Notes on the function gsw_CT_second_derivatives(SA,pt)

This function, **gsw_CT_second_derivatives**(SA,pt), evaluates the second derivatives of $\tilde{\Theta}\left(S_{\mathrm{A}},\theta\right)$, namely

$$\tilde{\Theta}_{S_{\mathrm{A}}S_{\mathrm{A}}}, \quad \tilde{\Theta}_{\theta\theta} \quad \text{and} \quad \tilde{\Theta}_{S_{\mathrm{A}}\theta}\,. \tag{1}$$

These second derivatives are found by mathematically differentiating Eqns. (A.12.3) of the TEOS-10 Manual, repeated here,

$$\Theta_{\theta}\big|_{S_{\mathrm{A}}} = c_p\left(S_{\mathrm{A}},\theta,0\right)/c_p^0\,, \qquad \Theta_{S_{\mathrm{A}}}\Big|_{\theta} = \left[\mu\left(S_{\mathrm{A}},\theta,0\right) - \left(T_0+\theta\right)\mu_T\left(S_{\mathrm{A}},\theta,0\right)\right]/c_p^0\,. \tag{A.12.3}$$

The outputs $\tilde{\Theta}_{\theta\theta}$ and $\tilde{\Theta}_{S_{\mathrm{A}}\theta}$ of this function, **gsw_CT_second_derivatives**(SA,pt), remain well-behaved as the input Absolute Salinity approaches zero, including at $S_{\mathrm{A}} = 0\ \mathrm{g\,kg^{-1}}$, but the output $\tilde{\Theta}_{S_{\mathrm{A}}S_{\mathrm{A}}}$ has a singularity at $S_{\mathrm{A}} = 0\ \mathrm{g\,kg^{-1}}$, and a nan is returned at $S_{\mathrm{A}} = 0\ \mathrm{g\,kg^{-1}}$.

References

IOC, SCOR and IAPSO, 2010: *The international thermodynamic equation of seawater – 2010: Calculation and use of thermodynamic properties*. Intergovernmental Oceanographic Commission, Manuals and Guides No. 56, UNESCO (English), 196 pp. Available from http://www.TEOS-10.org See Eqn. (A.12.3) of this TEOS-10 Manual.

Here follows appendix A.12 of the TEOS-10 Manual (IOC *et al*., 2010).

A.12 Differential relationships between η, θ, Θ and S_{A}

Evaluating the fundamental thermodynamic relation in the forms (A.11.6) and (A.11.12) and using the four boxed equations in appendix A.11, we find the relations

$$\begin{aligned}\left(T_0+t\right)\mathrm{d}\eta + \mu\left(p\right)\mathrm{d}S_{\mathrm{A}} &= \frac{\left(T_0+t\right)}{\left(T_0+\theta\right)}\,c_p\left(0\right)\,\mathrm{d}\theta \;+\; \left[\mu\left(p\right) - \left(T_0+t\right)\mu_T\left(0\right)\right]\mathrm{d}S_{\mathrm{A}} \\ &= \frac{\left(T_0+t\right)}{\left(T_0+\theta\right)}\,c_p^0\,\mathrm{d}\Theta \;+\; \left[\mu\left(p\right) - \frac{\left(T_0+t\right)}{\left(T_0+\theta\right)}\mu\left(0\right)\right]\mathrm{d}S_{\mathrm{A}}\,.\end{aligned} \tag{A.12.1}$$

The quantity $\mu\left(p\right)\mathrm{d}S_{\mathrm{A}}$ is now subtracted from each of these three expressions and the whole equation is then multiplied by $\left(T_0+\theta\right)/\left(T_0+t\right)$ obtaining

$$\left(T_0+\theta\right)\mathrm{d}\eta \;=\; c_p\left(0\right)\,\mathrm{d}\theta - \left(T_0+\theta\right)\mu_T\left(0\right)\,\mathrm{d}S_{\mathrm{A}} \;=\; c_p^0\,\mathrm{d}\Theta - \mu\left(0\right)\,\mathrm{d}S_{\mathrm{A}}\,. \tag{A.12.2}$$

