Section 3.3).

The term “hidden Markov model” is used to denote a broad class of stochastic processes; here we use a particular and somewhat restricted species of HMM to model a hydrological time series and present an approximate Expectation / Maximization (EM) algorithm to perform *Maximum Likelihood* (ML) segmentation. In addition to the standard probabilistic interpretation of the algorithm, a numerical optimization point of view is also possible and we use the latter to prove the convergence of the algorithm. Finally we discuss related algorithms and possible extensions.

3.1 HMM’s and Hydrological Time Series

We will use a pair of stochastic processes $(Z_t, X_t)$ to model a hydrological time series with change points. We start by considering a simple example.

The annual flow of a river is denoted by $X_t$. We assume that, for the years $t = 1, 2, ..., t_1$, $X_t$ is a normally distributed random variable with mean $\mu_1$ and standard deviation $\sigma$. In year $t_1$ a *transition* takes place and, for the years $t = t_1 + 1, t_1 + 2, ..., t_2$, $X_t$ is normally distributed with mean $\mu_2$ and standard deviation $\sigma$. This process continues with transitions taking place in years $t_2, t_3, ..., t_{K-1}$. This process is illustrated in Figure 1. We indicate the *states* of the river flow by circles and the possible transitions from state to state by arrows; note that the states are *unobservable*. We indicate the observable time series by the double arrows emanating from the states.

The above mechanism can be modeled by a pair of stochastic processes $(Z_t, X_t)$ (with $t = 0, 1, 2, ...$) defined as follows.

1. $Z_t$, which is the *state process*, is a finite state Markov chain with $K$ states; it has initial probability vector $\pi$ and transition probability matrix $P$. Hence, for any $T$, the joint probability function of $Z_0, Z_1, ..., Z_T$ is

$$
\Pr(Z_1 = z_1, Z_2 = z_2, ..., Z_T = z_T) = \pi_{z_0} \cdot P_{z_0, z_1} \cdot P_{z_1, z_2} \cdot \cdots \cdot P_{z_{T-1}, z_T}.
$$

For the specific example discussed above, it will also be true that: (a) $\pi_1 = 1, \pi_k = 0$ for $k = 2, 3, ..., K$, (b) $P_{k,j} = 0$ for $k = 1, 2, ..., K$ and all $j$ other than $k$, $k+1$. The parameters of this process are $K$ and $P$. 

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2. $X_t$, which is the \textit{observation process}, is a sequence of \textit{conditionally independent}, normally distributed random variables with mean $\mu_z$ and standard deviation $\sigma$. More precisely, for every $t$, the joint probability density of $X_1, X_2, ..., X_t$ conditioned on $Z_1, Z_2, ..., Z_t$ is

$$f_{X_1, X_2, ..., X_t | Z_1, Z_2, ..., Z_t}(x_1, x_2, ..., x_t | z_1, z_2, ..., z_t) = \prod_{i=1}^{n} e^{-(x_1 - \mu_z)^2/2\sigma^2}. \quad (5)$$

The parameters of this process are $\mu_1, \mu_2, \ldots, \mu_K$ and $\sigma$. We will often use the notation $\mathbf{M} = [\mu_1, \mu_2, \ldots, \mu_K]$. 

The $(Z_t, X_t)$ pair is a HMM, in particular a \textit{left-to-right continuous HMM} \cite{31}. “Left-to-right” refers to the structure of state transitions (as depicted in Figure 1) and “continuous” refers to the fact that the observation process is continuous valued. The model parameters are $K, \mathbf{P}, \mathbf{M}, \sigma$.

There is a one-to-one correspondence between state sequences $\mathbf{z} = (z_1, z_2, \ldots, z_T)$ and segmentations $\mathbf{t} = (t_0, t_1, \ldots, t_{K'}).$ For example, given a particular $\mathbf{z}$, we obtain the corresponding $\mathbf{t}$ by locating the times $t_k$ such that $z_k \neq z_{k+1}$, for $k = 1, 2, \ldots, K' - 1$ (and setting $t_0 = 0$ and $t_{K'} = T$). The postulated Markov chain only allows left-to-right transitions, hence $K' \leq K$, i.e. there will be at most $K$ segments, and every segment will be uniquely associated with a state.

The \textit{conditional likelihood} of a state sequence $\mathbf{z}$ (\textit{given} an observation sequence $\mathbf{x}$) is denoted by

$$L_{K,T}^1(\mathbf{z}; \mathbf{x}; \mathbf{P}, \mathbf{M}, \sigma) = L_{K,T}(z_1, z_2, ..., z_T | x_1, x_2, ..., x_T; P, \mathbf{M}, \sigma)$$

and the \textit{joint likelihood} of a state sequence $\mathbf{z}$ and an observation sequence $\mathbf{x}$ is denoted by

$$L_{K,T}^2(\mathbf{z}, \mathbf{x}; \mathbf{P}, \mathbf{M}, \sigma) = L_{K,T}^2(z_1, z_2, ..., z_T, x_1, x_2, ..., x_T; P, \mathbf{M}, \sigma).$$  \quad (7)

$L_{K,T}^1$ and $L_{K,T}^2$ are understood as functions of $\mathbf{z} = (z_1, z_2, ..., z_T)$; the observations $\mathbf{x} = (x_1, x_2, \ldots, x_T)$, the number of segments $K$, and the length of the time series $T$, as well as the parameters $\mathbf{P}$, $\mathbf{M}$, $\sigma$ are assumed \textbf{fixed}. In place of $T$ any $t$ can be used, to indicate the likelihood of the subsequence $(z_1, z_2, ..., z_t)$ given $(x_1, x_2, ..., x_t)$ etc. For example, we can write

$$L_{K,t}^2(z_1, z_2, ..., z_t, x_1, x_2, ..., x_t; P, \mathbf{M}, \sigma).$$ \quad (8)

Note also that

$$L_{K,T}^1 = A \cdot L_{K,T}^2$$ \quad (9)

where $A$ is a quantity independent of $(z_1, z_2, ..., z_T)$. Finally, from (4), (5) we have

$$L_{K,T}^2(\mathbf{z}, \mathbf{x}; \mathbf{P}, \mathbf{M}, \sigma) = \prod_{t=1}^{T} \left( P_{zt-1, z_t} \cdot e^{-(x_t - \mu_z)^2/2\sigma^2} \right), \quad (10)$$

where $z_0 = 1$, according to the previously stated assumption.

