Notes on the function gsw_entropy_second_derivatives(SA,CT)

This function, **gsw_entropy_second_derivatives**(SA,CT), evaluates the second order partial derivatives of entropy $\hat{\eta}(S_A,\Theta)$ with respect to Absolute Salinity and Conservative Temperature, as given in Eqns. (P.14b), (P.15a) and (P.15b) of the TEOS-10 Manual (IOC *et al.*, 2010), repeated here,

$$\hat{\eta}_\Theta = \frac{\tilde{\eta}_\theta}{\tilde{\Theta}_\theta} \equiv \frac{c_p^0}{(T_0+\theta)}, \quad \hat{\eta}_{\Theta\Theta} = -\frac{1}{\tilde{\Theta}_\theta}\frac{c_p^0}{(T_0+\theta)^2}, \quad \hat{\eta}_{S_A} = -\frac{\tilde{\mu}(S_A,\theta,0)}{(T_0+\theta)}, \qquad \text{(P.14a,b,c)}$$

$$\hat{\eta}_{S_A\Theta} = \frac{\tilde{\Theta}_{S_A}}{\tilde{\Theta}_\theta}\frac{c_p^0}{(T_0+\theta)^2}, \quad \text{and} \quad \hat{\eta}_{S_AS_A} = -\frac{\tilde{\mu}_{S_A}(S_A,\theta,0)}{(T_0+\theta)} - \frac{\left(\tilde{\Theta}_{S_A}\right)^2}{\tilde{\Theta}_\theta}\frac{c_p^0}{(T_0+\theta)^2}, \qquad \text{(P.15a,b)}$$

This function, **gsw_entropy_second_derivatives**(SA,CT), uses the full TEOS-10 Gibbs function $g(S_A,t,p)$ of IOC *et al.* (2010), being the sum of the IAPWS-09 and IAPWS-08 Gibbs functions. The function first calculates potential temperature θ and then evaluates both $\tilde{\Theta}_{S_A}$ and $\tilde{\Theta}_\theta$ from the GSW function **gsw_CT_first_derivatives**(SA,pt). This enables $\hat{\eta}_{\Theta\Theta}$ and $\hat{\eta}_{S_A\Theta}$ to be calculated directly from the above equations. In Eqn. (P.15b) $\tilde{\mu}_{S_A}(S_A,\theta,0) = g_{S_AS_A}(S_A,\theta,0)$ is evaluated directly from this second order partial derivative of the Gibbs function. This second order partial derivative, $g_{S_AS_A}(S_A,\theta,0)$, varies as S_A^{-1} as S_A tends to zero, so that $\hat{\eta}_{S_AS_A}$ has a singularity at $S_A = 0 \text{ g kg}^{-1}$.

References

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IAPWS, 2009: Supplementary Release on a Computationally Efficient Thermodynamic Formulation for Liquid Water for Oceanographic Use. The International Association for the Properties of Water and Steam. Doorwerth, The Netherlands, September 2009, available from http://www.iapws.org. This Release is referred to in the text as **IAPWS-09**.

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

Here follows appendix A.12 and an excerpt from appendix P 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

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

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

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

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

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

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

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

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

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

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

The three second order derivatives of $\hat{\eta}(S_\mathrm{A},\Theta)$ are listed in Eqns. (P.14) and (P.15) of appendix P. The corresponding derivatives of $\hat{\theta}(S_\mathrm{A},\Theta)$, 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

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

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

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 $\tilde{\Theta}(S_\mathrm{A},\theta)$ from the TEOS-10 Gibbs function.

And an excerpt from Appendix P of the TEOS-10 Manual (IOC *et al.*, 2010)

The partial derivatives with respect to Θ and with respect to θ, both at constant S_A and p, and the partial derivatives with respect to S_A, are related by

$$\left.\frac{\partial}{\partial\Theta}\right|_{S_\mathrm{A},p} \;=\; \frac{1}{\tilde{\Theta}_\theta}\left.\frac{\partial}{\partial\theta}\right|_{S_\mathrm{A},p}, \quad \text{and} \quad \left.\frac{\partial}{\partial S_\mathrm{A}}\right|_{\Theta,p} \;=\; \left.\frac{\partial}{\partial S_\mathrm{A}}\right|_{\theta,p} \;-\; \frac{\tilde{\Theta}_{S_\mathrm{A}}}{\tilde{\Theta}_\theta}\left.\frac{\partial}{\partial\theta}\right|_{S_\mathrm{A},p}. \qquad \text{(P.13a,b)}$$

Use of these expressions, acting on entropy yields (with $p = 0$ everywhere, and using Eqn. (P.7) [or Eqn. (A.12.8b)] and Eqn. (P.8))

$$\hat{\eta}_\Theta \;=\; \frac{\tilde{\eta}_\theta}{\tilde{\Theta}_\theta} \;\equiv\; \frac{c_p^0}{(T_0+\theta)}, \qquad \hat{\eta}_{\Theta\Theta} \;=\; -\,\frac{1}{\tilde{\Theta}_\theta}\,\frac{c_p^0}{(T_0+\theta)^2}, \qquad \hat{\eta}_{S_\mathrm{A}} \;=\; -\,\frac{\tilde{\mu}(S_\mathrm{A},\,\theta,\,0)}{(T_0+\theta)}, \qquad \text{(P.14a,b,c)}$$

$$\hat{\eta}_{S_\mathrm{A}\Theta} \;=\; \frac{\tilde{\Theta}_{S_\mathrm{A}}}{\tilde{\Theta}_\theta}\,\frac{c_p^0}{(T_0+\theta)^2}, \quad \text{and} \quad \hat{\eta}_{S_\mathrm{A}S_\mathrm{A}} \;=\; -\,\frac{\tilde{\mu}_{S_\mathrm{A}}(S_\mathrm{A},\theta,\,0)}{(T_0+\theta)} \;-\; \frac{\left(\tilde{\Theta}_{S_\mathrm{A}}\right)^2}{\tilde{\Theta}_\theta}\,\frac{c_p^0}{(T_0+\theta)^2}, \qquad \text{(P.15a,b)}$$

in terms of the partial derivatives of the exact polynomial expressions (P.11b) and (P.12).