From this follows all the following partial derivatives between η, θ, Θ and S_{A},

$$\Theta_{\theta}\big|_{S_{\mathrm{A}}} = c_p\left(S_{\mathrm{A}},\theta,0\right)/c_p^0\,, \qquad \Theta_{S_{\mathrm{A}}}\Big|_{\theta} = \left[\mu\left(S_{\mathrm{A}},\theta,0\right) - \left(T_0+\theta\right)\mu_T\left(S_{\mathrm{A}},\theta,0\right)\right]/c_p^0\,, \tag{A.12.3}$$

$$\Theta_{\eta}\big|_{S_{\mathrm{A}}} = \left(T_0+\theta\right)/c_p^0\,, \qquad \Theta_{S_{\mathrm{A}}}\Big|_{\eta} = \mu\left(S_{\mathrm{A}},\theta,0\right)/c_p^0\,, \tag{A.12.4}$$

$$\theta_{\eta}\big|_{S_{\mathrm{A}}} = \left(T_0+\theta\right)/c_p\left(S_{\mathrm{A}},\theta,0\right), \qquad \theta_{S_{\mathrm{A}}}\Big|_{\eta} = \left(T_0+\theta\right)\mu_T\left(S_{\mathrm{A}},\theta,0\right)/c_p\left(S_{\mathrm{A}},\theta,0\right), \tag{A.12.5}$$

$$\theta_{\Theta}\big|_{S_{\mathrm{A}}} = c_p^0/c_p\left(S_{\mathrm{A}},\theta,0\right), \quad \theta_{S_{\mathrm{A}}}\Big|_{\Theta} = -\left[\mu\left(S_{\mathrm{A}},\theta,0\right) - \left(T_0+\theta\right)\mu_T\left(S_{\mathrm{A}},\theta,0\right)\right]/c_p\left(S_{\mathrm{A}},\theta,0\right), \tag{A.12.6}$$

$$\eta_\theta\big|_{S_\mathrm{A}} = c_p\left(S_\mathrm{A},\theta,0\right)\big/\left(T_0+\theta\right), \qquad \eta_{S_\mathrm{A}}\big|_\theta = -\mu_T\left(S_\mathrm{A},\theta,0\right), \tag{A.12.7}$$

$$\eta_\Theta\big|_{S_\mathrm{A}} = c_p^0\big/\left(T_0+\theta\right), \qquad \eta_{S_\mathrm{A}}\big|_\Theta = -\mu\left(S_\mathrm{A},\theta,0\right)\big/\left(T_0+\theta\right). \tag{A.12.8}$$

The three second order derivatives of $\hat{\eta}\left(S_\mathrm{A},\Theta\right)$ are listed in Eqns. (P.14) and (P.15) of appendix P. The corresponding derivatives of $\hat{\theta}\left(S_\mathrm{A},\Theta\right)$, namely $\hat{\theta}_\Theta$, $\hat{\theta}_{S_\mathrm{A}}$, $\hat{\theta}_{\Theta\Theta}$, $\hat{\theta}_{S_\mathrm{A}\Theta}$ and $\hat{\theta}_{S_\mathrm{A}S_\mathrm{A}}$ can also be derived using Eqn. (P.13), obtaining

$$\hat{\theta}_\Theta = \frac{1}{\tilde{\Theta}_\theta}, \quad \hat{\theta}_{S_\mathrm{A}} = -\frac{\tilde{\Theta}_{S_\mathrm{A}}}{\tilde{\Theta}_\theta}, \quad \hat{\theta}_{\Theta\Theta} = -\frac{\tilde{\Theta}_{\theta\theta}}{\left(\tilde{\Theta}_\theta\right)^3}, \quad \hat{\theta}_{S_\mathrm{A}\Theta} = -\frac{\tilde{\Theta}_{\theta S_\mathrm{A}}}{\left(\tilde{\Theta}_\theta\right)^2} + \frac{\tilde{\Theta}_{S_\mathrm{A}}\tilde{\Theta}_{\theta\theta}}{\left(\tilde{\Theta}_\theta\right)^3}, \tag{A.12.9a,b,c,d}$$

$$\text{and} \quad \hat{\theta}_{S_\mathrm{A}S_\mathrm{A}} = -\frac{\tilde{\Theta}_{S_\mathrm{A}S_\mathrm{A}}}{\tilde{\Theta}_\theta} + 2\,\frac{\tilde{\Theta}_{S_\mathrm{A}}}{\tilde{\Theta}_\theta}\,\frac{\tilde{\Theta}_{\theta S_\mathrm{A}}}{\tilde{\Theta}_\theta} - \left(\frac{\tilde{\Theta}_{S_\mathrm{A}}}{\tilde{\Theta}_\theta}\right)^2 \frac{\tilde{\Theta}_{\theta\theta}}{\tilde{\Theta}_\theta}, \tag{A.12.10}$$

in terms of the partial derivatives $\tilde{\Theta}_\theta$, $\tilde{\Theta}_{S_\mathrm{A}}$, $\tilde{\Theta}_{\theta\theta}$, $\tilde{\Theta}_{\theta S_\mathrm{A}}$ and $\tilde{\Theta}_{S_\mathrm{A}S_\mathrm{A}}$ which can be obtained by differentiating the polynomial $\tilde{\Theta}\left(S_\mathrm{A},\theta\right)$ from the TEOS-10 Gibbs function.