\subsection*{3.2 The Segmentation Algorithm}

The ML segmentation $\hat{\mathbf{t}}$ can be obtained from the ML state sequence $\hat{\mathbf{z}} = (\hat{z}_1, \hat{z}_2, \ldots, \hat{z}_T)$. Since state sequences are unobservable, we will estimate $\hat{\mathbf{z}}$ in terms of the observable sequence $\mathbf{x} = (x_1, x_2, \ldots, x_T)$ and the parameters $K, \mathbf{P}, \mathbf{M}, \sigma$. Note that in practice $K, \mathbf{P}, \mathbf{M}, \sigma$ will also be unknown. Hence the computation of the maximum likelihood HMM segmentation must be divided into two subtasks: (a) estimating the HMM parameters and (b) computing the actual segmentation. We follow the standard approach used in HMM problems: a parameter estimation phase is followed by a time series segmentation phase and the process is repeated until convergence. This is the Expectation / Maximization (EM) approach. First we discuss estimation and segmentation in more detail; then we will return to a discussion of the EM approach.
3.2.1 Parameter Estimation

Suppose, for the time being, that a segmentation \( t = (t_0, t_1, ..., t_m) \) is given. A reasonable estimate of \( \mathbf{M} = [\mu_1, \mu_2, ..., \mu_K] \), dependent on the given segmentation, is (for \( k = 1, 2, ..., K \))

\[
\hat{\mu}_k = \frac{\sum_{t=t_{k-1}+1}^{t_k} x_t}{T_k}. \tag{11}
\]

Similarly we could use the following segmentation-dependent estimates of \( \sigma \) (for \( k = 1, 2, ..., K \))

\[
\hat{\sigma}_k = \sqrt{\frac{\sum_{t=t_{k-1}+1}^{t_k} (x_t - \hat{\mu}_k)^2}{T_k - 1}}. \tag{12}
\]

However, to maintain compatibility with Hubert’s approach, we will use the segmentation-independent estimate

\[
\hat{\sigma} = \sqrt{\frac{\sum_{t=1}^{T} (x_t - \hat{\mu})^2}{T - 1}} = \sqrt{\frac{\sum_{k=1}^{K} \sum_{t=t_{k-1}+1}^{t_k} (x_t - \hat{\mu})^2}{T - 1}}. \tag{13}
\]

where

\[
\hat{\mu} = \frac{\sum_{t=1}^{T} x_t}{T}.
\]

Let us now turn to the transition probability matrix \( P \). In a left-to-right HMM, for \( k = 1, 2, ..., K \) and all \( j \) different from \( k \) and \( k+1 \), we will have \( P_{k,j} = 0 \). Also, for \( k = 1, 2, ..., K - 1 \) we will have \( P_{k,k+1} = 1 - P_{k,k} \). Hence \( P \) only has \( K - 1 \) free parameters, namely \( P_{1,1}, P_{2,2}, ..., P_{K-1,K-1} \). These could be estimated from the given segmentation. However, in this paper we use a simpler approach. Namely, we assume

\[
P = \begin{bmatrix}
p & 1 - p & 0 & 0 & 0 & 0 \\
0 & p & 1 - p & 0 & 0 & 0 \\
... & ... & ... & ... & ... & ... \\
0 & 0 & 0 & ... & p & 1 - p \\
0 & 0 & 0 & 0 & 0 & 1
\end{bmatrix}. \tag{14}
\]

Hence \( P \) is determined in terms of a single parameter \( p \), which will be chosen a priori, rather than estimated. We have found by numerical experimentation that the exact value of \( p \) is not critical; in all the examples of Section 4, the segmentation algorithm performs very well using \( p \) in the range \([0.85,0.95]\).

Finally, we must make a choice regarding the number of segments \( K \). We will use Hubert’s approach, and take a sequence of increasing values: \( K = 2, 3, ... \) until a value of \( K \) is reached which yields statistically nonsignificant segmentations (statistical significance is evaluated by Scheffe’s contrast criterion, [16, 33]).

3.2.2 Segmentation

Given observations \( \mathbf{x} = (x_1, x_2, ..., x_T) \) and assuming the parameters \( K, P, \mathbf{M}, \sigma \) to be known, the Maximum Likelihood (ML) state sequence is the \( \hat{\mathbf{z}} = (\hat{z}_1, \hat{z}_2, ..., \hat{z}_T) \) which maximizes \( L_{1,K,T}^1(\mathbf{z} | \mathbf{x} ; P, \mathbf{M}, \sigma) \) as function of \( \mathbf{z} \). The ML segmentation \( \hat{\mathbf{t}} = (\hat{t}_0, \hat{t}_1, ..., \hat{t}_{K'}) \) is obtained from \( \hat{\mathbf{z}} \). It will be seen in
Section 3.2.4 that, under certain circumstances, \( \hat{z} \) also minimizes the segmentation cost \( D_K \) defined in Section 2.

\( \hat{z} = (\hat{z}_1, \hat{z}_2, ..., \hat{z}_T) \) can be found by the Viterbi algorithm [11], a computationally efficient dynamic programming approach. In view of (9) we have

\[
(\hat{z}_1, \hat{z}_2, ..., \hat{z}_T) = \arg \max_{z_1, z_2, ..., z_T} L^2_{K,T}(z_1, z_2, ..., z_T, x_1, x_2, ..., x_T; P, M, \sigma). \tag{15}
\]

Now, for \( t = 1, 2, ..., T \) and \( k = 1, 2, ..., K \) define

\[
q_{k,t} = \max_{z_1, z_2, ..., z_{t-1}} L^2_{K,t}(z_1, z_2, ..., z_{t-1}, k, x_1, x_2, ..., x_t; P, M, \sigma) \tag{16}
\]

It can be shown by standard dynamic programming arguments [5] that both \( \hat{z} = (\hat{z}_1, \hat{z}_2, ..., \hat{z}_T) \) and the \( q_{k,t} \)'s of (16) can be computed recursively as follows.

**Viterbi Algorithm**

**Input:** The time series \( x_1, x_2, ..., x_T \); the parameters \( K, P, M \) and \( \sigma \).

**Forward Recursion**

Set \( q_{1,0} = 1, q_{2,0} = q_{3,0} = ... = q_{k,0} = 0 \).

For \( t = 1, 2, ..., T \)

For \( k = 1, 2, ..., K \)

\[
q_{k,t} = \max_{1 \leq j \leq K} \left( q_{j,t-1} \cdot P_{j,k} \cdot e^{-\left(x_t - \mu_k\right)^2/2\sigma^2} \right)
\]

\[
r_{k,t} = \arg \max_{1 \leq j \leq K} \left( q_{j,t-1} \cdot P_{j,k} \cdot e^{-\left(x_t - \mu_k\right)^2/2\sigma^2} \right).
\]

End

End

**Backtracking**

\[
\hat{L}^2_{K,T} = \max_{1 \leq k \leq K} (q_{k,T})
\]

\[
\hat{z}_T = \arg \max_{1 \leq k \leq K} (q_{k,T}).
\]

For \( t = T, T - 1, ..., 2 \)

\[
\hat{z}_{t-1} = r_{\hat{z}_t,t}.
\]

End

Upon completion of the forward recursion, \( \hat{L}^2_{K,T} \), the maximum value of \( L^2_{K,T} \), is obtained. The backtracking phase produces the state sequence which maximizes \( L^2_{K,T} \) (and hence also \( L^1_{K,T} \)). Execution time is of order \( O(T \cdot K^2) \) which is linear (rather than exponential) in the length of the time series \( T \). This makes the algorithm computationally feasible even for long time series. For more details on the Viterbi algorithm see [11].
3.2.3 Combined Parameter Estimation and Segmentation

Parameter estimation and segmentation can be combined in an algorithm which maximizes the likelihood viewed as a function of both the state sequence \( z = (z_1, z_2, ..., z_T) \) and the parameters \( \mathbf{M} \). The algorithm presented below is an iterative \textit{Expectation / Maximization} (EM) algorithm [9] which produces a converging sequence of segmentations.

