

RBF-WHITE Kernel

Covariance functions:

This Kernel is the result of having a white Gaussian noise latent process, with an auto-covariance function defined by

$$K_{frfr}(t, t') = \sigma_f^2 \delta(t - t'), \quad (1)$$

for the r -th latent function, convolved with a Gaussian smoothing Kernel,

$$h_q(t, t') = h_q(t - t') = \frac{1}{\sqrt{2\pi l_q^2}} \exp\left(-\frac{(t - t')^2}{2l_q^2}\right) \quad (2.a)$$

$$= \frac{\sqrt{\sigma_q}}{\sqrt{2\pi}} \exp\left(-\frac{\sigma_q}{2} (t - t')^2\right) \quad (2.b)$$

where l_q is the length (or time) scale of the q -th smoothing kernel, and $\sigma_q = 1/l_q^2$ (i.e. $l_q = 1/\sigma_q$) is its inverse width.

The resulting output is given by

$$y_{rq}(t) = \int_0^t f_r(\tau) h_q(t - \tau) d\tau. \quad (3)$$

Given the linearity of the convolution and the fact that $f_r(t)$ is a GP, then $y_{rq}(t)$ is also a GP defined by its mean function,

$$E\{y_{rq}(t)\} = \mu_{rq}(t) = \int_0^t h_q(t - \tau) E\{f_r(\tau)\} d\tau = 0, \quad (4)$$

and the Cross-Covariance between $y_{rp}(t)$ and $y_{rq}(t')$, since $y_{rp}(t)$ is uncorrelated with $y_{rq}(t')$ whenever $p \neq r$ for any p, q :

$$\begin{aligned} K_{y_p y_q}^{(r)}(t, t') &= E\{y_{rp}(t) y_{rq}(t')\} \\ &= \int_0^t \int_0^{t'} h_p(t - \tau) h_q(t' - \tau') K_{frfr}(\tau, \tau') d\tau d\tau' \\ &= \sigma_f^2 \int_0^{t \wedge t'} h_p(t - \tau) h_q(t' - \tau) d\tau, \end{aligned} \quad (5)$$

where the upper limit of integration is due to the fact for $t > t + \Delta t'$
or $t' > t + \Delta t'$, $K_{fr}^r(t, t') = 0$. Replacing $\eta_p(t - \tau)$ and $\eta_q(t' - \tau)$ by
their values we obtain

$$\begin{aligned} K_{\eta_p \eta_q}^{(r)}(t, t') &= \sigma_r^2 \int_0^{t+\Delta t'} \sqrt{\frac{\sigma_p}{2\pi}} \exp\left(-\frac{\sigma_p(t-\tau)^2}{2}\right) \cdot \sqrt{\frac{\sigma_q}{2\pi}} \exp\left(-\frac{\sigma_q(t'-\tau)^2}{2}\right) d\tau \\ &= \frac{\sigma_r^2 \sqrt{\sigma_p \sigma_q}}{2\pi} \int_0^{t+\Delta t'} \exp\left(-\frac{\sigma_p(t^2 - 2t\tau + \tau^2) + \sigma_q((t')^2 - 2t'\tau + \tau^2)}{2}\right) d\tau \\ &= \frac{\sigma_r^2 \sqrt{\sigma_p \sigma_q}}{2\pi} \int_0^{t+\Delta t'} \exp\left(-\frac{(\sigma_p + \sigma_q)\tau^2 - 2(\sigma_p t + \sigma_q t')\tau + \sigma_p t^2 + \sigma_q (t')^2}{2}\right) d\tau \end{aligned}$$

$$= \frac{\sigma_r^2 \sqrt{\sigma_p \sigma_q}}{2\pi} \int_0^{t+\Delta t'} \exp\left(-\frac{\tau^2 - 2 \frac{\sigma_p t + \sigma_q t'}{\sigma_p + \sigma_q} \tau + \frac{\sigma_p t^2 + \sigma_q (t')^2}{\sigma_p + \sigma_q}}{2/(2(\sigma_p + \sigma_q))}\right) d\tau$$

$$= \frac{\sigma_r^2 \sqrt{\sigma_p \sigma_q}}{2\pi} \int_0^{t+\Delta t'} \exp\left(-\frac{(\tau - (\sigma_p t + \sigma_q t') / (\sigma_p + \sigma_q))^2}{2/(2(\sigma_p + \sigma_q))}\right) d\tau$$

$$\times \exp\left(-\frac{\frac{\sigma_p t^2 + \sigma_q (t')^2}{2(\sigma_p + \sigma_q)} + \frac{(\sigma_p t + \sigma_q t')^2}{2(\sigma_p + \sigma_q)}}{\frac{(\sigma_p + \sigma_q)}{2(\sigma_p + \sigma_q)}}\right)$$

$$= \frac{\sigma_r^2 \sqrt{\sigma_p \sigma_q}}{2\pi} \int_0^{t+\Delta t'} \exp\left(-\frac{\sigma_p + \sigma_q}{2} \left(\tau - \frac{\sigma_p t + \sigma_q t'}{\sigma_p + \sigma_q}\right)^2\right) d\tau$$

$$\times \exp\left(-\frac{\cancel{\sigma_p^2 t^2} + \sigma_p \sigma_q t^2 + \cancel{\sigma_p \sigma_q (t')^2} + \cancel{\sigma_q^2 (t')^2}}{2(\sigma_p + \sigma_q)}\right)$$

$$\times \exp\left(-\frac{\cancel{\sigma_p^2 t^2} + 2 \sigma_p \sigma_q t t' + \cancel{\sigma_q^2 (t')^2}}{2(\sigma_p + \sigma_q)}\right) \Rightarrow$$

$$K_{\text{p}\text{q}}^{(r)}(t, t') = \frac{\sigma_r^2 \sqrt{\sigma_p \sigma_q}}{2\pi} \exp\left(-\frac{\sigma_p \sigma_q}{2(\sigma_p + \sigma_q)} (t - t')^2\right)$$

$$\times \underbrace{\int_0^{t-t'} \exp\left(-\frac{\sigma_p \sigma_q}{2} \left(t - \frac{\sigma_p t + \sigma_q t'}{\sigma_p + \sigma_q}\right)^2\right) dt}_{I}$$
(6)

