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Remote detection of water property changes from a time series of oceanographic data

A. Henry-Edwards and M. Tomczak

School of Chemistry Physics and Earth Sciences, Flinders University of South Australia, Australia

Abstract. A water mass analysis method based on a constrained minimization technique is developed to derive water property changes in water mass formation regions from oceanographic station data taken at significant distance from the formation regions. The method is tested with two synthetic data sets, designed to mirror conditions in the North Atlantic at the Bermuda BATS time series station.

The method requires careful definition of constraints before it produces reliable results. It is shown that an analysis of the error fields under different constraint assumptions can identify which properties vary most over the period of the observations. The method reproduces the synthetic data sets extremely well if all properties other than those that are identified as undergoing significant variations are held constant during the minimization.

1 Introduction

In recent years, the general acceptance of global warming and the importance of long-range weather forecasting for modern agriculture have made climate change and variability an important issue. The interactions of the atmosphere and the ocean are of great importance for climate research, and many countries have made these processes a primary focus of their research programs. This has led to increased recognition of the role of the oceanic circulation for climate research and of water masses as elements of climate stability.

Within the broader category of climate research there are two major types of change to be investigated. Climate variability takes place over time scales of months, years or decades and is largely affected by year to year changes in oceanographic water mass formation. Climate change occurs over longer time periods of centuries or thousands of years. Prior to the 1980s, most climate research largely ignored both of these variations to instead focus on the mean climate, gaining an understanding of how the ocean and atmosphere interact, with little consideration of temporal variability.

With increasingly powerful computers becoming available to oceanographers a large number of climate and ocean models have been developed, often on global scales. One of the key problems facing modellers is the accurate representation of water mass formation (England and Maier-Reimer, 2001). To this end, numerous tracers have been incorporated into ocean models, either for data assimilation studies, model validation or as part of studies into the oceanic carbon cycle. Water masses integrate changes taking place in the surface flux in ocean and climate models. This makes them attractive tools for the detection of climate change in a climate model (Banks et al., 2002).

Many water masses are formed in sub-polar regions, where continuous monitoring of air and sea properties can be both expensive and hazardous. This is especially the case during the winter months when most of the water mass formation occurs. As a result of this, the properties of some water masses are only poorly understood. A greater understanding of the production of these water masses over long time periods and changes in their properties is therefore of great interest to climate researchers.

After the second world war a series of weather ships were deployed across the Atlantic and Pacific to provide time series of atmospheric measurements for weather forecasts. Many of these ships also collected oceanographic data as standard procedure, leading to some extensive time series of temperature and salinity. With the deployment of weather satellites for the same purpose, many of the weather ships were phased out and the oceanographic time series were stopped.

Increased interest in climate variability has seen a renewed interest in time series of oceanographic data. The Bermuda

Correspondence to: M. Tomczak
(matthias.tomczak@flinders.edu.au)

Table 1. Source water definitions used in the data simulation model. Temperatures are in °C, oxygen and nutrient data in μmol/L.

Water Type	potential temperature	salinity	oxygen	phosphate	nitrate	silicate
simWNACW (upper)*	18.9	36.6	190.0	0.25	6.0	2.0
simWNACW (lower)	9.40	35.1	135.0	1.70	24.0	15.0
simLSW	3.165	34.832	305.0	1.09	16.4	9.1
simISOW	3.060	34.970	280.0	1.12	17.0	14.6

* only used in data set 2.
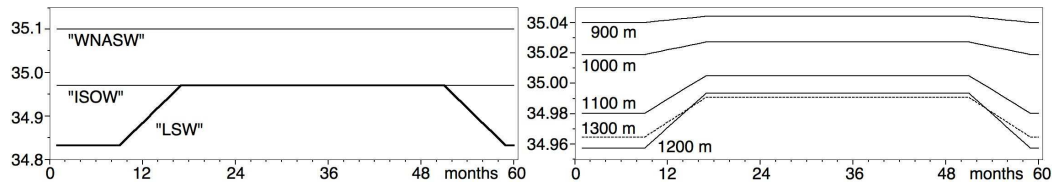
Fig. 1. Simulated data set 1 as a function of time. Left: Salinity of the SWTs; right: salinity at five depth levels.