### HMM Segmentation Algorithm

**Input:** The time series \( x = (x_1, x_2, ..., x_T) \); the parameters \( K, P \); a termination variable \( \varepsilon \).

Choose randomly a state sequence \( \hat{z}^{(0)} = (z_1^{(0)}, z_2^{(0)}, ..., z_T^{(0)}) \).

Compute \( \hat{\sigma} \) from (13).

For \( i = 1, 2, ... \)

- Compute \( t^{(i)} \) from \( \hat{z}^{(i-1)} \).
- Compute \( \hat{\mathbf{M}}^{(i)} \) from \( t^{(i)} \) and (11).
- Compute \( \hat{z}^{(i)} \) by the Viterbi algorithm using \( x, K, P, \hat{\mathbf{M}}^{(i)}, \hat{\sigma} \).

If \( |L_{K,T}^2(\hat{z}^{(i)}, x; P, \hat{\mathbf{M}}^{(i)}, \hat{\sigma}) - L_{K,T}^2(\hat{z}^{(i-1)}, x; P, \hat{\mathbf{M}}^{(i-1)}, \hat{\sigma})| < \varepsilon \),

\[ \hat{z} = \hat{z}^{(i)} \]

Exit the loop

EndIf

End

In Section 3.2.4 we will show that the above algorithm is a very close approximation to an EM algorithm and that, under certain conditions, every iteration increases the likelihood function. In all the examples presented in Section 4 the algorithm converges to the \textit{global} maximum with very few iterations (typically 3 or 4). In other words, the outer loop of the algorithm is executed only a few times; in each execution we perform a parameter reestimation according to (11) (with execution time \( O(T) \)) and a segmentation by the Viterbi algorithm (with execution time \( O(T \cdot K^2) \)). Hence the total execution time for a fixed \( K \) value is \( O(T \cdot K^2) \).

For a complete segmentation procedure the above algorithm is run for a sequence of increasing values \( K = 2, 3, ... \). First the algorithm is used to obtain the ML segmentation of order \( K = 2 \); the difference of the means of the two segments is tested for statistical significance by the Scheffe criterion (for details see [16] and [33]). If the difference is not significant, then it is concluded that the entire time series consists of a single segment. If the difference is significant, the algorithm is run with \( K = 3 \) and the Scheffe test is applied to the resulting segments. The process is continued until, for some value of \( K \), a segmentation is obtained which fails the Scheffe test (or until we reach \( K = T \), an unlikely case).

The use of Scheffe’s contrast criterion to determine the true value of \( K \) is somewhat problematic. This point is discussed in some detail in [16]. Many methods for the determination of \( K \) have been proposed in the literature, but none of these completely resolves the problem. In cases of doubt, a
pragmatic approach would be to use human judgement to evaluate segmentations with different $K$’s. In the case of hydrological and environmental time series which involve a rather small number of segments, this is relatively easy. The short execution time of the segmentation algorithm favors this approach, since experimentation in an “interactive” mode is feasible.

3.2.4 Convergence

The goal of this section is to show that, for a fixed $K$, every iteration of the HMM segmentation algorithm increases the likelihood; since the likelihood is bounded above by one, this also implies that the algorithm converges.

Two approaches can be used. The first approach is based upon the probabilistic interpretation of the algorithm; since this is a routinely applied analysis of EM algorithms, it will be presented only in outline. In the second approach, the segmentation algorithm is viewed from a numerical optimization point of view and convergence is proved without using any probabilistic assumptions; furthermore this approach shows clearly the connection of our segmentation algorithm to Hubert’s procedure.

**Probabilistic Approach.** As explained in [9], the basic ingredient of the EM family of algorithms is the iterative application of an expectation step followed by a likelihood maximization step. In our case the expectation step consists in estimating $\hat{M}^{(i)}$ by (11) and the maximization step consists in finding $z^{(i)}$ by the Viterbi algorithm.

While the Viterbi algorithm computes exactly the global maximum of the likelihood (viewed as a function of $z$ only!), the estimation step used in this paper is approximate. The exact step would involve computing estimates of $\hat{\mu}_1, \hat{\mu}_2, ... , \hat{\mu}_K$ for every possible segmentation and then combining these estimates in a sum weighted by the respective probability of each segmentation (a similar approach should be used for $\sigma$, using the estimates of (12)). This approach is used in [10] and elsewhere; while it is computationally more expensive than the approach used here, it is still viable. At any rate, in most cases the two approaches yield very similar results.

If it is assumed that the estimate of (11) is a close approximation to the maximum likelihood estimate of $M$, then convergence can be established by a standard EM argument presented in [9, 24] and several other places. This argument shows that a certain cross entropy $Q(z^{(i)}, z^{(i-1)})$ is decreased by every iteration of an EM algorithm. Since $Q$ is always nonnegative, it must converge to a nonnegative number, and this suffices for the algorithm to terminate. Furthermore, by relating $Q(z^{(i)}, z^{(i-1)})$ to the likelihood, it can be shown that the sequence $L_{K,T}(z^{(i)})$ is monotonically increasing.

**Numerical Approach.** In what follows we will consider $K, P, x, \sigma$ to be fixed. We will denote the set of all possible state sequences by $\Phi$ and the set of all state sequences with $K$ transitions by $\Phi_K$; we will also use the standard notation $R^K$ for the set of all $K$-dimensional real vectors.