Now, to obtain the final expression of $K_{\text{p}\text{q}}^{(r)}(t, t')$ we just need to solve I, which is easy, since, making the change of variable

$$z = \sqrt{\frac{\sigma_p \sigma_q}{2}} \left(t - \frac{\sigma_p t + \sigma_q t'}{\sigma_p + \sigma_q}\right) \Rightarrow$$

$$dz = \sqrt{\frac{\sigma_p \sigma_q}{2}} dt,$$

we obtain the familiar expression of the error function:

$$I = \frac{\sqrt{\pi}}{2} \cdot \sqrt{\frac{2}{\sigma_p \sigma_q}} \cdot \frac{2}{\sqrt{\pi}} \int_{-\frac{\sqrt{\sigma_p \sigma_q}}{2} \cdot \frac{\sigma_p t + \sigma_q t'}{\sigma_p + \sigma_q}}^{\frac{\sqrt{\sigma_p \sigma_q}}{2} \cdot \left(t - t' - \frac{\sigma_p t + \sigma_q t'}{\sigma_p + \sigma_q}\right)} \exp(-z^2) dz$$

$$= \sqrt{\frac{\pi}{2\sigma_p \sigma_q}} \left[\operatorname{erf}\left(\frac{\sqrt{\sigma_p \sigma_q}}{2} \left(t - t' - \frac{\sigma_p t + \sigma_q t'}{\sigma_p + \sigma_q}\right)\right) + \operatorname{erf}\left(\frac{\sqrt{\sigma_p \sigma_q}}{2} \cdot \frac{\sigma_p t + \sigma_q t'}{\sigma_p + \sigma_q}\right) \right].$$

The first term can be rewritten to emphasize that it corresponds to the stationary part, since

$$t - t' - \frac{\sigma_p t + \sigma_q t'}{\sigma_p + \sigma_q} = -\frac{\sigma_p(t - t') + \sigma_q(t' - t)}{\sigma_p + \sigma_q}$$

$$= \begin{cases} -\frac{\sigma_q(t' - t)}{\sigma_p + \sigma_q}, & t < t' \text{ [i.e. } t - t' = t], \\ -\frac{\sigma_p(t - t')}{\sigma_p + \sigma_q}, & t > t' \text{ [i.e. } t - t' = t']. \end{cases}$$

$$t_1 t' - \frac{\tau_{\varphi_p} t + \tau_{\varphi_q} t'}{\tau_{\varphi_p} + \tau_{\varphi_q}} = -\tau_{\varphi_v} |t - t'| / (\tau_{\varphi_p} + \tau_{\varphi_q}), \quad (7)$$

where

$$(8.a) \quad \tau_{\varphi_v} = \begin{cases} \tau_{\varphi_q}, & t < t'; \\ \tau_{\varphi_p}, & t > t'. \end{cases} = \tau_{\varphi_q} (1 - u(t-t')) + \tau_{\varphi_p} u(t-t') \quad (8.b)$$

$$= \tau_{\varphi_q} + (\tau_{\varphi_p} - \tau_{\varphi_q}) u(t-t'). \quad (8.c)$$

Therefore, I can be re-expressed as

$$I = \sqrt{\frac{\pi}{2\tau_{\varphi_p}\tau_{\varphi_q}}} \left[\operatorname{erf} \left(\sqrt{\frac{\tau_{\varphi_p}\tau_{\varphi_q}}{2}} \cdot \frac{\tau_{\varphi_p} t + \tau_{\varphi_q} t'}{\tau_{\varphi_p} + \tau_{\varphi_q}} \right) - \operatorname{erf} \left(\sqrt{\frac{\tau_{\varphi_p}\tau_{\varphi_q}}{2}} \cdot \frac{\tau_{\varphi_v} |t - t'|}{\tau_{\varphi_p} + \tau_{\varphi_q}} \right) \right],$$

and the kernel becomes

$$K_{Y_p Y_q}^{(r)}(t, t') = \frac{\sigma_r^2}{\sqrt{8\pi}} \exp \left(-\frac{\tau_{\varphi_p} \tau_{\varphi_q}}{2(\tau_{\varphi_p} + \tau_{\varphi_q})} (t - t')^2 \right) \times \left[\operatorname{erf} \left(\sqrt{\frac{\tau_{\varphi_p}\tau_{\varphi_q}}{2}} \cdot \frac{\tau_{\varphi_p} t + \tau_{\varphi_q} t'}{\tau_{\varphi_p} + \tau_{\varphi_q}} \right) - \operatorname{erf} \left(\sqrt{\frac{\tau_{\varphi_p}\tau_{\varphi_q}}{2}} \cdot \frac{\tau_{\varphi_v} |t - t'|}{\tau_{\varphi_p} + \tau_{\varphi_q}} \right) \right] \quad (9)$$

To complete the description of the Kernel it is interesting to separate the stationary,

$$K_{Y_p Y_q}^{st(r)}(t, t') = \frac{\sigma_r^2}{\sqrt{8\pi}} \exp \left(-\frac{\tau_{\varphi_p} \tau_{\varphi_q}}{2(\tau_{\varphi_p} + \tau_{\varphi_q})} (\tilde{t} - \tilde{t}')^2 \right) \left[1 - \operatorname{erf} \left(\sqrt{\frac{\tau_{\varphi_p}\tau_{\varphi_q}}{2}} \cdot \frac{\tau_{\varphi_v} |\tilde{t} - \tilde{t}'|}{\tau_{\varphi_p} + \tau_{\varphi_q}} \right) \right] \quad (10)$$

and non-stationary versions of the kernel,

$$K_{Y_p Y_q}^{non-st(r)}(t, t') = \frac{\sigma_r^2}{\sqrt{8\pi}} \exp \left(-\frac{\tau_{\varphi_p} \tau_{\varphi_q}}{2(\tau_{\varphi_p} + \tau_{\varphi_q})} (t - t')^2 \right) \left[\operatorname{erf} \left(\sqrt{\frac{\tau_{\varphi_p}\tau_{\varphi_q}}{2}} \cdot \frac{\tau_{\varphi_p} t + \tau_{\varphi_q} t'}{\tau_{\varphi_p} + \tau_{\varphi_q}} \right) - 1 \right] \quad (11)$$