Atlantic Time-series Study (BATS) from the Sargasso Sea (Michaels and Knap, 1996; Steinberg et al., 2001) and the Hawaii Ocean Time-Series (HOTS) from Hawaii (Karl and Lukas, 1996) are two prominent oceanographic time series, both of which have been running for quite some time collecting high quality monthly data. With the growing availability of these and other time series, it is important to develop methods with which to analyse and utilise the increasing volume of time dependent oceanographic data.

Many existing water mass analysis techniques, in particular Optimum Multi-Parameter (OMP) analysis and isopycnal analysis, assume constant water mass properties and are designed for looking at water mass contributions over a wide area without any temporal variation (Hinrichsen and Tomczak, 1993; Karstensen and Tomczak, 1998; Tomczak and Large, 1989). This approach is valid for analyses of individual cruises or data sets with no time dependence but is not always appropriate when looking at an oceanographic time series. Indeed, one of the primary principles of modern climate research is that oceanographic and atmospheric properties vary with time.

In a recent OMP analysis of the BATS data set in the Sargasso Sea near Bermuda in the North Atlantic, Leffanue and Tomczak (2004) found that the Labrador Sea Water (LSW) signal apparently disappeared from the data set for a number of years, at the same time as an increase in analysis error values was observed. They noticed that by introducing a time dependence of LSW salinity the error values were reduced and the LSW signal remained present throughout the entire time period. They concluded that changes in the weather conditions over the Labrador Sea during water mass formation had resulted in variations in the properties of LSW

which were then propagated throughout the North Atlantic, and which OMP analysis was unable to resolve.

With this in mind, this paper describes the development of a new water mass analysis tool which can be used to identify changes in source water properties as well as water mass contributions from observations of temperature, salinity and other parameters such as oxygen and nutrients. We generate a simple simulated data set for this purpose, in which all source water properties as well as all relative contributions are prescribed and thus vary in a known manner. We then apply a technique based on OMP analysis to the data set to test the feasibility of the analysis. We have chosen to call the new technique Time Resolving OMP (TROMP) analysis to indicate its derivation from the original OMP analysis technique. In a companion paper (Henry-Edwards and Tomczak, 2006) we apply the new method to the BATS data and show that it is capable of extracting information on variations of water mass properties in the Labrador Sea from observations taken near Bermuda.

2　Data and method

Two simulated time series of station data were created to test the feasibility of a TROMP analysis. Both reflect conditions in the North Atlantic Ocean but with different degree of closeness to observations. In each data set the water properties P_i for all source water masses were predefined through source water types SWT_i, as were the relative contributions x_i at which the water masses contribute to the simulated time series. These values were then combined using the linear mixing equation to produce the "measured" property values $P_{\mathrm{meas}} = \Sigma x_i P_i$ to generate the time series. A time step of one

month between each simulated time step was used to replicate the monthly observations from the BATS data set. The effects of nutrient remineralisation were not included in these data sets, as they had no impact on the method development.

The first simulated time series used source water properties for three simulated water masses, Western North Atlantic Central Water (simWNACW), Labrador Sea Water (simLSW) and Iceland-Scotland Overflow Water (simISOW). The SWT definitions were taken from Leffanue and Tomczak (2004), and simWNACW was represented as a single SWT through values at the lower end of its distribution range. Time variations in the time series were produced by varying the salinity of Labrador Sea Water to match that of Iceland-Scotland Overflow Water for a period and letting it return to its initial value thereafter. Table 1 gives the SWT definitions at the start of the time series; Fig. 1 shows the time development.

The second data set was based on more realistic variations of simLSW temperature and salinity. It prescribed the same time-invariable oxygen and nutrient SWTs, included an upper definition for simWNACW, and simulated time variations of temperature as well as salinity, following the observations from the Labrador Sea described by Dickson et al. (1996).