Taking the negative logarithm of (10) we obtain

$$- \log \left[ L_{K,T}^2(z, x; P, M, \sigma) \right] = - \sum_{t=1}^{T} \log \left( P_{z_{t-1}, z_t} \right) + \sum_{t=1}^{T} \frac{(x_t - \mu_{z_t})^2}{2\sigma^2}.$$  \hspace{1cm} (17)

We define $\phi(z) =$ “number of times $z_{t-1} \neq z_t$”; in other words, $\phi(z)$ is the number of transitions in the state sequence $z$. If we limit ourselves to state sequences $z \in \Phi_K$, then obviously $\phi(z) = K$. Now, for
Now, using first (24) and then (23), we obtain
\[ -\log \left[ L_{K,T}^2(z, x; P, M, \sigma) \right] = - \left( (T - \phi(z)) \cdot \log(p) + \phi(z) \cdot \log(1-p) \right) + \sum_{t=1}^{T} \frac{(x_t - \mu_{zt})^2}{2\sigma^2} \]
(18)
\[ = - \left( (T - K) \cdot \log(p) + K \cdot \log(1-p) \right) + \sum_{t=1}^{T} \frac{(x_t - \mu_{zt})^2}{2\sigma^2} \Rightarrow \]
(19)
\[ = C(T, K, P) + \sum_{t=1}^{T} \frac{(x_t - \mu_{zt})^2}{2\sigma^2}. \]
(20)
where \( C(T, K, P) = - [ (T - K) \cdot \log(p) + K \cdot \log(1-p) ] \). Now we define the function
\[ J(z, M) = \sum_{t=1}^{T} (x_t - \mu_{zt})^2 \]
(21)
and note that
\[ J(z, M) = -2\sigma^2 \cdot \left( \log \left[ L_{K,T}^2(z, x; P, M, \sigma) \right] + C(T, K, P) \right). \]
(22)
Note that, for simplicity of notation, we write \( J(z, M) \) as a function only of \( z, M \); the quantities \( T, K, P, x, \sigma \) can be considered fixed.

Now consider a run of the segmentation algorithm which produces a sequence \( z^{(0)}, z^{(1)}, z^{(2)} \ldots, z^{(i)}, \ldots \). Suppose that for every \( s \) we have \( z^{(i)} \in \Phi_K \). By the reestimation formula for \( M^{(i)} \) we will have for every \( s \):
\[ \forall M \in R^K : J(z^{(i-1)}; M^{(i)}) \leq J(z^{(i-1)}; M). \]
(23)
Furthermore, note that the Viterbi algorithm yields the global maximum of the likelihood as a function of \( z \). Hence, from (22) and the reestimation formula for \( z^{(i)} \) we will have for every \( i \):
\[ \forall z \in \Phi_K : J(z^{(i)}; M^{(i)}) \leq J(z; M^{(i)}). \]
(24)
Now, using first (24) and then (23), we obtain
\[ J(z^{(i)}; M^{(i)}) \leq J(z^{(i-1)}; M^{(i)}) \leq J(z^{(i-1)}; M^{(i-1)}) \]
(25)
and, from (25) and (22),
\[ L_{K,T}^2(z^{(i)}, x; P, M^{(i)}, \sigma) \geq L_{K,T}^2(z^{(i-1)}, x; P, M^{(i-1)}, \sigma) \]
(26)
Hence, if for every \( i \) we have \( z^{(i)} \in \Phi_K \), then the sequence \( \left\{ L_{K,T}^2(z^{(i)}, x; P, M^{(i)}, \sigma) \right\}_{i=0}^{\infty} \) is increasing; since it is also bounded from above by one, it must converge. It follows that the HMM segmentation algorithm produces a sequence of segmentations with increasing and convergent likelihood; from convergence of the likelihood we also conclude that the algorithm will eventually terminate. Furthermore, if \( t^{(i)} \) is the segmentation obtained from \( z^{(i)} \) it is easy to check that
\[ D_K(t^{(i)}) = J(z^{(i)}; M^{(i)}). \]
(27)
From (23), (27) follows that Hubert’s segmentation cost is decreased in every iteration of the HMM segmentation algorithm.
For the above analysis to hold, we have required that $z(t) \in \Phi_K$ for every $i$. This condition is easy to check; it is usually satisfied in practice; and it can be enforced by choosing the parameter $p$ to be not too close to 1 (if $p \approx 1$, then the cost of state transitions is very high and transitions are avoided).

One way to interpret the above analysis is the following: using an appropriate value of $p$, the segmentation algorithm presented here becomes an iterative, approximate way to find Hubert’s optimal segmentation. The approximation is usually very good, as will be seen in Section 4. This interpretation is completely nonprobabilistic and does not depend on the use of the hidden Markov model.

**Computational Issues.** We must also mention that successful implementation of the Viterbi algorithm requires a normalization of the $q_{k,t}$’s to avoid numerical underflow; alternatively one can work with the logarithms of the the $q_{k,t}$’s and perform additions rather than multiplications.

### 3.3 Discussion and Extensions

An extensive mathematical, statistical and engineering literature covers both the theoretical and applied aspects of HMM’s. The reader can use [10, 31] as starting points for a broader overview of the subject. EM-like algorithms for HMM’s were introduced in [4, 3, 2, 24]. The EM family of algorithms was introduced in great generality in [9]; work on HMM’s also appears in the econometrics [13, 23], as well as in the biological [22] literature. These references are merely starting points; the literature is very extensive.

As already mentioned, the EM segmentation algorithm used here is a variation of algorithms which are well-established in the field of speech recognition; for example see [18, 19]. Taking into account the extensive HMM literature, as well as various ideas reported in the hydrological literature, the algorithm of Section 3.2.4 can be extended in several directions.

1. The assumption that the observations are normally distributed is not essential. Other forms of probability density can be used in (10). Similarly, by a simple modification of (10) the algorithm can handle vector valued observations.

2. A basic idea of the algorithm is that each segment must be homogeneous. Assuming that the observations within a segment are generated independently and normally, segment homogeneity is evaluated by the deviation of $x_{t_k-1+1}, x_{t_k-1+2}, \ldots, x_{t_k}$ from the segment mean $\bar{x}_k$. But alternative assumptions can be used. For example, assume that the observations are generated by an autoregressive mechanism, i.e. that, for $t = t_{k-1} + 1, t_{k-1} + 2, \ldots, t_k$ and $k = 1, 2, \ldots, K$, we have

$$x_t = a_{0,k} + a_{1,k}x_{t-1} + a_{2,k}x_{t-2} + \ldots + a_{l,k}x_{t-l} + \epsilon_t$$  \hspace{1cm} (28)

(where $\epsilon_t$ is a white noise term). The segmentation algorithm can be used within this framework. In this case the reestimation phase computes the AR coefficients $a_{1,k}, a_{2,k}, \ldots, a_{l,k}$, which can be estimated from $x_{t_{k-1}+1}, x_{t_{k-1}+2}, \ldots, x_{t_k}$ using a least squares fitting algorithm. This approach is used in Section 4.3 to fit a HMM autoregressive model to global temperature data.