It is also interesting to observe the behaviour of the main diagonal of the Kernel matrix (i.e. $t = t'$):

$$K_{Y_p Y_q}^{(r)}(t, t) = \frac{\sigma_r^2}{\sqrt{8\pi}} \operatorname{erf} \left(\sqrt{\frac{\tau_{\varphi_p}\tau_{\varphi_q}}{2}} t \right) \quad (12)$$

And the auto-covariance function (i.e. $p=q$):

$$K_{Y_p Y_p}(t, t') = \frac{\sigma_r^2}{\sqrt{8\pi}} \exp\left(\frac{-\varphi_p(t-t')^2}{2}\right) \left[\operatorname{erf}\left(\frac{\varphi_p(t+t')}{2\sqrt{2}}\right) - \operatorname{erf}\left(\frac{\varphi_p|t-t'|}{2\sqrt{2}}\right) \right] \quad (13)$$

We also need to obtain the Cross-covariance matrix between $y_{rp}(t)$ and $f_r(t')$:

$$\begin{aligned} K_{y_{rp} f_r}(t, t') &= \int_0^t h_p(t-\tau) K_{f_r f_r}(t', \tau) d\tau \\ &= \sigma_r^2 h_p(t-t') u(t-t') \\ &= \frac{\sigma_r^2 \sqrt{\varphi_p}}{\sqrt{2\pi}} \exp\left(-\frac{\varphi_p}{2}(t-t')^2\right) u(t-t'), \end{aligned} \quad (14)$$

which means that $f_r(t')$ only has influence on $y_p(t)$ for $t > t'$, as expected, since it is a white noise process.

Gradients:

$$\begin{aligned} \nabla_{\sigma_r^2} K_{y_{rp} f_r}(t, t') &= \sqrt{\frac{\varphi_p}{2\pi}} \exp\left(-\frac{\varphi_p}{2}(t-t')^2\right) u(t-t') \\ &= \frac{K_{y_{rp} f_r}(t, t')}{\sigma_r^2} \end{aligned} \quad (14.a) \quad (14.b) \quad \frac{1}{2} \varphi_p^{-1/2}$$

$$\begin{aligned} \nabla_{\varphi_p} K_{y_{rp} f_r}(t, t') &= \frac{\sigma_r^2}{\sqrt{2\pi}} \exp\left(-\frac{\varphi_p}{2}(t-t')^2\right) u(t-t') \nabla_{\varphi_p} \sigma_r^{1/2} \cdot \frac{\sqrt{\varphi_p}}{\sqrt{2\varphi_p}} \\ K_{y_{rp} f_r}(t, t') &= + \frac{\sigma_r^2 \sqrt{\varphi_p}}{\sqrt{2\pi}} \exp\left(-\frac{\varphi_p}{2}(t-t')^2\right) \left(-\frac{1}{2}(t-t')^2\right) u(t-t') \\ &= \left[\frac{1}{\sqrt{2\varphi_p}} - \sqrt{\varphi_p}(t-t')^2 \right] \frac{\sigma_r^2}{2\sqrt{2\pi}} \exp\left(-\frac{\varphi_p}{2}(t-t')^2\right) u(t-t') \\ &= \frac{1}{2} \left(\frac{1}{\sqrt{2\varphi_p}} - (t-t')^2 \right) K_{y_{rp} f_r}(t, t') \end{aligned} \quad (15.a) \quad (15.b)$$

Now, before obtaining the gradients of $K_{\text{Pyq}}^{(r)}(t, t')$ we define

$$E_{pq}^{(r)}(t, t') = \operatorname{erf}\left(\sqrt{\frac{\sigma_p \sigma_q}{2}} \cdot \frac{\sigma_p t + \sigma_q t'}{\sigma_p + \sigma_q}\right) - \operatorname{erf}\left(\sqrt{\frac{\sigma_p \sigma_q}{2}} \cdot \frac{\sigma_q |t - t'|}{\sigma_p + \sigma_q}\right),$$

so that

$$K_{\text{Pyq}}^{(r)}(t, t') = \frac{\sigma_r^2}{\sqrt{8\pi}} \exp\left(-\frac{\sigma_p \sigma_q}{2(\sigma_p + \sigma_q)} (t - t')^2\right) E_{pq}^{(r)}(t, t'). \quad (17)$$

And hence,

$$\nabla_{\sigma_r^2} K_{\text{Pyq}}^{(r)}(t, t') = \frac{1}{\sqrt{8\pi}} \exp\left(-\frac{\sigma_p \sigma_q}{2(\sigma_p + \sigma_q)} (t - t')^2\right) \nabla_{\sigma_q}^{(r)}(t, t') \quad (18.a)$$

$$= \frac{K_{\text{Pyq}}^{(r)}(t, t')}{\sigma_r^2} \quad (18.b)$$

$$\begin{aligned} \nabla_{\sigma_p} K_{\text{Pyq}}^{(r)}(t, t') &= \frac{\sigma_r^2}{\sqrt{8\pi}} \exp\left(-\frac{\sigma_p \sigma_q}{2(\sigma_p + \sigma_q)} (t - t')^2\right) \nabla_{\sigma_q}^{(r)}(t, t') \\ K_{\text{Pyq}}^{(r)}(t, t') &= \times \left(-\frac{(t - t')^2}{2}\right) \cdot \nabla_{\sigma_p} \frac{\sigma_p \sigma_q}{\sigma_p + \sigma_q} \\ &\quad + \frac{\sigma_r^2}{\sqrt{8\pi}} \exp\left(-\frac{\sigma_p \sigma_q}{2(\sigma_p + \sigma_q)} (t - t')^2\right) \nabla_{\sigma_p} \nabla_{\sigma_q}^{(r)}(t, t'), \end{aligned} \quad (19)$$

