## Notes on the function gsw\_stabilise\_SA\_CT (SA,CT,p)

## Stabilisation of hydrographic profiles

## 1. Introduction

The vertical stability of a water column is described by the square of the buoyancy frequency ( $N^2$ ). In this paper we follow the  $N^2$  definition similar to that used in Jackett and McDougall (1995), now defined in terms of the vertical gradients of Absolute Salinity and Conservative Temperature (these being the salinity and temperature variables of TEOS-10, IOC et al. (2010))

$$g^{-2}N^{2} = -\frac{\alpha^{\Theta}}{v} \frac{\partial \Theta}{\partial P}\Big|_{x,y} + \frac{\beta^{\Theta}}{v} \frac{\partial S_{A}}{\partial P}\Big|_{x,y}, \tag{1}$$

where the vertical derivatives are taken at constant latitude and longitude with respect to absolute pressure P. The gravitational acceleration is given the symbol g and v is the specific volume of seawater, being the reciprocal of in situ density  $\rho$ , and the thermal expansion and haline contraction coefficients defined with respect to Absolute Salinity  $S_A$  and Conservative Temperature  $\Theta$  are given by

$$\alpha^{\Theta} = \frac{1}{v} \frac{\partial v}{\partial \Theta} \Big|_{S_{A}, p} \quad \text{and} \quad \beta^{\Theta} = -\frac{1}{v} \frac{\partial v}{\partial S_{A}} \Big|_{\Theta, p}.$$
 (2)

There are many ways to evaluate  $N^2$  and McDougall and Barker (2014) list six of the most commonly used definitions and they show that they are all equivalent. In this paper we will also use the expression for  $N^2$  written in terms of the vertical gradient of in situ temperature, namely

$$g^{-2}N^{2} = -\frac{\alpha^{t}}{v} \left[ \frac{\partial T}{\partial P} \Big|_{x,y} - \Gamma \right] + \frac{\beta^{t}}{v} \frac{\partial S_{A}}{\partial P} \Big|_{x,y}, \tag{3}$$

where  $\Gamma$  is the adiabatic lapse rate, and the thermal expansion and haline contraction coefficients defined with respect to Absolute Salinity  $S_A$  and in situ temperature are given by

$$\alpha^{t} = \frac{1}{v} \frac{\partial v}{\partial T} \Big|_{S_{A}, p} \quad \text{and} \quad \beta^{t} = -\frac{1}{v} \frac{\partial v}{\partial S_{A}} \Big|_{T, p}.$$
 (4)

Throughout this paper we follow the naming convention used in Jackett and McDougall (1995) so that we use the word "cast" to describe a vertical profile of either hydrographic data or data from a gridded product, and the word "bottle" to describe a data point at a particular pressure on such a cast. An instability is detected on a part of the cast where the square of the buoyancy frequency evaluated between a bottle pair is negative.

## 3. Stabilisation by adjusting both Absolute Salinity and Conservative Temperature

The second method of correcting for instabilities is more complex and involves minimally adjusting both Absolute Salinity and Conservative Temperature. This time a single cast contains Absolute Salinity  $S_A$ , Conservative Temperature  $\Theta$ , and pressure p recorded for n bottles, i.e.  $\left(S_{Aj},\Theta_j,p_j\right),j=1,2,...,n$ , and we minimally adjust both the Absolute Salinity by  $S'_{Aj}$  and Conservative Temperature by  $\Theta'_j$  to achieve a stable cast which has  $N^2$  greater than a predefined value  $N^2_{lower\_limit}$  between each pair of bottles. In this case the unknown vector in the inequality constraint  $A_{ij}x_j \leq b_i$  involves the perturbations of both Absolute Salinity and Conservative Temperature and the matrix A consists of four stripes, with elements of  $+\beta^{\Theta}$ ,  $-\beta^{\Theta}$ ,  $+\alpha^{\Theta}$  and  $-\alpha^{\Theta}$ , while  $b_i$  is defined by

$$b = \beta^{\Theta} \Delta S_{A} - \alpha^{\Theta} \Delta \Theta - \frac{\Delta P \, v}{g^{2}} N_{lower\_limit}^{2}$$

$$= \frac{\Delta P \, v}{g^{2}} \left( N^{2} - N_{lower\_limit}^{2} \right). \tag{7}$$