Optimum Multi-Parameter (OMP) analysis was first introduced in Tomczak (1981) as an extension of the temperature-salinity mixing triangle of Helland- Hansen (1918). We refer the reader to available descriptions for full details of the OMP analysis procedure (for example Karstensen and Tomczak, 1998) and restrict ourselves to a brief summary, as TROMP analysis is based on OMP analysis. OMP analysis solves a system of linear mixing equations to identify the relative contributions of a number of SWTs in a given data set. In an analysis of a data set in which four SWTs are present and measurements for salinity (S), potential temperature (Θ), oxygen (O), nitrate (N), phosphate (P) and silicate (Si) are used as tracers, the system of equations would take the form:

$$
\begin{aligned}
\Theta_1 x_1 + \Theta_2 x_2 + \Theta_3 x_3 + \Theta_4 x_4 &= \Theta_{obs} + R_\Theta \\
S_1 x_1 + S_2 x_2 + S_3 x_3 + S_4 x_4 &= S_{obs} + R_S \\
O_1 x_1 + O_2 x_2 + O_3 x_3 + O_4 x_4 - \alpha r_O &= O_{obs} + R_O \\
N_1 x_1 + N_2 x_2 + N_3 x_3 + N_4 x_4 + \alpha r_N &= N_{obs} + R_N \\
P_1 x_1 + P_2 x_2 + P_3 x_3 + P_4 x_4 + \alpha r_P &= P_{obs} + R_P \\
Si_1 x_1 + Si_2 x_2 + Si_3 x_3 + Si_4 x_4 + \alpha r_{Si} &= Si_{obs} + R_{Si} \\
x_1 + x_2 + x_3 + x_4 &= 1 + R_\Sigma
\end{aligned}
$$

Here x_i are the relative contributions from each SWT in the observed property distribution, α is the amount of remineralised material in the water sample, $r_{nutrient}$ are the Redfield ratios (Redfield et al., 1963; not used for the simulated data) and R are the residuals that are minimised to solve the equation. The last line of the equation is the mass constraint function to ensure that the sum of water type contributions adds up to 100%. To make water properties commensurable all variables are non-dimensionalised by dividing through the difference between the largest and smallest SWT in each row.

In the minimisation, a non-dimensional weighting function W is added and the equation is re-arranged to take the form:

$$
R = W \times (\mathbf{A}x - b)
$$

where R is the residual, $\mathbf{A}$ is the matrix of SWTs, x is the vector of relative contributions and b is the vector of measured water properties. A non-negativity constraint is introduced to avoid negative water mass contributions. By ensuring the number of water properties exceed the number of SWTs in the analysis, the minimisation becomes an over-determined problem and is solved in a straightforward manner.

Time Resolving Optimum Multi-Parameter (TROMP) analysis was designed to identify changes in source water properties from the mixing analysis of a time series of data. TROMP analysis solves a similar system of equations to OMP. The main difference is that a TROMP analysis varies the source water properties as well as the relative contributions.

The inclusion of source water properties as variables in the analysis means that the minimisation function becomes nonlinear and highly under-determined. Such systems have an infinite set of solutions, and it is necessary to impose additional constraints upon the minimisation in order to achieve a viable result. The main problem faced during the development of the TROMP method was the identification of suitable minimisation constraints and criteria to establish a procedure that leads to physically realistic and trustworthy results.

The TROMP analysis operates in two alternating stages, which are performed at each time step; the first defines initial values, while the second performs the actual minimisation. Stage 1 uses SWT values from the previous time step to determine the relative contributions of each water mass at the current time step through OMP analysis. Stage 2 takes the relative contributions determined from stage 1 and the SWT values from the previous time step as starting values for a constrained minimisation. Initialisation of the procedure, i.e. definition of SWTs for the first time step, is either based on water type definitions from the literature or found through recourse to data from the water mass formation regions. The SWTs from the second stage are then carried through to the first stage of the following time step, meaning that the SWTs can change smoothly with time.