where

$$\nabla_{\sigma_p} \frac{\sigma_p \sigma_q}{\sigma_p + \sigma_q} = \frac{\sigma_q (\sigma_p + \sigma_q) - \sigma_p \sigma_q}{(\sigma_p + \sigma_q)^2} = \frac{\sigma_q^2}{(\sigma_p + \sigma_q)^2} \quad (20)$$

$$\begin{aligned} \nabla_{\sigma_p} \nabla_{\sigma_q}^{(r)}(t, t') &= \frac{2}{\sqrt{\pi}} \left\{ \exp\left(-\frac{\sigma_p \sigma_q}{2} \cdot \left(\frac{\sigma_p t + \sigma_q t'}{\sigma_p + \sigma_q}\right)^2\right) \cdot \sqrt{\sigma_q} \right. \\ &\quad \times \nabla_{\sigma_p} \left(\frac{\sigma_p t + \sigma_q t'}{\sigma_p + \sigma_q} \sqrt{\sigma_p} \right) \\ &\quad \left. - \exp\left(-\frac{\sigma_p \sigma_q}{2} \cdot \left(\frac{\sigma_q |t - t'|}{\sigma_p + \sigma_q}\right)^2\right) \cdot \sqrt{\frac{\sigma_q}{2}} \cdot \nabla_{\sigma_p} \left(\frac{\sigma_q \sqrt{\sigma_p}}{\sigma_p + \sigma_q} \right) \right\} \end{aligned} \quad (21)$$

and

$$\begin{aligned}
 \boxed{\nabla_{\varphi_p} \left(\sqrt{\varphi_p} \cdot \frac{\varphi_p t + \varphi_q t'}{\varphi_p + \varphi_q} \right)} &= \frac{\left[\frac{1}{2} (\varphi_p)^{-1/2} (\varphi_p t + \varphi_q t') + \varphi_p^{1/2} t \right] (\varphi_p + \varphi_q)}{(\varphi_p + \varphi_q)^2} \\
 &\quad - \frac{\varphi_p^{1/2} (\varphi_p t + \varphi_q t')}{(\varphi_p + \varphi_q)^2} \\
 &= \left[\cdot, (\varphi_p t + \varphi_q t') (\varphi_p + \varphi_q) / 2 \right. \\
 &\quad \left. + \varphi_p t (\varphi_p + \varphi_q) - \varphi_p (\varphi_p t + \varphi_q t') \right] \\
 &\quad \times (\varphi_p + \varphi_q)^{-2} \varphi_p^{-1/2} \\
 &= \left[\overline{\varphi_p^2 t / 2} + \overline{\varphi_p \varphi_q t / 2} + \overline{\varphi_p \varphi_q t' / 2} + \overline{\varphi_q^2 t' / 2} \right. \\
 &\quad \left. + \overline{\varphi_p \varphi_q t} - \overline{\varphi_p \varphi_q t'} \right] / [(\varphi_p + \varphi_q)^2 \sqrt{\varphi_p}] \\
 &= \frac{\overline{\varphi_p^2 t / 2} + \overline{\varphi_p \varphi_q (3t - t') / 2} + \overline{\varphi_q^2 t' / 2}}{(\varphi_p + \varphi_q)^2 \sqrt{\varphi_p}}
 \end{aligned} \tag{22}$$

$$\begin{aligned}
 \nabla_{\varphi_p} \left(\frac{\varphi_v \sqrt{\varphi_p}}{\varphi_p + \varphi_q} \right) &= \frac{\frac{1}{2} \varphi_p^{-1/2} \varphi_v (\varphi_p + \varphi_q) + \varphi_p^{1/2} (\varphi_p + \varphi_q) \nabla_{\varphi_p} \varphi_v}{(\varphi_p + \varphi_q)^2} \\
 &\quad - \frac{\varphi_v (\varphi_p)^{1/2}}{(\varphi_p + \varphi_q)^2},
 \end{aligned}$$

where, remembering that

$$\varphi_v = \varphi_q (1 - u(t-t')) + \varphi_p u(t-t'),$$

we get

$$\boxed{\nabla_{\varphi_p} \varphi_v = u(t-t')} \tag{23}$$

so that

$$\nabla_{\vartheta_p} \left(\frac{\vartheta_q \sqrt{2\vartheta_p}}{2\vartheta_p + 2\vartheta_q} \right) = \boxed{[2\vartheta_p \vartheta_q (1 - u(t-t'))/2 + 2\vartheta^2_p (u(t-t'))/2] + \boxed{2\vartheta_p^2 u(t-t')}} \\ + \boxed{2\vartheta_p \vartheta_q u(t-t')} - \boxed{2\vartheta_p \vartheta_q (1 - u(t-t'))} - \boxed{2\vartheta_p^2 u(t-t')} \\ \times (2\vartheta_p + 2\vartheta_q)^{-2} \vartheta_p^{-1/2}$$

Missing terms:

$$2\vartheta_q^2 (1 - u(t-t'))/2 \\ + \vartheta_p \vartheta_q u(t-t')/2$$

Missing terms:

$$2\vartheta_q^2/2 - 2\vartheta_q^2 u(t-t')/2 \\ + 2\vartheta_p \cdot u(t-t') \vartheta_q/2$$