3. Similarly, it may be assumed that the observations are generated by a polynomial regression of the form (for $t = t_{k-1} + 1, t_{k-1} + 2, \ldots, t_k$ and $k = 1, 2, \ldots, K$)

$$x_t = a_{0,k} + a_{1,k} \cdot (t - t_{k-1}) + \ldots + a_{l,k} \cdot (t - t_{k-1})^l + \epsilon_t$$  \hspace{1cm} (29)

where $\epsilon_t$ is a noise term. Again, the coefficients $a_{0,k}, a_{1,k}, \ldots, a_{l,k}$ can be computed at every reestimation phase by a least squares fitting algorithm. Additional constraints can be used to enforce continuity across segments. In the case of 1st order polynomials there are only two coefficients, $a_{0,k}, a_{1,k}$, which are determined by the continuity assumptions; the iterative reestimation of the change points can still be performed. This case may be of interest for detection of trends.
4. It has been mentioned in Section 3.2.1 that $P$ can also be reestimated in every iteration of the EM algorithm. Preserving the left-to-right structure implies that for $k = 1, 2, ..., K$ and for all $j$ different from $k$ and $k + 1$, we have $P_{k,j} = 0$; furthermore, for $k = 1, 2, ..., K - 1$ we have $P_{k,k+1} = 1 - P_{k,k}$. The $P_{k,k}$ parameters can be estimated by $\hat{P}_{k,k} = \frac{\sum_{t=1}^{T_k} z_t}{T_k}$. However, some preliminary experiments indicate that this approach does not yield improved segmentations.

5. On the other hand, the treatment of the state transition can be modified in a more substantial manner by dropping the left-to-right assumption. In the current model each state of the Markov chain corresponds to a single segment and, because of the left-to-right structure, it is visited at most once. An alternate approach would be to assign some physical significance to the states. For instance, states could be chosen to correspond to climate regimes such as “dry”, “wet” etc. In this case a state could be visited more than once. This approach allows the choice of models which incorporate expert knowledge about the evolution of climate regimes. On the other hand, if the left-to-right structure is dropped, the number of free parameters in the $P$ matrix increases. These parameters could be estimated (conditional on a particular state sequence) by

$$\hat{P}_{kj} = \frac{\text{no. of times that } z_t = k \text{ and } z_{t+1} = j}{\text{no. of times that } z_t = k}. \tag{30}$$

The enhancements of arbitrary transition structure and transition probability estimation are easily accommodated by our algorithm.

4 Experiments

In this section we evaluate the segmentation algorithm by numerical experiments. The first experiment involves an annual river discharge time series which contains 86 points. The second example involves the reconstructed annual mean global temperature time series and contains 282 points. Both of these examples involve segmentation by minimization of total deviation from segment means. The third example again involves the annual mean global temperature time series, but performs segmentation by minimization of autoregressive prediction error. The fourth example involves artificially generated time series with up to 1500 points.

4.1 Annual Discharge of the Senegal River

In this experiment we use the time series of the Senegal river annual discharge data, measured at the Bakel station for the years 1903-1988. The length of the time series is 86. The same data set has been used by Hubert [16, 17]. The goal is to find the segmentation which is optimal with respect to total deviation from the segment means, has the highest possible order and is statistically significant according to Scheffe’s criterion.

We run the segmentation algorithm for increasing values of $K$. In the experiments reported here we have always used $p = 0.9$ (similar results are obtained for other values of $p$ in the interval $[0.85, 0.95]$. For every value of $K$, convergence is achieved by the 3rd or 4th iteration of the algorithm. The optimal segmentations are presented in Table 1. The segmentations which were validated by the Scheffe criterion appear in bold letters.
Hence it can be seen that the optimal and statistically significant segmentation is that of order 5, i.e. the segments are [1903,1921], [1922,1936], [1937,1949], [1950,1967], [1967,1988]. That this is the globally optimal segmentation, has been shown by Hubert in [16, 17] using his exact segmentation procedure. A plot of the time series, indicating the 5 segments and the respective means appears in Figure 2.

Figure 2 to appear here

We have verified that the HMM algorithm finds the globally optimal segmentation for all values of $K$ (as listed in Table 1). We performed this verification by use of the exact dynamic programming algorithm presented in the Appendix. The conclusion is that, in this experiment, the HMM segmentation algorithm finds the optimal segmentations considerably faster than the exact algorithm. Specifically, running the entire experiment (i.e. obtaining the HMM segmentations of all orders) with a MATLAB implementation of the HMM segmentation algorithm took 1.1 second on a Pentium III 1 GHz personal computer; we expect that a FORTRAN or C implementation would take about 10% to 20% of this time.

4.2 Annual Mean Global Temperature

In this experiment we use the time series of annual mean global temperature for the years 1700 – 1981. Only the temperatures for the period 1902 – 1981 come from actual measurements; the remaining temperatures were reconstructed according to a procedure described in [26] and also at the Internet address http://www.ngdc.noaa.gov/paleo/ea/eaintro.html. The length of the time series is 282. The goal is again to find the segmentation which is optimal with respect to total deviation from the segment-means, has the highest possible order and is statistically significant according to Scheffe’s criterion.

We run the segmentation algorithm for $K = 2, 3, ..., 6$, using $p = 0.9$. Convergence takes place in 4 iterations or less. The optimal segmentations are presented in Table 2. The segmentations which were validated by Scheffe’s criterion appear in bold letters.

| $K$ | Segment Boundaries (Change Points) |
|-----|-----------------------------------|
| 1   | 1700 1981                         |
| 2   | 1700 1930 1981                    |
| 3   | 1700 1812 1930 1981               |
| 4   | 1700 1720 1812 1930 1981          |
| 5   | 1700 1720 1812 1926 1935 1981     |
| 6   | 1700 1720 1812 1926 1934 1977 1981|

Table 2
Hence it can be seen that the optimal and statistically significant segmentation is of order 4, i.e. the segments are [1700,1720], [1721,1812], [1813,1930], [1931,1981]. A plot of the time series, indicating the 4 segments and the respective means appears in Figure 3.

The total execution time for the experiment (i.e. to obtain optimal segmentations of all orders) is 2.97 sec. The segmentations of Table 2 are the globally optimal ones, as we have verified using the dynamic programming segmentation algorithm.

4.3 Annual Mean Global Temperature with AR model

In this experiment we again use the annual mean global temperature time series, but now we assume that it is generated by a switching regression HMM. Specifically, we assume a model of the form

\[ x_t = a_{0,k} + a_{1,k}x_{t-1} + a_{2,k}x_{t-2} + a_{3,k}x_{t-3} + \epsilon_t \]  

(31)

where the parameters \(a_{0,k}, a_{1,k}, a_{2,k}, a_{3,k}\) are specific to the \(k\)-th state of the underlying Markovian process. Given a particular segmentation, these parameters can be estimated by a least squares fitting algorithm. Hence the segmentation algorithm can be modified to obtain the optimal segmentation with respect to the model of (31).

Once again we run the segmentation algorithm for \(K = 2, 3, ..., 6\), using \(p = 0.9\). The optimal segmentations thus obtained are presented in Table 3.

| \(K\) | Segment Boundaries (Change Points) |
|------|-------------------------------------|
| 1    | 1700 1981                           |
| 2    | 1700 1926 1981                      |
| 3    | 1700 1833 1926 1981                 |
| 4    | 1700 1769 1833 1926 1981            |
| 5    | 1700 1769 1833 1895 1926 1981       |
| 6    | 1700 1769 1825 1877 1904 1926 1981  |

Table 3

In this case segment validation is not performed by the Scheffé criterion; instead we use a prediction error correlation criterion. This indicates the maximum statistically significant number of segments is \(K=4\) and the segments are [1700,1769], [1770,1833], [1834,1926], [1927,1981]. A plot of the time series, indicating the 4 segments and the respective autoregressions appears in Figure 3.