A sequential quadratic programming method was used in the second stage to calculate relative contributions for each SWT and new definitions for selected SWTs as required. The method solves a quadratic programming sub-program at each iteration and is implemented in the Matlab function fmincon.m, which was used for this project. Fixed variation limits are defined around each SWT and relative contribution.

Sequential Quadratic Programming is generally considered the current state of the art in nonlinear programming methods. It uses an approximation of the Hessian (the square matrix of second partial derivatives) of the Lagrangian function, a process that is most efficiently performed by solving
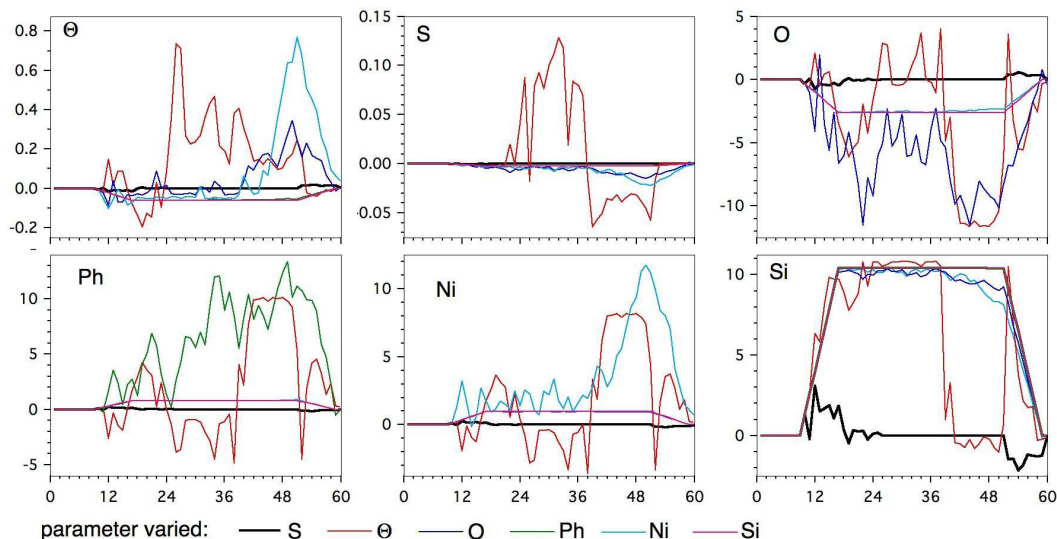
Fig. 2. Time development of the residuals for potential temperature Θ (°C), salinity S, oxygen O (μmol/L), phosphate Ph (μmol/L), nitrate Ni (μmol/L) and silicate Si (μmol/L) at the 1200 m depth level if one source water property is varied in all SWTs. Where curves cannot be seen they are duplicated by curves of another varied property.

the Kuhn-Tucker equations, which express necessary conditions for optimality for a constrained optimization problem. This procedure leads to a quadratic programming problem. The solution to this quadratic sub-problem is then used to form a search direction for a line search procedure, the result of which is used for the next iteration. The method is outlined in more detail in Gill et al. (1981) and Fletcher (1980).

In first attempts to use the TROMP analysis we allowed all source water properties to vary and placed only limits on their range of variation. This proved to be effective for very simple data series with relatively large variations but was not suitable for data sets with more realistic source water variations. Experimentation with a range of constraints and careful evaluation of the error fields led us to define an approach in which TROMP analysis only uses SWTs as variables that can reasonably be expected to have undergone significant variations, while keeping all other SWTs as constants. As we will show, information from the error fields can be used to identify which water type properties have to be set as variables, and which properties can be considered constants.

3   Results and discussion

An essential aspect of any application of a constraint minimisation is the identification of suitable constraints. In an oceanographic context it is rarely obvious from the data which water type variations are the most important contributors to the observed variations of water properties. The first task of a TROMP analysis is therefore the relative ranking of possible variables in terms of their importance to the de-

termination of a solution that comes as close as possible to reality.

