

Notes on the function `gsw_pt_second_derivatives(SA,CT)`

This function, `gsw_pt_second_derivatives(SA,CT)`, evaluates the second derivatives of $\hat{\theta}(S_A, \Theta)$, namely

$$\hat{\theta}_{S_A S_A}, \quad \hat{\theta}_{\Theta \Theta} \quad \text{and} \quad \hat{\theta}_{S_A \Theta} \quad (1)$$

in terms of the partial derivatives $\tilde{\Theta}_\theta$, $\tilde{\Theta}_{S_A}$, $\tilde{\Theta}_{\theta\theta}$, $\tilde{\Theta}_{\theta S_A}$ and $\tilde{\Theta}_{S_A S_A}$ using Eqns. (A.12.9c,d) and (A.12.10), repeated here,

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

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

So the present code first calls `gsw_CT_first_derivatives(SA,CT)` and `gsw_CT_second_derivatives(SA,CT)` to evaluate $\tilde{\Theta}_\theta$, $\tilde{\Theta}_{S_A}$, $\tilde{\Theta}_{\theta\theta}$, $\tilde{\Theta}_{\theta S_A}$ and $\tilde{\Theta}_{S_A S_A}$.

The output $\hat{\theta}_{S_A S_A}$ of this function, `gsw_pt_second_derivatives(SA,CT)`, has a singularity at $S_A = 0 \text{ g kg}^{-1}$, where a nan is returned.

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 Eqns. (A.12.9) and (A.12.10) 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

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

The quantity $\mu(p)dS_A$ is now subtracted from each of these three expressions and the whole equation is then multiplied by $(T_0+\theta)/(T_0+t)$ obtaining

$$(T_0+\theta)d\eta = c_p(0) d\theta - (T_0+\theta)\mu_T(0) dS_A = c_p^0 d\Theta - \mu(0) dS_A. \quad (\text{A.12.2})$$

From this follows all the following partial derivatives between η , θ , Θ and S_A ,

$$\Theta_\theta|_{S_A} = c_p(S_A, \theta, 0)/c_p^0, \quad \Theta_{S_A}|_\theta = [\mu(S_A, \theta, 0) - (T_0 + \theta)\mu_T(S_A, \theta, 0)]/c_p^0, \quad (\text{A.12.3})$$

$$\Theta_\eta|_{S_A} = (T_0 + \theta)/c_p^0, \quad \Theta_{S_A}|_\eta = \mu(S_A, \theta, 0)/c_p^0, \quad (\text{A.12.4})$$

$$\theta_\eta|_{S_A} = (T_0 + \theta)/c_p(S_A, \theta, 0), \quad \theta_{S_A}|_\eta = (T_0 + \theta)\mu_T(S_A, \theta, 0)/c_p(S_A, \theta, 0), \quad (\text{A.12.5})$$

$$\theta_\Theta|_{S_A} = c_p^0/c_p(S_A, \theta, 0), \quad \theta_{S_A}|_\Theta = -[\mu(S_A, \theta, 0) - (T_0 + \theta)\mu_T(S_A, \theta, 0)]/c_p(S_A, \theta, 0), \quad (\text{A.12.6})$$

$$\eta_\theta|_{S_A} = c_p(S_A, \theta, 0)/(T_0 + \theta), \quad \eta_{S_A}|_\theta = -\mu_T(S_A, \theta, 0), \quad (\text{A.12.7})$$

$$\eta_\Theta|_{S_A} = c_p^0/(T_0 + \theta), \quad \eta_{S_A}|_\Theta = -\mu(S_A, \theta, 0)/(T_0 + \theta). \quad (\text{A.12.8})$$

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

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

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

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