The constrained least squares technique minimizes the salinity and temperature perturbations,

$$\sum_{j=1}^{n} \left[ \left( S_{Aj}' \right)^2 + \left( \Theta_j' \right)^2 \left( \frac{\alpha^{\Theta}}{\beta^{\Theta}} \right)^2 \right]. \tag{8}$$

Note that we have weighted the Conservative Temperature perturbations by the ratio  $\alpha^{\Theta}/\beta^{\Theta}$  to arrive at the same units as Absolute Salinity.

As described by Jackett and McDougall (1995) the above constrained least squares problem achieves a stable vertical water column but oftentimes at the expense of making

unphysical changes to the water-mass structure of the water column. That is, the resulting  $S_A - \Theta$  curve of the water column can be perturbed in a way that does not seem realistic. Here we address this issue by adding a requirement that the Absolute Salinity and Conservative Temperature perturbations,  $S'_{Aj}$  and  $\Theta'_{j}$  of each bottle must exactly obey the linear constraint

$$S'_{Aj} \delta \Theta + \Theta'_{j} \delta S_{A} = 0, \qquad (9)$$

where the differences of Conservative Temperature and Absolute Salinity,  $\delta\Theta$  and  $\delta S_{\rm A}$ , are chosen so that the ratio  $\delta\Theta/\delta S_{\rm A}$  is representative of a smoothed version of the  $S_{\rm A}-\Theta$  curve of the water column.

We developed a multi-step procedure to implement the above method in the GSW code (GSW Oceanographic toolbox, version 3.06),  $gsw\_stabilise\_SA\_CT$ . Initially the vertical  $(S_{Aj}, \Theta_j, P_j)$  profile is stabilised by adjusting Absolute Salinity  $S_A$  and Conservative Temperature  $\Theta$ , without the linear constraint of Eqn. 9 to have a  $N_{lower\_limit}^2$  of  $1x10^{-9}$  s<sup>-2</sup>. This very small lower limit enables the calculation of the mixed-layer pressure (MLP) as described in de Boyer Montégut et al. (2004). A background cast is constructed to have bottles regularly spaced in vertically integrated  $-\rho g^{-1}N^2$  with a resolution of about 0.1 kg m<sup>-3</sup>, this is achieved by using the data below the MLP and vertically averaging over a range of ~0.2 kg m<sup>-3</sup> such that each average has an overlap by 0.05 kg m-3. This sparse, smoothed cast is then stabilised without the individual bottle constraints (Eqn. 9) such that the minimum stability is greater than the user defined  $N_{lower\_limit}^2$ . The resulting cast is used to calculate  $\delta\Theta$  and  $\delta S_A$  of Eqn (9).

In the GSW code, the default  $N_{lower\_limit}^2$  for each bottle pair is set to be  $1x10^{-9}$  s<sup>-2</sup> which is approximately one fifth of the square of the earth's rotation rate. Also included is a pressure dependent polynomial that is based on the lowest 10 % of the buoyancy frequencies in observed profiles collected in the Southern Ocean, south of 50°S, where the lowest  $N_{lower\_limit}^2$  values are typically found. This code is called  $gsw\_Nsquared\_lowerlimit$ , in future releases of GSW it is intended that this function will be expanded to include a  $N_{lower\_limit}^2$  polynomial that is a function of pressure, latitude and longitude.

In the code, *gsw\_stabilise\_SA\_CT*, we have included the option to conserve heat or salt. We have set the default to conserve neither heat nor salt on our calculations, as we found that sometimes stabilising the water column at one height caused changes far above or below this height. In the case of observed data, correcting for spikes in the data and conserving properties can cause the profile to shift away from the observed profile shape.