An extensive series of trials produced pointers how to proceed. It easily confirmed our expectation that analyses that include all SWTs as variables do not produce sensible results. Reducing the level of complexity only slightly, however, can provide leads on how to proceed: If one source water property is allowed to vary in all SWTs (while all other source water properties are kept constant), the analysis produced a distinct pattern in the error fields. This is clearly seen in the results from our first simulated data set, in which the only source water property that varied was salinity (and this variation was restricted to LSW). Figure 2 shows the residual error for the six properties as functions of time. In most situations the errors vary wildly and at times grow well beyond reasonable bounds, but they become quite small when salinity is allowed to vary in all SWTs (heavy curves in Fig. 2). Notice that this is true for all properties and not just for salinity, although only salinity was allowed to vary. This is a strong indication that the most important change in the source water properties occurred in salinity.

Having identified the most important time-varying property (or properties, ranked in order of importance) it is then possible to proceed with a better targeted TROMP analysis by limiting the number of variables to one or two source water properties for a single SWT. The TROMP algorithm allows us to set limits on the variation of all variables, and the proposed procedure can be implemented by setting extremely narrow (or zero) variation limits for all SWT definitions except the one of interest (in our case simLSW salinity). The results of this approach were satisfactory for our first simulated data set, particularly when the analysis was
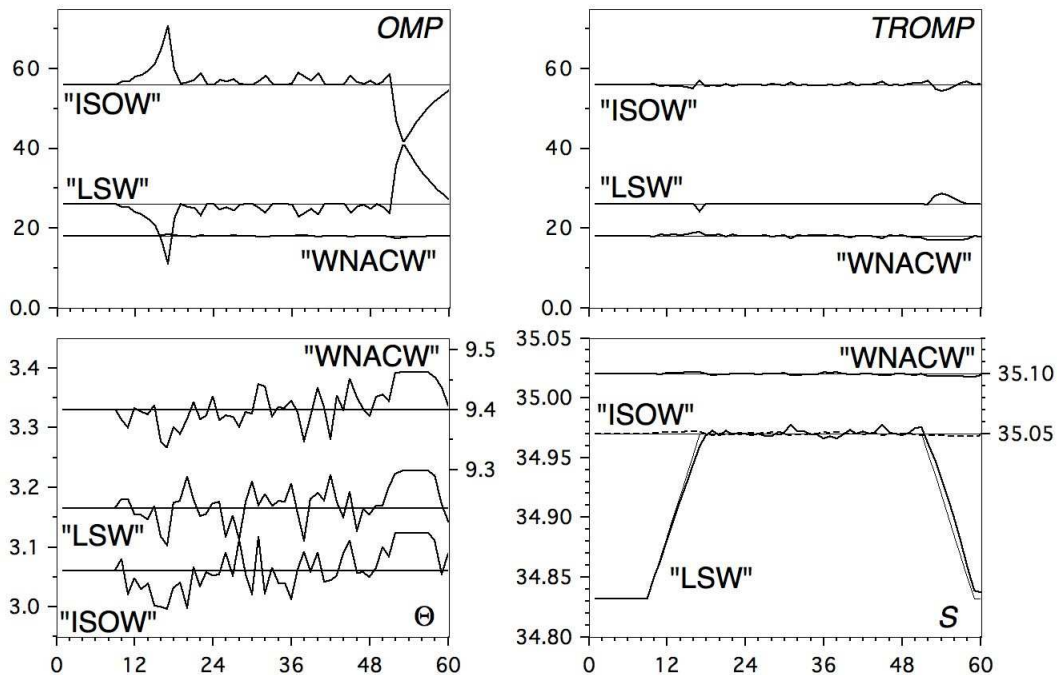
Fig. 3. Results of the analysis of data set 1 for the 1200 m depth level when simLSW salinity is allowed to vary, all other source water properties are handled as variables with near-zero tolerance, and stages 1 and 2 go through 3 iterations at every time step. Relative water mass contributions (%) from the results of stage 1 (OMP analysis, top left) and after three iterations through stages 1 and 2 (TROMP analysis, top right); time development of potential temperature (°C, bottom left) and salinity (bottom right). Thin lines indicate the target values.

implemented in two or more iterations of stages 1 and 2 for every time step. However, the analysis produced not only the correct time evolution of salinity but also apparent variations in potential temperature, a property that was set to remain constant in the simulated data set (Fig. 3).