See p. 8'

$$= \boxed{[2\vartheta_p \vartheta_q/2 - 2\vartheta_p \vartheta_q u(t-t')/2 + 2\vartheta_p^2 u(t-t')/2] \\ + 2\vartheta_p \vartheta_q u(t-t') - \boxed{2\vartheta_p \vartheta_q} + \boxed{2\vartheta_p \vartheta_q u(t-t')}} \quad (24)$$

$$\times (2\vartheta_p + 2\vartheta_q)^{-2} \vartheta_p^{-1/2}$$

$$= \boxed{\frac{2\vartheta_p \vartheta_q/2 + [2\vartheta_p^2 - 32\vartheta_p \vartheta_q] u(t-t')/2}{(2\vartheta_p + 2\vartheta_q)^2 \sqrt{2\vartheta_p}}} \quad (24)$$

And finally, the gradient w.r.t. ϑ_q :

$$\nabla_{\vartheta_q} K_{ypq}^{(r)}(t, t') = \boxed{\frac{\partial r^2}{\sqrt{8\pi}} \left(-\frac{(t-t')^2 2\vartheta_p}{2} \right) \exp \left(-\frac{2\vartheta_p \vartheta_q}{2(2\vartheta_p + 2\vartheta_q)} (t-t')^2 \right)}$$

$$K_{ypq}^{(r)}(t, t') = \boxed{\begin{aligned} & \times E_{pq}^{(r)}(t, t') \nabla_{\vartheta_q} \frac{\vartheta_q}{2\vartheta_p + 2\vartheta_q} \\ & + \frac{\partial r^2}{\sqrt{8\pi}} \exp \left(-\frac{2\vartheta_p \vartheta_q}{2(2\vartheta_p + 2\vartheta_q)} (t-t')^2 \right) \nabla_{\vartheta_q} E_{pq}^{(r)}(t, t') \end{aligned}} \quad (25)$$

where

$$\boxed{\nabla_{\vartheta_q} \frac{\vartheta_q}{2\vartheta_p + 2\vartheta_q} = \frac{\vartheta_p + \cancel{\vartheta_q} - \cancel{\vartheta_q}}{(2\vartheta_p + 2\vartheta_q)^2} = \frac{\vartheta_p}{(2\vartheta_p + 2\vartheta_q)^2}} \quad (26)$$

and

$$\begin{aligned}
 \nabla_{v_p} \left(\frac{v_r \sqrt{v_p}}{v_p + v_q} \right) &= \left\{ \left[v_p^{1/2} u(t-t') + (v_q + (v_p - v_q) u(t-t')) \frac{1}{2} v_p^{-1/2} \right] (v_p + v_q)^{-1} \right. \\
 &\quad \left. - [v_q + (v_p - v_q) u(t-t')] v_p^{1/2} \right\} (v_p + v_q)^{-2} \\
 &= \left\{ v_p^2 u(t-t') + v_p v_q u(t-t') + \frac{v_p v_q}{2} + \frac{v_q^2}{2} \right. \\
 &\quad \left. + \frac{v_p^2 u(t-t')}{2} - \frac{v_q^2 u(t-t')}{2} - v_p v_q - v_p^2 u(t-t') \right. \\
 &\quad \left. + v_p v_q u(t-t') \right\} (v_p + v_q)^2 \sqrt{v_p}^{-1} \\
 &= \frac{v_q (v_q - v_p)/2 + (v_p^2 + 4 v_p v_q - v_q^2) u(t-t')/2}{(v_p + v_q)^2 \sqrt{v_p}}
 \end{aligned}$$

Alternatively this could be written as

$$\begin{aligned}
 \nabla_{v_p} \left(\frac{v_r \sqrt{v_p}}{v_p + v_q} \right) &= \left\{ \left[v_p^{1/2} u(t-t') + (v_q (1-u(t-t')) + v_p u(t-t')) \frac{1}{2} v_p^{-1/2} \right] \right. \\
 &\quad \times (v_p + v_q) - (v_q (1-u(t-t')) + v_p u(t-t')) v_p^{1/2} \\
 &\quad \times \left. \left\{ (v_p + v_q)^2 \right\}^{-1} \right\} \\
 &= \left\{ v_p^2 u(t-t') + v_p v_q u(t-t') + \frac{1}{2} v_p v_q (1-u(t-t')) \right. \\
 &\quad \left. + \frac{1}{2} v_p^2 u(t-t') + \frac{1}{2} v_q^2 (1-u(t-t')) + \frac{1}{2} v_p v_q u(t-t') \right\} \\
 &\quad - v_p v_q (1-u(t-t')) - v_p^2 u(t-t') \left\{ (v_p + v_q)^2 \sqrt{v_p} \right\}^{-1} \\
 &= \left\{ \overbrace{v_p v_q u(t-t')} + \overbrace{\frac{1}{2} v_p v_q} - \overbrace{\frac{1}{2} v_p v_q u(t-t')} + \overbrace{\frac{1}{2} v_p^2 u(t-t')} \right. \\
 &\quad \left. + \overbrace{\frac{1}{2} v_q^2} - \overbrace{\frac{1}{2} v_q^2 u(t-t')} + \overbrace{\frac{1}{2} v_p v_q u(t-t')} - v_p v_q \right\} \\
 &\quad + v_p v_q u(t-t') \left\{ (v_p + v_q)^2 \sqrt{v_p} \right\}^{-1} \\
 &= \left\{ \frac{1}{2} (v_q^2 - v_p v_q) + \frac{1}{2} (4 v_p v_q + v_p^2 - v_q^2) u(t-t') \right. \\
 &\quad \left. \times \left\{ (v_p + v_q)^2 \sqrt{v_p} \right\}^{-1} \right\}
 \end{aligned}$$

missing in p.8

$$\begin{aligned}
 \nabla_{\vartheta_q} E_{pq}^{(r)}(t, t') &= \frac{2}{\sqrt{\pi}} \left\{ \exp \left(-\frac{\vartheta_p \vartheta_q}{2} \left(\frac{\vartheta_p t + \vartheta_q t'}{\vartheta_p + \vartheta_q} \right)^2 \right) \right. \\
 &\quad \times \sqrt{\frac{\vartheta_p}{2}} \times \nabla_{\vartheta_q} \left. \frac{(\vartheta_p t + \vartheta_q t') \sqrt{\vartheta_q}}{\vartheta_p + \vartheta_q} \right) \\
 &\quad - \exp \left(-\frac{\vartheta_p \vartheta_q}{2} \left(\frac{\vartheta_q |t-t'|}{\vartheta_p + \vartheta_q} \right)^2 \right) \\
 &\quad \times \left. \frac{|t-t'| \sqrt{\vartheta_p}}{\sqrt{2}} \nabla_{\vartheta_q} \frac{\vartheta_q \sqrt{\vartheta_q}}{\vartheta_p + \vartheta_q} \right\}, \tag{27}
 \end{aligned}$$