Recall that the segments obtained by means-based segmentation are [1700,1720], [1721, 1812], [1813, 1930], [1931, 1981]. This seems to be in reasonable agreement with the AR-based segmentation, excepting the discrepancy of 1720 and 1769. From a numerical point of view, there is no a priori reason to expect that the AR-based segmentation and means-based segmentation should give the same results. The fact that the two segmentations are in reasonable agreement, supports the hypothesis that actual climate changes have occurred approximately at the transition times indicated by both segmentation methods.

Finally, let us note that the total execution time for the experiment (i.e. to obtain optimal segmentations of every order) is 3.07 sec and that the segmentations of Table 3 are the globally optimal ones, as we have verified using the dynamic programming segmentation algorithm.
4.4 Artificial Time Series

The goal of the final experiment is to investigate the scaling properties of the algorithm, specifically the scaling of execution time with respect to time series length $T$ and the scaling of accuracy with respect to noise in the observations. To obtain better control over these factors, artificial time series are used, which have been generated by the following mechanism.

The time series are generated by a 5-th order HMM. Every time series is generated by running the HMM from state no.1 until state no.5. Hence, every time series involves 5 state transitions and, for the purposes of this experiment, this is assumed to be known a priori. On the other hand, it can be seen that the length of the time series is variable. With a slight change of notation, in this section $T$ will denote the expected length of the time series, which can be controlled by choice of the probability $p$. The values of $p$ were chosen to generate time series of average lengths 200, 250, 500, 750, 1000, 1250, 1500.

The observations are generated by a normal distribution with mean $\mu_k$ ($k=1, 2, ..., 5$) and standard deviation $\sigma$. In all experiments the values $\mu_1=\mu_3=\mu_5=1, \mu_2=\mu_4=-1$ were used. Several values of $\sigma$ were used, namely $\sigma=0.00, 0.10, 0.20, 0.30, 0.50, 0.75, 1.00, 1.25, 1.50, 1.75, 2.00$.

For each combination of $T$ and $\sigma$, 20 time series were generated and the HMM segmentation algorithm was run on each one. For each run two quantities were computed: $c$, accuracy of segmentation, and $T_e$, execution time. Segmentation accuracy is computed by the formula

$$c = \frac{\sum_{t=1}^{T} 1(z_t = \hat{z}_t)}{T}$$

where the indicator function $1(z_t = \hat{z}_t)$ is equal to 1 when $z_t = \hat{z}_t$ and equal to 0 otherwise.

From these data two tables are compiled. Table 4 lists $T_e$ (in seconds) as a function of $T$ (i.e. $T_e$ is averaged over all time series of the same $T$). Table 5 lists average segmentation accuracy $c$ as a function of $T$ and $\sigma$ (i.e. $c$ is averaged over the 20 time series with the same $T$ and $\sigma$). As expected, segmentation accuracy is generally a decreasing function of $\sigma$.

| $T$ | 200 | 250 | 500 | 750 | 1000 | 1250 | 1500 |
|-----|-----|-----|-----|-----|------|------|------|
| $T_e$ | 0.193 | 0.249 | 0.585 | 1.024 | 1.845 | 3.026 | 4.60 |

Table 4. Average execution time $T_e$ (in seconds) as a function of average time series length $T$.

| $T$ | 200 | 250 | 500 | 750 | 1000 | 1250 | 1500 |
|-----|-----|-----|-----|-----|------|------|------|
| $\sigma$ | c |
| 0.00 | 1.0000 | 1.0000 | 1.0000 | 0.9692 | 1.0000 | 1.0000 | 0.9902 |
| 0.10 | 1.0000 | 1.0000 | 1.0000 | 0.9814 | 1.0000 | 1.0000 | 1.0000 |
| 0.20 | 1.0000 | 0.9806 | 1.0000 | 1.0000 | 1.0000 | 0.9716 | 1.0000 |
| 0.30 | 1.0000 | 1.0000 | 0.9999 | 0.9792 | 1.0000 | 0.9807 | 1.0000 |
| 0.50 | 0.9989 | 0.9993 | 0.9994 | 0.9976 | 1.0000 | 0.9977 | 1.0000 |
| 0.75 | 0.9945 | 0.9979 | 0.9663 | 0.9521 | 0.9988 | 0.9992 | 0.9991 |
| 1.00 | 0.9881 | 0.9880 | 0.9863 | 0.9974 | 0.9517 | 0.9981 | 0.9711 |
| 1.25 | 0.9778 | 0.9710 | 0.9762 | 0.9924 | 0.9965 | 0.9843 | 0.9781 |
| 1.50 | 0.9561 | 0.9701 | 0.9874 | 0.9341 | 0.9507 | 0.9362 | 0.9956 |
| 1.75 | 0.9337 | 0.8985 | 0.9494 | 0.9341 | 0.9708 | 0.9272 | 0.9942 |
| 2.00 | 0.8628 | 0.8617 | 0.8255 | 0.9141 | 0.8600 | 0.9523 | 0.8297 |

Table 5. Average classif. accuracy $c$ as a function of average time series length $T$ and noise level $\sigma$.  

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5 Conclusion

In this paper we have used hidden Markov models to represent hydrological and enviromental time series with multiple change points. Inspired by Hubert’s pioneering work and by methods of speech recognition, we have presented a fast iterative segmentation algorithm which belongs to the EM family. The quality of a particular segmentation is evaluated by the deviation from segment means, but extensions involving autoregressive HMM’s, trend-generating HMM’s etc. can also be used. Because execution time is \(O(T \cdot K^2)\), our algorithm can be used to explore various possible segmentations in an interactive manner. We have presented a convergence analysis which shows that under appropriate conditions every iteration of our algorithm increases the likelihood of the resulting segmentation. Furthermore, numerical experiments (involving river flow and global temperature time series) indicate that the algorithm can be expected to converge to the globally optimal segmentation.

A Appendix: A Dynamic Programming Segmentation Algorithm

In this appendix we present an alternative time series segmentation algorithm which, unlike the HMM algorithm, is guaranteed to produce the globally optimal segmentation of a time series. This superior performance, however, is obtained at the price of longer execution time. Still, the algorithm is computationally viable for time series of several hundred terms. We describe the algorithm briefly here; a more detailed report appears in [20].