The problem becomes more acute when the range of SWT variations is small, as in the actual time development of simLSW properties, on which we based our second simulated data set. With the smaller SWT variations it took TROMP analysis longer to converge on a solution and so more iterations were required. In this case, it took five iterations to converge on a result with residuals comparable to those achieved with the first simulated data set. Figure 4 shows the results when TROMP analysis is applied to the second data set in the manner just described. It is seen that the analysis traces the actual evolution of simLSW potential temperature and salinity closely but contains much unrealistic noise. TROMP analysis improves on the first guesses derived from OMP analysis; it reduces the departure from the correct relative contributions and the noise, but the reduction is rather small.

Applying a low-pass filter to the results can of course improve the agreement between our simulated observations and analysis. A better way to improve the result can be obtained by restricting the number of variables in the analysis: When all water type properties that are considered unimportant for

the explanation of the observed property variations are not handled as variables with extremely narrow variation limits but are declared constants, the TROMP analysis is forced to concentrate on the variable of interest and produces excellent agreement between the simulated data and the results from the analysis. Figure 5 shows the result of such procedure. The reduced number of variables leads to a faster and more accurate analysis, with no need for iterations at each time step. This improved method is used in Henry-Edwards and Tomczak (2006).

An important aspect of TROMP analysis is the choice of weights. In OMP analysis, the problem is over-determined and has only one solution. Weights are introduced to take account of the quality of the data and the relative usefulness of the various parameters for the minimization of the residuals (depending on measurement error, degree of environmental variability, and difference in SWT values). In a TROMP analysis, we are solving an under-determined problem that has a multitude of solutions, and the choice of weights can affect the direction of the line search procedure of the constrained optimization. Increasing the weighting of a selected variable skews the minimisation function, so that gradients with respect to that variable are steeper. This can result in a faster analysis, but whether the resulting minimization represents the physically correct solution depends on the closeness of the starting point to the correct solution. Slow evolution