with

$$\begin{aligned}
 \nabla_{\vartheta_q} \frac{(\vartheta_p t + \vartheta_q t') \sqrt{\vartheta_q}}{\vartheta_p + \vartheta_q} &= \frac{\frac{1}{2} \vartheta_q^{-1/2} (\vartheta_p t + \vartheta_q t') (\vartheta_p + \vartheta_q) + \vartheta_q^{1/2} t' (\vartheta_p + \vartheta_q)}{(\vartheta_p + \vartheta_q)^2} \\
 &= \frac{\vartheta_q^{1/2} (\vartheta_p t + \vartheta_q t')}{(\vartheta_p + \vartheta_q)^2} \\
 &= \left[\underbrace{\vartheta_p^2 t / 2}_{+} + \underbrace{\vartheta_p \vartheta_q t / 2}_{+} + \underbrace{\vartheta_p \vartheta_q t' / 2}_{+} + \underbrace{\vartheta_q^2 t' / 2}_{+} \right. \\
 &\quad \left. + \cancel{\vartheta_p \vartheta_q t'} + \cancel{\vartheta_q^2 t} - \cancel{\vartheta_p \vartheta_q t} - \cancel{\vartheta_q^2 t'} \right] \\
 &\quad \times (\vartheta_p + \vartheta_q)^{-2} (\vartheta_q)^{-1/2} \\
 &= \frac{\vartheta_p^2 t / 2 + \vartheta_p \vartheta_q (3t' - t) / 2 + \vartheta_q^2 t' / 2}{(\vartheta_p + \vartheta_q)^2 \sqrt{\vartheta_q}} \tag{28}
 \end{aligned}$$

and

$$\boxed{\nabla_{v_q} \frac{v_v \sqrt{v_p}}{v_p + v_q} = \frac{\frac{1}{2} v_q^{-1/2} v_v (v_p + v_q) + v_q^{1/2} (v_p + v_q) \nabla_{v_q} v_v}{(v_p + v_q)^2}}$$

$$\rightarrow \frac{v_v v_q^{1/2}}{(v_p + v_q)^2}$$

$$= [v_p v_v / 2 + v_q v_v / 2 + (v_p v_q + v_q^2) (1 - u(t-t')) - v_q v_v] / [(v_p + v_q)^2 \sqrt{v_q}]$$

$$= [v_p v_q (\overbrace{1 - u(t-t')} / 2 + \overbrace{v_p^2 u(t-t')} / 2 + v_q^2 (\overbrace{1 - u(t-t')} / 2 + v_p v_q u(t-t')) + v_p v_q (\overbrace{1 - u(t-t')} + v_q^2 (\overbrace{1 - u(t-t')} - v_q^2 (\overbrace{1 - u(t-t')} - v_p v_q u(t-t')))]$$

$$\times (v_p + v_q)^{-2} v_q^{-1/2}$$

$$= [v_p v_q / 2 + v_q^2 / 2 + v_p v_q + \cancel{v_q^2 - v_q^2} + ((\cancel{v_p^2 / 2}) v_p v_q / 2 - \cancel{v_q^2 / 2} + v_p v_q / 2 u(t-t') - v_p v_q - \cancel{v_q^2 + v_q^2} - v_p v_q)] / [(v_p + v_q)^2 \sqrt{v_q}]$$

$$= \frac{[3 v_p v_q + v_q^2] / 2 + (v_p^2 / 2 - 2 v_p v_q - v_q^2 / 2) u(t-t')}{(v_p + v_q)^2 \sqrt{v_q}}$$

where we have used the fact that

(29)

$$\boxed{\nabla_{v_q} v_v = 1 - u(t-t')} \quad (30)$$

(30)

$$\begin{aligned}
 \nabla_{\varphi_p} K_{Y_p Y_q}^{(r)}(t, t') &= -\frac{1}{2} \cdot \frac{\partial r^2}{\sqrt{8\pi}} (t-t')^2 \exp\left(-\frac{\varphi_p \varphi_q}{2(\varphi_p + \varphi_q)} (t-t')^2\right) \\
 &\quad \times E_{pq}^{(r)}(t, t') \times \nabla_{\varphi_p} \frac{\varphi_p \varphi_q}{\varphi_p + \varphi_q} \\
 &\quad + \frac{\partial r^2}{\sqrt{8\pi}} \exp\left(-\frac{\varphi_p \varphi_q}{2(\varphi_p + \varphi_q)} (t-t')^2\right) \nabla_{\varphi_p} E_{pq}^{(r)}(t, t') \\
 &= -\frac{1}{2} (t-t')^2 K_{Y_p Y_q}^{(r)}(t, t') \nabla_{\varphi_p} \frac{\varphi_p \varphi_q}{\varphi_p + \varphi_q} \\
 &\quad + \frac{\partial r^2}{\sqrt{8\pi}} \exp\left(-\frac{\varphi_p \varphi_q}{2(\varphi_p + \varphi_q)} (t-t')^2\right) \nabla_{\varphi_p} E_{pq}^{(r)}(t, t')
 \end{aligned}$$

$$\nabla_{\varphi_p} \frac{\varphi_p \varphi_q}{\varphi_p + \varphi_q} = \frac{(\varphi_q \nabla_{\varphi_p} \varphi_p + \varphi_p \nabla_{\varphi_p} \varphi_q)(\varphi_p + \varphi_q) - \varphi_p \varphi_q}{(\varphi_p + \varphi_q)^2} \Rightarrow$$

