1

$1,2$

R

T

$$reso(resampled)/reso(input)$$

$$t \times f_{\mathrm{res}} / T_{\mathrm{sys}}^2$$

t

$$f_{\mathrm{res}}$$

T_{sys}

$$1/\sigma^2$$

σ

S

$$(N-1)^{th}$$

N^{th}

$$\gamma_R$$

$$\gamma_T$$

$$r_S = \max(|r_R|, |r_T|)$$

$$x_{\min,S}$$

$$\min(x_{\min,R}, x_{\min,T})$$

$$x_{\max,S}$$

$$\max(x_{\max,R}, x_{\max,T})$$

$$\max(x_{\min,R}, x_{\min,T})$$

$$\min(x_{\max,R}, x_{\max,T})$$

N

$$N_S = \mathrm{int}(\frac{x_{\max,S} - x_{\min,S}}{r_S} + 1.5),$$

0

$$x_{\mathrm{val},S} = x_{\mathrm{min},S} - 1. \times r_S,$$

$$x_{\min,S}$$

x

$$[x_{\min,S}, x_{\max,S}]$$

N_S

$$T(i)$$

$$w(i)$$

Averaged channel intensity and weight (aligned spectra):

$$T_S(i) = \frac{w_R(i) \times T_R(i) + w_T(i) \times T_T(i)}{w_R(i) + w_T(i)} \tag{1}$$

$$w_S(i) = w_R(i) + w_T(i) \tag{2}$$

R'

T'

$j\min$

$j\max$

$$k_{\min}$$

$$k_{\max}$$

$$S(i)$$

$$T_R$$

i

$$N(\mu_R, {\sigma_R}^2)$$

$$\mathrm{pdf}_R(x) = \frac{1}{\sigma_R\sqrt{2\pi}} \exp\left(-\frac{(x-\mu_R)^2}{2{\sigma_R}^2}\right)$$

$$\mu_R$$

$$\sigma_R$$

$$\mathrm{var}(T_R(i)) = \sigma_R(i)^2$$

$$w_R(i)$$

$$w_R(i) = \frac{1}{\sigma_R(i)^2}$$

Resampled channel intensity (all weights):

$$T_{R'}(i) = \frac{\sum_{j=j_{\min}}^{j_{\max}} f_R(j) \times w_R(j) \times T_R(j)}{\sum_{j=j_{\min}}^{j_{\max}} f_R(j) \times w_R(j)} \tag{3}$$

$$f(j)$$

$$f(j) = 0$$

$$f(j) = 1$$

$$0 < f(j) < 1$$

β

$$\alpha(j)$$

$$\beta = \sum_{j=j_{\mathrm{min}}}^{j_{\mathrm{max}}} f_R(j) \times w_R(j)$$

$$\alpha_R(j) = \frac{f_R(j) \times w_R(j)}{\beta}$$

$$T_{R'}(i)$$

$$T_{R'}(i) = \sum_{j=j_{\min}}^{j_{\max}} \alpha_R(j) \times T_R(j)$$

$$w_{R'}(i)$$

$$\mathrm{var}(T_{R'}(i))$$

$$\mathrm{var}\left(\sum_{j=j_{\min}}^{j_{\max}} \alpha_R(j) \times T_R(j)\right)$$

$$\sum_{j=j_{\min}}^{j_{\max}} \alpha_R(j)^2 \times \mathrm{var}\left(T_R(j)\right)$$

$$\frac{1}{\beta^2} \sum_{j=j_{\min}}^{j_{\max}} f_R(j)^2 \, w_R(j)$$

$$\mathrm{var}(aX + bY) = a^2\mathrm{var}(X) + b^2\mathrm{var}(Y)$$

a

b

X

Y

Resampled channel weight (weights `TIME` and SIGMA):

$$w_{R'}(i) = \frac{\left(\sum_{j=j_{\min}}^{j_{\max}} f_R(j) w_R(j)\right)^2}{\sum_{j=j_{\min}}^{j_{\max}} f_R(j)^2 \, w_R(j)} \tag{4}$$

R'