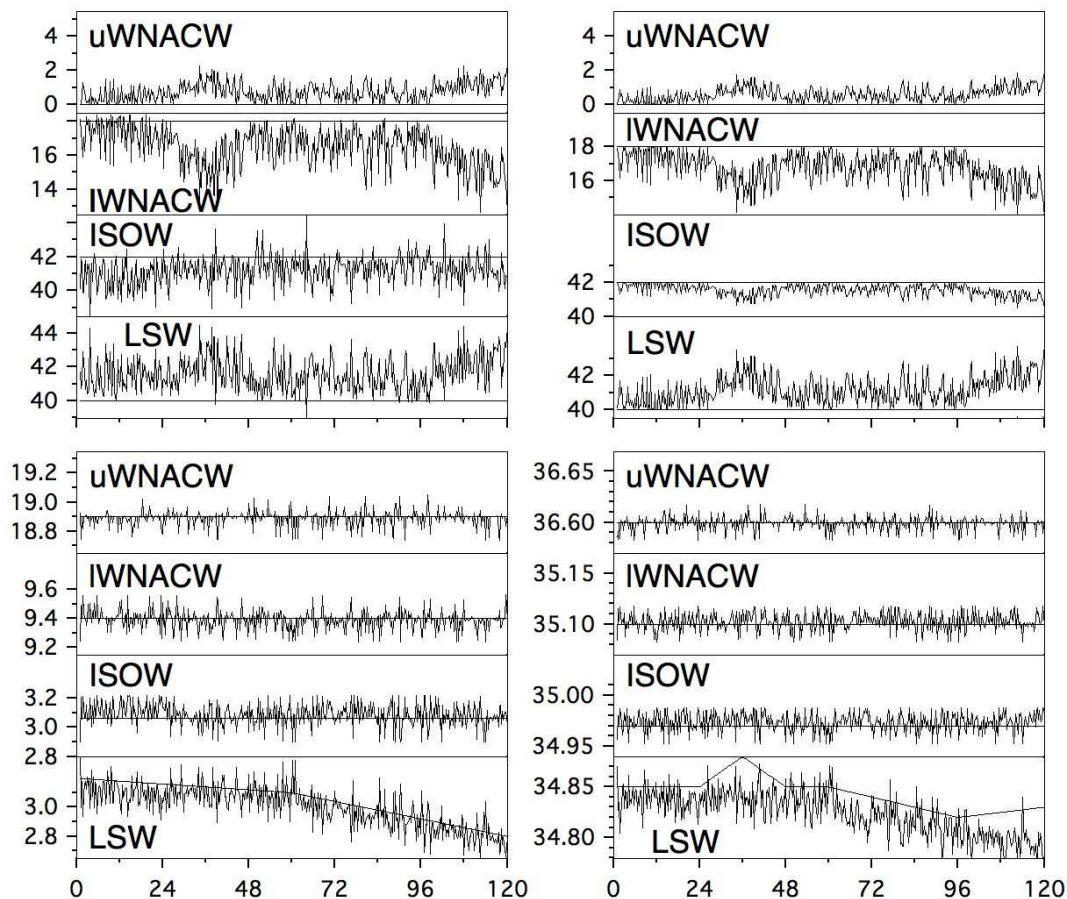
Fig. 4. Results of the analysis of data set 2 for the 1200 m depth level. Variation limits were set to zero for oxygen and nutrients, 3 for LSW temperature and salinity, and 1 for temperature and salinity of all other water masses. Stages 1 and 2 went through 5 iterations at every time step. Relative water mass contributions (%) from the results of stage 1 (OMP analysis, top left) and after five iterations through stages 1 and 2 (TROMP analysis, top right); time development of potential temperature (°C, bottom left) and salinity (bottom right). Thin lines indicate the target values. (At 1200 m the target value for the simulated uWNACW is zero).

of STWs is therefore critical for a successful TROMP analysis. The effect is more obvious when analysing an actual data set and is discussed further in Henry-Edwards and Tomczak (2006).

4   Conclusion

A sequential quadratic programming method named TROMP analysis was applied to two synthetic data sets to simulate an analysis aimed at extracting variations of Labrador Sea Water properties from observations near Bermuda. The results demonstrate the potential effectiveness of the method and a procedure how it can be applied to oceanographic time series without a priori knowledge of time variations in the water mass formation regions. It suggests that when TROMP analysis is applied to field data it should follow a sequence of steps consisting of:

– a series of TROMP analyses in which one source water property is allowed to vary across all SWTs simultaneously, while all other source water properties are kept constant;

– inspection of the resulting error fields and analysis output, to identify source water properties which may be varying during the analysis period;

– a targeted TROMP analysis in which variations are restricted to the source water properties and SWTs identified as likely to change.

In a companion paper (Henry-Edwards and Tomczak, 2006) we follow the above procedure in an application of the TROMP analysis to the BATS data set in the Sargasso Sea.