A.1 A General Segmentation Cost

A generalization of the time series segmentation problem discussed in previous sections is the following. Given a time series \(x = (x_1, x_2, \ldots, x_T)\) and a fixed \(K\), find a sequence of times \(t = (t_0, t_1, \ldots, t_K)\) which satisfies \(0 = t_0 < t_1 < \ldots < t_{K-1} < t_K = T\), and minimizes

\[
J_K(t) = \sum_{k=1}^{K} f_k(t_{k-1}, t_k; x).
\]  

(32)

\(J_K(t)\) consists of a sum of terms \(f_k(t_{k-1}, t_k; x)\). For example, Hubert’s cost function can be obtained by setting

\[f_K(s, t; x) = \sum_{\tau=s+1}^{t} \left( x_{\tau} - \frac{\sum_{\tau=s+1}^{t} x_{\tau}}{t-s} \right)^2.\]

(33)

Hence Hubert’s segmentation cost (3) is a special case of (32).

Similarly, consider autoregressive models of the form

\[x_t = u_t A_k + \epsilon_t,\]

(34)

where \(t = t_{k-1} + 1, t_{k-1} + 2, \ldots, t_k\) and \(u_t = [1, x_{t-1}, x_{t-2}, \ldots, x_{t-l}]\), \(A_k = [a_{k,1}, a_{k,2}, \ldots, a_{k,l}]^T\) (the superscript \(T\) denotes transpose of a matrix). Then we can set

\[
f_K(s, t; x) = \sum_{\tau=s+1}^{t} (x_{\tau} - u_\tau A_k)^2.
\]

(35)
Then the segmentation cost becomes

$$J_K(t) = \sum_{\tau=s}^{t} \epsilon_{\tau}^2 = \sum_{k=1}^{K} \sum_{t=t_{k-1}+1}^{t_k} (x_t - u_t A_k)^2 .$$

(36)

The \(a_{k,1}, a_{k,2}, \ldots, a_{k,l}\) (elements of \(A_k\)) are unknown, but can be determined by least squares fitting on \(x_{t_{k-1}+1}, x_{t_{k-1}+2}, \ldots, x_{t_k}\). A similar formulation can be used for regressive models of the form \(x_t = u_t A_k + \epsilon_t\) where \(A_k = [a_{k,0}, a_{k,1}, \ldots, a_{k,l}]^t\), \(u_t = [1, (t - t_{k-1}), (t - t_{k-1})^2, \ldots, (t - t_{k-1})^l]\). Hence we see that (32) is sufficiently general to subsume many cost functions of practical interest.

### A.2 Dynamic Programming Segmentation Algorithm

The following dynamic programming algorithm can be used to minimize (32); it has been presented in [1] and applies to very general versions of the time series segmentation problem.

---

**Dynamic Programming Segmentation Algorithm**

**Input:** The time series \(x = (x_1, x_2, \ldots, x_T)\); a termination number \(K\).

**Initialization**

For \(t = 1, 2, \ldots, T\)

For \(s = 1, 2, \ldots, t\)

\[d_{s,t} = f_K(s - 1, t; x)\]

End

\(c_{t,0} = d_{1,t}\)

End

**Minimization**

For \(k = 1, 2, \ldots, K\)

For \(t = k, k+1, \ldots, T\)

For \(s = 0, 1, \ldots, t - 1\)

\[e_s = c_{s,k-1} + d_{s+1,t}\]

End

\(c_{t,k} = \min_{1 \leq s \leq t} (e_s)\)

\(z_{t,k} = \arg \min_{1 \leq s \leq t} (e_s)\)

End

End

**Backtracking**

For \(k = 1, 2, \ldots, K\)
\( \hat{t}_{k,k} = T \)
For \( n = k - 1, k - 2, \ldots, 1 \)
\( \hat{t}_{n,k} = z_{\hat{t}_{n+1,k},n} \)
End
\( \hat{t}_{0,k} = 0 \)
End

On termination, the dynamic programming segmentation algorithm has computed

\[
c_{T,k} = \min_{t=(t_0,t_1,\ldots,t_k)} J_k(t) \quad (37)
\]

for \( k = 1, 2, \ldots, K \); in other words it has recursively solved a sequence of minimization problems. For \( k = 1, 2, \ldots, K \), the optimal segmentation \( \hat{t}_k = (t_{0,k}, t_{1,k}, \ldots, t_{k,k}) \) has been obtained by backtracking.

The recursive minimization is performed in the second part of the algorithm; it is seen that computation time is \( O(K \cdot T^2) \). This is not as good as the \( O(K^2 \cdot T) \) obtained by the HMM algorithm (note that usually \( K \) is significantly less than \( T \), but is still computationally viable for \( T \) in the order of a few hundreds. The backtracking part of the algorithm has execution time \( O(K^2) \).

However, in many cases the computationally most expensive part of the algorithm is the initialization phase, i.e. the computation of \( d_{s,t} \). This involves \( O(T^2) \) computations of \( d_{s,t} = f_K(s-1,t;x) \) and can increase the computation cost by one or more orders of magnitude. For example, if we apply the algorithm to detect changes in the mean, then

\[
d_{s,t} = f_K(s-1,t;x) = \sum_{\tau=s}^t \left( x_{\tau} - \frac{\sum_{\tau=s}^t x_{\tau}}{t-s+1} \right)^2 \quad (38)
\]

which involves \( t - s + 1 \) additions; if (38) is used in the initialization phase, then this phase requires \( O(T^3) \) computations and this severely limits computational viability to relatively short time series.

Hence, to enhance the computational viability of the dynamic programming segmentation algorithm, it is necessary to find efficient ways to perform the initialization phase. In the next two sections, we will deal with this question for two specific forms of \( f_K(s,t;x) \): the first form pertains to the computation of means and the second to the computation of regressions and autoregressions.

A.3 Fast Computation of Means

The computation of means can be performed recursively, as will now be shown. For \( t = 1, 2, \ldots, T \), \( s = 1, 2, \ldots, t-1 \), we must compute

\[
M_{s,t} = \sum_{\tau=s}^t x_{\tau}, \quad d_{s,t} = f_K(s-1,t;x) = \sum_{\tau=s}^t \left( x_{\tau} - \frac{M_{s,t}}{t-s+1} \right)^2. \quad (39)
\]