$$\nabla_{\varphi_p} \frac{\varphi_p \varphi_q}{\varphi_p + \varphi_q} = \frac{\varphi_q (\varphi_p + \varphi_q) - \cancel{\varphi_p} \cancel{\varphi_q}}{(\varphi_p + \varphi_q)^2} = \frac{\cancel{\varphi_q}^2}{(\varphi_p + \varphi_q)^2}$$

$$\nabla_{\varphi_q} \frac{\varphi_p \varphi_q}{\varphi_p + \varphi_q} = \frac{\varphi_p (\varphi_p + \cancel{\varphi_q}) - \cancel{\varphi_p} \varphi_q}{(\varphi_p + \varphi_q)^2} = \frac{\cancel{\varphi_p}^2}{(\varphi_p + \varphi_q)^2}$$

$$\begin{aligned}
 \nabla_{\varphi_p} E_{pq}^{(r)}(t, t') &= \frac{\sqrt{2}}{\sqrt{\pi}} \left\{ \exp\left(-\frac{\varphi_p \varphi_q}{2} \left(\frac{\varphi_p t + \varphi_q t'}{\varphi_p + \varphi_q}\right)^2\right) \right. \\
 &\quad \times \nabla_{\varphi_p} \left[\sqrt{\varphi_p \varphi_q} \cdot \frac{\varphi_p t + \varphi_q t'}{\varphi_p + \varphi_q} \right] \\
 &\quad \left. - \frac{1}{\sqrt{2}} \exp\left(-\frac{\varphi_p \varphi_q}{2} \left(\frac{\varphi_p |t-t'|}{\varphi_p + \varphi_q}\right)^2\right) \right. \\
 &\quad \left. \times \nabla_{\varphi_p} \left[\sqrt{\varphi_p \varphi_q} \cdot \frac{\varphi_p |t-t'|}{\varphi_p + \varphi_q} \right] \right\}
 \end{aligned}$$

$$\begin{aligned}
 \nabla_{\varphi_p} \frac{(\varphi_p t + \varphi_q t') \varphi_p^{1/2} \varphi_q^{1/2}}{\varphi_p + \varphi_q} &= \left\{ \left[(\varphi_p t + \varphi_q t') \varphi_p^{1/2} \varphi_q^{1/2} \right. \right. \\
 &\quad + (\varphi_p t + \varphi_q t') \varphi_q^{1/2} \nabla_{\varphi_p} \varphi_p^{1/2} \\
 &\quad + (\varphi_p t + \varphi_q t') \varphi_p^{1/2} \nabla_{\varphi_q} \varphi_q^{1/2} \left. \left. \right] \right. \\
 &\quad \times (\varphi_p + \varphi_q) \\
 &\quad - (\varphi_p t + \varphi_q t') \varphi_p^{1/2} \varphi_q^{1/2} \left\{ (\varphi_p + \varphi_q)^{-2} \right. \\
 \\
 &= \left\{ \left[(\varphi_p t + \varphi_q t') \varphi_p \varphi_q \right. \right. \\
 &\quad + \frac{1}{2} (\varphi_p t + \varphi_q t') (\varphi_q \delta_{\varphi_p} + \varphi_p \delta_{\varphi_q}) \left. \left. \right] \right. \\
 &\quad \times (\varphi_p + \varphi_q) - (\varphi_p t + \varphi_q t') \varphi_p \varphi_q \left. \left. \right\} \\
 &\quad \times \left[(\varphi_p + \varphi_q)^2 \varphi_p^{1/2} \varphi_q^{1/2} \right]^{-1}
 \end{aligned}$$

Therefore,

$$\begin{aligned}
 \nabla_{\varphi_p} \frac{(\varphi_p t + \varphi_q t') \varphi_p^{1/2} \varphi_q^{1/2}}{\varphi_p + \varphi_q} &= \left\{ \left[\varphi_p \varphi_q t + \frac{1}{2} \varphi_q (\varphi_p t + \varphi_q t') \right] \right. \\
 &\quad \times (\varphi_p + \varphi_q) - (\varphi_p t + \varphi_q t') \varphi_p \varphi_q \left. \left. \right\} \\
 &\quad \times \left[(\varphi_p + \varphi_q)^2 \varphi_p^{1/2} \varphi_q^{1/2} \right]^{-1} \\
 \\
 &= \frac{\varphi_p^2 \varphi_q^2 t + \varphi_p \varphi_q^2 t + \frac{1}{2} \varphi_p^2 \varphi_q t + \frac{1}{2} \varphi_p \varphi_q^2 t + \frac{1}{2} \varphi_p \varphi_q^2 t' + \frac{1}{2} \varphi_q^3 t'}{(\varphi_p + \varphi_q)^2 \sqrt{\varphi_p \varphi_q}} \\
 \\
 &= \frac{\cancel{\varphi_p^2 \varphi_q^2 t} + \varphi_p \varphi_q^2 t + \frac{1}{2} \varphi_p^2 \varphi_q t + \frac{1}{2} \varphi_p \varphi_q^2 t + \frac{1}{2} \varphi_p \varphi_q^2 t' + \frac{1}{2} \varphi_q^3 t'}{(\varphi_p + \varphi_q)^2 \sqrt{\varphi_p \varphi_q}} \Rightarrow
 \end{aligned}$$

$$\nabla_{v_p} \frac{(v_p t + v_q t') v_p^{1/2} v_q^{1/2}}{v_p + v_q} = \frac{(3 v_p^2 v_q^2 + v_p^2 v_q^2) t + (v_q^3 - v_p v_q^2) t'}{2 (v_p + v_q)^2 \sqrt{v_p v_q}}$$

$$\nabla_{v_q} \frac{(v_p t + v_q t') v_p^{1/2} v_q^{1/2}}{v_p + v_q}$$

$$= \left\{ [v_p v_q t' + \frac{1}{2} (v_p t + v_q t') v_p] (v_p + v_q) - (v_p t + v_q t') v_p v_q \right\} \\ \times [(v_p + v_q)^2 \sqrt{v_p v_q}]^{-1}$$