0.0

0.25

0.5

$$x_{\mathrm{val}}$$

$$\mathcal{W}_{R'}$$

$$\sigma_{R'}$$

$$x_{\mathrm{val}} \rightarrow x_{\mathrm{val}} + 0.00$$

$$w_{R'} = w_R$$

$$\sigma_{R'} = \sigma_R$$

$$x_{\mathrm{val}} \rightarrow x_{\mathrm{val}} + 0.25$$

$$w_{R'} = 1.6 \times w_R$$

$$\sigma_{R'} = \sigma_R / \sqrt{1.6}$$

$$x_{\mathrm{val}} \rightarrow x_{\mathrm{val}} + 0.50$$

$$w_{R'} = 2 \times w_R$$

$$\sigma_{R'} = \sigma_R / \sqrt{2}$$

$$\sigma_R(j)$$

$$\mathcal{W}_{R'} / \mathcal{W}_{R}$$

$$\sqrt{2}$$

$$R' \to R''$$

Resampled channel weight (weight `EQUAL`):

$$w_{R'}(i) = \frac{\sum_{j=j_{\min}}^{j_{\max}} f_R(j) w_R(j)}{\sum_{j=j_{\min}}^{j_{\max}} f_R(j)} \tag{5}$$

$$w_R(j)$$

1.0

T_S

w_S

Averaged channel intensity and weight (non-aligned spectra):

$$T_S(i) = \frac{w_{R'}(i) \times T_{R'}(i) + w_{T'}(i) \times T_{T'}(i)}{w_{R'}(i) + w_{T'}(i)} \tag{6}$$

$$w_S(i) = w_{R'}(i) + w_{T'}(i) \tag{7}$$

$$f \neq 0$$

''

obs

S_{in}

S_{out}

$$t_{S_{\mathrm{out}}}$$

$$t_{S_{\mathrm{out}}} = t_{S_{\mathrm{in}}} + t_{\mathrm{obs}}$$

$$T_{\mathrm{sys}}, S_{\mathrm{out}}$$

$$t \times |r| / T_{\mathrm{sys}}^2$$

γ

$$\frac{t_{S_{\mathrm{out}}} \times |r_{S_{\mathrm{out}}}|}{T^2_{\mathrm{sys},S_{\mathrm{out}}}} = \frac{t_{S_{\mathrm{in}}} \times |r_{S_{\mathrm{in}}}|}{T^2_{\mathrm{sys},S_{\mathrm{in}}}} + \frac{t_{\mathrm{obs}} \times |r_{\mathrm{obs}}|}{T^2_{\mathrm{sys,obs}}}$$

$$f_{\mathrm{res},S_{\mathrm{out}}}$$

$$f_{\mathrm{off}}, S_{\mathrm{out}}$$

$$f_{\mathrm{off}}, S_{\mathrm{in}}$$

$$f_{\text{off}}$$

$$(f_{\mathrm{off},S_{\mathrm{out}}} - x_{\mathrm{val},S_{\mathrm{out}}})/f_{\mathrm{res},S_{\mathrm{out}}}$$

$$f(i_{\mathrm{chan}}) = f_{\mathrm{res}} \times (i_{\mathrm{chan}} - r_{\mathrm{chan}}) + f_{\mathrm{off}}$$

$$i_{\mathrm{chan}} = 0$$

$$x_{\mathrm{val}} = f_{\mathrm{res}} \times (0 - r_{\mathrm{chan}}) + f_{\mathrm{off}}$$

$$v_{\mathrm{res},S_{\mathrm{out}}}$$

$$-c \times f_{\mathrm{res},S_{\mathrm{out}}} / f_{\mathrm{rest},S_{\mathrm{out}}}$$

C

f_{rest}

$$v_{\mathrm{off}}, S_{\mathrm{out}}$$

$$v_{\mathrm{off}}, S_{\mathrm{in}}$$

$$v_{\mathrm{off}}$$

$$(v_{\mathrm{off},S_{\mathrm{out}}} - x_{\mathrm{val},S_{\mathrm{out}}})/v_{\mathrm{res},S_{\mathrm{out}}}$$

$$-f_{\mathrm{rest},S_{\mathrm{out}}} \times v_{\mathrm{res},S_{\mathrm{out}}}/c$$