For \( t = 1, 2, \ldots, T \), \( s = 1, 2, \ldots, t \), define the following additional quantities:

\[
p_{s,t} = \frac{\sum_{\tau=s}^t x_{\tau}}{\sum_{\tau=s}^1 1}, \quad q_{s,t} = p_{s+1,t} - p_{s,t}. \quad (40)
\]
Then we have

\[ d_{s,t} = \sum_{\tau=s}^{t} (x_\tau - p_{s,t})^2 = (x_s - p_{s,t})^2 + \sum_{\tau=s+1}^{t} (x_\tau - p_{s,t})^2 \]  \hspace{1cm} (41)

and

\[ \sum_{\tau=s+1}^{t} (x_\tau - p_{s,t})^2 = \sum_{\tau=s+1}^{t} (x_\tau - p_{s+1,t} - p_{s+1,t} - p_{s,t})^2 \]
\[ = \sum_{\tau=s+1}^{t} (x_\tau - p_{s+1,t})^2 + \sum_{\tau=s+1}^{t} (p_{s+1,t} - p_{s,t})^2 + 2 \cdot \sum_{\tau=s+1}^{t} (x_\tau - p_{s+1,t})(p_{s+1,t} - p_{s,t}) \]
\[ = d_{s+1,t} + (t - s) \cdot (q_{s,t})^2 + 2 \cdot (p_{s+1,t} - p_{s,t}) \cdot \left( \sum_{\tau=s+1}^{t} x_\tau - (t - s)p_{s+1,t} \right) \Rightarrow \]
\[ \sum_{\tau=s+1}^{t} (x_\tau - p_{s,t})^2 = d_{s+1,t} + (t - s) \cdot (q_{s,t})^2 \]  \hspace{1cm} (42)

From (41), (42) follows that (for \(t = 1, 2, ..., T\), \(s = 1, 2, ..., t - 1\))

\[ d_{s,t} = d_{s+1,t} + (t - s) \cdot (q_{s,t})^2 + (x_s - p_{s,t})^2. \]  \hspace{1cm} (43)

The above computations can be implemented in time \(O(T^2)\) by the following algorithm.

---

**Recursive Computation of \(d_{s,t}\)**

For \(t = 1, 2, ..., T\)

\[ M_{t,t} = x_t \]
\[ p_{t,t} = M_{t,t} \]

For \(s = t - 1, t - 2, ..., 1\)

\[ M_{s,t} = x_s + M_{s+1,t} \]
\[ p_{s,t} = \frac{M_{s,t}}{t-s+1} \]

End

End

For \(t = 1, 2, ..., T\)

For \(s = 1, 2, ..., t - 1\)

\[ q_{s,t} = (p_{s+1,t} - p_{s,t}) \]

End

End

For \(t = 1, 2, ..., T\)
\[ d_{t,t} = 0 \]

For \( s = t - 1, t-2, ..., 1 \)
\[ d_{s,t} = d_{s+1,t} + (t-s) \cdot (q_{s,t})^2 + (x_s - p_{s,t})^2. \]

End

End

Hence, if the above code replaces the initialization phase of the dynamic programming algorithm in Section A.2, we obtain an \( O(K \cdot T^2) \) implementation of the entire algorithm. In other words, we obtain an algorithm which, given a time series of length \( T \), computes the global minimum of Hubert’s segmentation cost (for all segmentations of orders \( K = 1, 2, 3, ..., T \)) in time \( O(K \cdot T^2) \).

### A.4 Fast Computation of Regression Coefficients

Consider now autoregressive models described by (34). As already mentioned, in this case we have
\[ f_k(t_{k-1}, t_k; x) = \sum_{t=t_{k-1}+1}^{t_k} (x_t - u_t A_k)^2. \] (44)

Hence \( d_{s,t} = f_k(s-1, t; x) \) is given by
\[ d_{s,t} = \sum_{\tau=s}^{t} (x_\tau - u_\tau A(s,t))^2. \] (45)

where \( u_t = [1, x_{t-1}, x_{t-2}, ..., x_{t-l}] \) and \( A(s,t) \) is obtained by solving the least squares equation
\[ A(s,t) = (U(s,t)' \cdot U(s,t))^{-1} \cdot U(s,t)' \cdot X(s,t) \] (46)

with
\[ X(s,t) = \begin{bmatrix} x_s \\ x_{s+1} \\ ... \\ x_t \end{bmatrix} \quad \text{and} \quad U(s,t) = \begin{bmatrix} u_s \\ u_{s+1} \\ ... \\ u_t \end{bmatrix}. \] (47)

Note that to solve (46) the matrix multiplications \( U(s,t)' \cdot U(s,t), U(s,t)' \cdot X(s,t) \) must be performed. For \( t = 1, 2, ..., T, s = 1, 2, ..., t \), these multiplications require \( O(T^5) \) time. However, the solution of (46) can be approximated by a fast recursive algorithm reported in [12]. Choose some small number \( \delta \) and set
\[ P_0 = \frac{1}{\delta} \cdot I \] (48)

(\( I \) is the \((l+1) \times (l+1)\) unit matrix). Then, consider the following recursion for \( s = 1, 2, ..., T \) and \( t = s + 1, ..., T \):
\[ u_t = [1, x_{t-1}, x_{t-2}, ..., x_{t-l}], \] (49)
\[ n = t - s, \] (50)
\[ P_n = P_{n-1} - P_{n-1} \cdot u_t' \cdot u_t \cdot \frac{1}{1 + u_t \cdot P_{n-1} \cdot u_t'}, \] (51)
\[ \hat{A}(s,t) = \hat{A}(s,t-1) + P_n \cdot u_t' \cdot \left( x_t - u_t \cdot \hat{A}(s,t-1) \right). \] (52)
Using the arguments of [12] for a fixed $s$ and increasing $t$ it can be shown that $\hat{A}(s, t)$ converges very quickly to $A(s, t)$, the true solution of (46). Furthermore, the computations of (49)-(52) can be implemented in time $O(T^2)$. Hence, for the case of autoregressive models, the $d_{s,t}$ computation can be programmed as follows.

**Recursive Computation of $d_{s,t}$**

For $s = 1, 2, ..., T$

\[ P_0 = \frac{1}{\delta} \cdot I \]

Initialize $\hat{A}(s, s)$ randomly

\[ d_{s,s} = 0 \]

For $t = s + 1, s + 2, ..., T$

\[ u_t = [1, x_{t-1}, x_{t-2}, ..., x_{t-l}] \]

\[ n = t - s \]

\[ P_n = P_{n-1} - P_{n-1} \cdot u_t' \cdot u_t \cdot P_{n-1} \cdot \frac{1}{1+u_t' \cdot P_{n-1} \cdot u_t'} \]

\[ \hat{A}(s, t) = \hat{A}(s, t - 1) + P_n \cdot u_t' \cdot \left( x_t - u_t \cdot \hat{A}(s, t - 1) \right) \]

\[ d_{s,t} = d_{s,t-1} + \left( x_t - u_t \cdot \hat{A}(s, t) \right)^2 \]

End

End

Hence, if the above code replaces the initialization phase of the dynamic programming segmentation algorithm in Section A.2, we have an $O(K \cdot T^2)$ implementation of the entire algorithm for autoregressive models. A similar modification is possible for regressive models of the form (34).

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Figure 1. A diagrammatic representation of a hidden Markov model.

Figure 2. Plot of the Senegal river annual discharge and the segment means. This figure was obtained from the optimal 5-th order segmentation.

Figure 3. Plot of the annual mean global temperature and the segment means. This figure corresponds to the optimal fourth order segmentation.
Figure 4. Plot of the annual mean global temperature and the AR estimate. This figure corresponds to the optimal fourth order segmentation.