$$= \frac{\overbrace{v_p^2 v_q^2 t' + v_p v_q^2 t'} + \frac{1}{2} \overbrace{v_p^3 t + \frac{1}{2} v_p^2 v_q^2 t + \frac{1}{2} v_p^2 v_q^2 t' + \frac{1}{2} v_p^2 v_q^2 t'}}{(v_p + v_q)^2 \sqrt{v_p v_q}}$$

$$- \frac{\overbrace{v_p^2 v_q^2 t} + \overbrace{v_p v_q^2 t'}}{(v_p + v_q)^2 \sqrt{v_p v_q}} \Rightarrow$$

$$\nabla_{v_q} \frac{(v_p t + v_q t') \sqrt{v_p v_q}}{v_p + v_q} = \frac{(v_p^3 - v_p^2 v_q^2) t + (3 v_p^2 v_q^2 + v_p v_q^2) t'}{2 (v_p + v_q)^2 \sqrt{v_p v_q}}$$

And finally,

$$\nabla_{v_p} \frac{v_v \sqrt{v_p v_q} |t - t'|}{v_p + v_q} = \nabla_{v_p} \frac{[v_q + (v_p - v_q) u(t-t')] \sqrt{v_p v_q} |t - t'|}{v_p + v_q}$$

$$= \left\{ \left[\nabla_{v_p} v_q + (\nabla_{v_p} v_p - \nabla_{v_p} v_q) u(t-t') \right] \sqrt{v_p v_q} |t - t'| \right. \\ + [v_q + (v_p - v_q) u(t-t')] |t - t'| \left(v_q^{1/2} \cdot \frac{1}{2} v_p^{-1/2} \nabla_{v_p} v_p \right. \\ \left. + v_p^{1/2} \cdot \frac{1}{2} v_q^{-1/2} \nabla_{v_p} v_q \right) \left. \right) (v_p + v_q) \\ - [v_q + (v_p - v_q) u(t-t')] \sqrt{v_p v_q} |t - t'| \times (v_p + v_q)^{-2} \Rightarrow$$

$$\nabla_{\varphi_q} \frac{\varphi_v \sqrt{\varphi_p \varphi_q} |t-t'|}{\varphi_p + \varphi_q} = \left\{ \begin{aligned} & \left[(1-u(t-t')) \delta_{\varphi_q} + u(t-t') \delta_{\varphi_p} \right] \varphi_p \varphi_q (\varphi_p + \varphi_q) |t-t'| \\ & + \frac{1}{2} \left[\varphi_q (1-u(t-t')) + \varphi_p u(t-t') \right] (\varphi_q \delta_{\varphi_p} + \varphi_p \delta_{\varphi_q}) \\ & \times (\varphi_p + \varphi_q) |t-t'| \\ & - \left[\varphi_q (1-u(t-t')) + \varphi_p u(t-t') \right] \varphi_p \varphi_q |t-t'| \end{aligned} \right\} \\ & \times \left\{ (\varphi_p + \varphi_q)^2 \sqrt{\varphi_p \varphi_q} \right\}^{-1}$$

Now, let's focus on the gradient w.r.t. φ_p :

$$\nabla_{\varphi_p} \frac{\varphi_v \sqrt{\varphi_p \varphi_q} |t-t'|}{\varphi_p + \varphi_q} = \left\{ \begin{aligned} & \left[\varphi_p \varphi_q (\varphi_p + \varphi_q) u(t-t') + \frac{1}{2} \varphi_q^2 (\varphi_p + \varphi_q) (1-u(t-t')) \right. \\ & \left. + \frac{1}{2} \varphi_p \varphi_q (\varphi_p + \varphi_q) u(t-t') \right. \\ & \left. - \varphi_p \varphi_q^2 (1-u(t-t')) - \cancel{\varphi_p^2 \varphi_q u(t-t')} \right] |t-t'| \end{aligned} \right\} \\ & \times \left\{ (\varphi_p + \varphi_q)^2 \sqrt{\varphi_p \varphi_q} \right\}^{-1} \\ = & \left\{ \left[\frac{\varphi_q^2}{2} (\varphi_q - \varphi_p) + \frac{\varphi_q}{2} (4\varphi_p \varphi_q + \varphi_p^2 - \varphi_q^2) u(t-t') \right] \right. \\ & \left. \times |t-t'| \right\} \left\{ (\varphi_p + \varphi_q)^2 \sqrt{\varphi_p \varphi_q} \right\}^{-1}$$

And w.r.t. φ_q :

$$\nabla_{\varphi_q} \frac{\varphi_v \sqrt{\varphi_p \varphi_q} |t-t'|}{\varphi_p + \varphi_q} = \left\{ \begin{aligned} & \left[\varphi_p \varphi_q (\varphi_p + \varphi_q) (1-u(t-t')) + \frac{1}{2} \varphi_p \varphi_q (\varphi_p + \varphi_q) (1-u(t-t')) \right. \\ & \left. + \frac{1}{2} \varphi_p^2 (\varphi_p + \varphi_q) u(t-t') - \varphi_p \varphi_q^2 (1-u(t-t')) \right. \\ & \left. - \varphi_p^2 \varphi_q u(t-t') \right] |t-t'| \right\} \left\{ (\varphi_p + \varphi_q)^2 \sqrt{\varphi_p \varphi_q} \right\}^{-1} \\ = & \left\{ \left[\frac{\varphi_p \varphi_q}{2} (3\varphi_p + \varphi_q) + \frac{\varphi_p}{2} (\varphi_p^2 - 4\varphi_p \varphi_q - \varphi_q^2) u(t-t') \right] \right. \\ & \left. \times |t-t'| \right\} \left\{ (\varphi_p + \varphi_q)^2 \sqrt{\varphi_p \varphi_q} \right\}^{-1}$$