The choice of weights and the number of iterations required depends on the circumstances and requires both insight into the oceanographic situation and experimentation. Mathematically the issue is the specification of the search
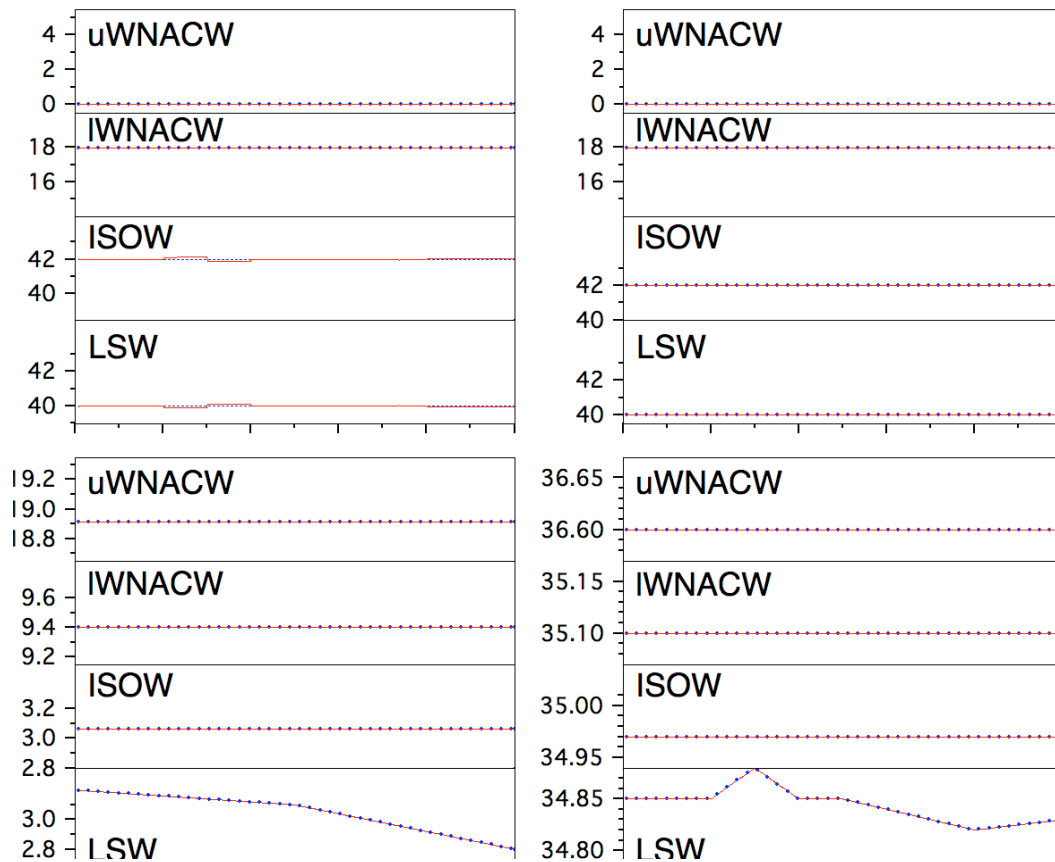
Fig. 5. Results of the analysis of data set 2 for the 1200 m depth level. Oxygen and nutrients were declared constants for all water masses, temperature and salinity for all water masses but the simulated LSW. Temperature and salinity of the simulated LSW were allowed to vary by up to 3% at every time step. Stages 1 and 2 went through 5 iterations at every time step. Relative water mass contributions (%) from the results of stage 1 (OMP analysis, top left) and after five iterations through stages 1 and 2 (TROMP analysis, top right); time development of potential temperature (°C, bottom left) and salinity (bottom right). Red lines indicate calculated values. Dotted blue lines indicate the target values; where the difference between calculated and target values is not resolved in the graph, the target values are indicated by heavy blue dots. (At 1200 m the target value for the simulated uWNACW is zero). Axes are scaled to compare directly with Fig. 4.

direction for the minimization procedure. Experience with different data sets indicates that there may not be a single best recipe to determine the most appropriate weights and iteration sequence. Henry-Edwards and Tomczak (2006) found that in their particular case the weights determined by OMP analysis gave the most physically realistic results. An application to the Southern Ocean (Tomczak and Liefrink, 2006[1]) gave realistic results if the source water properties that were allowed to vary alternated between potential temperature and oxygen for successive iterations. Experience with the method in different oceanographic situations may produce clearer guidelines for the best definition of weights and the most appropriate iteration sequence.

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