gaussian_int((nxa-i+nxb-j), gamma)

$$\int dx\left(x - X_p\right)^{nx_a + nx_b - (i+j)} \exp(-\gamma_{ab}(x - X_{ab})^2)$$

double gaussian_overlap_ref(int nxa, double alp_a, double Xa, int nxb, double alp_b, double Xb) computes $\langle (x - X_a)^{nx_a} G_a(x;\alpha_a, X_a) | (x - X_b)^{nx_b} G_b(x;\alpha_b, X_b) \rangle$

Consider that Gaussians are given as:

$$G(x;\alpha, X) = \exp(-\alpha(x - X)^2)$$

Then:

$$\begin{aligned} G_a(x;\alpha_a, X_a) G_b(x;\alpha_b, X_b) &= \exp(-\alpha_a(x - X_a)^2) \exp(-\alpha_b(x - X_b)^2) \\ &= \exp\left(-\frac{\alpha_a \alpha_b}{(\alpha_a + \alpha_b)}(X_b - X_a)^2\right) \exp(-\gamma_{ab}(x - X_{ab})^2) \end{aligned}$$

The basic overlap is:

$$\begin{aligned} S_{ab} &= \langle G_a(x;\alpha_a, X_a) | G_b(x;\alpha_b, X_b) \rangle \\ &= \exp\left(-\frac{\alpha_a \alpha_b}{(\alpha_a + \alpha_b)}(X_b - X_a)^2\right) \int dx \exp(-\gamma_{ab}(x - X_{ab})^2) \end{aligned}$$

Because:

$$\begin{aligned} \alpha_a(x - X_a)^2 + \alpha_b(x - X_b)^2 &= \alpha_a(x^2 - 2xX_a + X_a^2) + \alpha_b(x^2 - 2xX_b + X_b^2) \\ &= (\alpha_a + \alpha_b)x^2 - 2(\alpha_a X_a + \alpha_b X_b)x + (\alpha_a X_a^2 + \alpha_b X_b^2) \\ &= (\alpha_a + \alpha_b)\left[x^2 - \frac{2(\alpha_a X_a + \alpha_b X_b)}{(\alpha_a + \alpha_b)}x + \frac{(\alpha_a X_a^2 + \alpha_b X_b^2)}{(\alpha_a + \alpha_b)}\right] \\ &= \gamma_{ab}\left[x^2 - 2X_{ab}x + \frac{(\alpha_a X_a^2 + \alpha_b X_b^2)}{(\alpha_a + \alpha_b)}\right] \\ &= \gamma_{ab}\left[x^2 - 2X_{ab}x + X_{ab}^2 - X_{ab}^2 + \frac{(\alpha_a X_a^2 + \alpha_b X_b^2)}{(\alpha_a + \alpha_b)}\right] \\ &= \gamma_{ab}(x - X_{ab})^2 + \gamma_{ab}\left[\frac{(\alpha_a X_a^2 + \alpha_b X_b^2)}{(\alpha_a + \alpha_b)} - X_{ab}^2\right] \\ &= \gamma_{ab}(x - X_{ab})^2 + \frac{\alpha_a \alpha_b}{(\alpha_a + \alpha_b)}(X_b - X_a)^2 \end{aligned}$$

Where:

$$\gamma = \alpha_a + \alpha_b$$

$$X_{ab} = \frac{(\alpha_a X_a + \alpha_b X_b)}{(\alpha_a + \alpha_b)}$$

Because:

$$\frac{(\alpha_a X_a^2 + \alpha_b X_b^2)}{(\alpha_a + \alpha_b)} - X_{ab}^2 = \frac{(\alpha_a X_a^2 + \alpha_b X_b^2)}{(\alpha_a + \alpha_b)} - \frac{(\alpha_a X_a + \alpha_b X_b)^2}{(\alpha_a + \alpha_b)^2}$$
$$= \frac{(\alpha_a X_a^2 + \alpha_b X_b^2)(\alpha_a + \alpha_b) - (\alpha_a X_a + \alpha_b X_b)^2}{(\alpha_a + \alpha_b)^2} = \frac{\alpha_a \alpha_b (X_b - X_a)^2}{(\alpha_a + \alpha_b)^2}$$

Because:

$$(\alpha_a X_a^2 + \alpha_b X_b^2)(\alpha_a + \alpha_b) - (\alpha_a X_a + \alpha_b X_b)^2$$
$$= \alpha_a^2 X_a^2 + \alpha_a \alpha_b X_b^2 + \alpha_b \alpha_a X_a^2 + \alpha_b^2 X_b^2 - (\alpha_a^2 X_a^2 + 2\alpha_a X_a \alpha_b X_b + \alpha_b^2 X_b^2)$$
$$= +\alpha_a \alpha_b X_b^2 + \alpha_b \alpha_a X_a^2 - (2\alpha_a X_a \alpha_b X_b) = \alpha_a \alpha_b (X_b - X_a)^2$$

Now consider:

$$(x - X_a)^{nx_a} = (x - X_{ab} + X_{ab} - X_a)^{nx_a} = \sum_{i=0}^{nx_a} C_{nx_a}^i (x - X_{ab})^{nx_a - i} (X_{ab} - X_a)^i$$

Thus, without normalization:

$$\langle (x - X_a)^{nx_a} G_a(x; \alpha_a, X_a) | (x - X_b)^{nx_b} G_b(x; \alpha_b, X_b) \rangle$$
$$= \sum_{i=0}^{nx_a} \sum_{j=0}^{nx_b} \int dx C_{nx_a}^i (x - X_{ab})^{nx_a - i} (X_{ab} - X_a)^i C_{nx_b}^j (x - X_{ab})^{nx_b - j} (X_{ab}$$
$$- X_b)^j \exp\left(-\frac{\alpha_a \alpha_b}{(\alpha_a + \alpha_b)} (X_b - X_a)^2\right) \exp(-\gamma_{ab}(x - X_{ab})^2)$$
$$= \sum_{i=0}^{nx_a} \sum_{j=0}^{nx_b} C_{nx_a}^i C_{nx_b}^j (X_{ab} - X_a)^i (X_{ab}$$
$$- X_b)^j \exp\left(-\frac{\alpha_a \alpha_b}{(\alpha_a + \alpha_b)} (X_b - X_a)^2\right) \int dx (x$$
$$- X_{ab})^{nx_a + nx_b - (i+j)} \exp(-\gamma_{ab}(x - X_{ab})^2)$$

This is done by the function:

double gaussian_moment_ref(int nx, double alp, double X, int nxa,double alp_a, double Xa, int nxb,double alp_b, double Xb) computes

$$\langle (x - X_a)^{nx_a} G_a(x; \alpha_a, X_a) | (x - X_c)^{nx_c} G_c(x; \alpha_c, X_c) | (x - X_b)^{nx_b} G_b(x; \alpha_b, X_b) \rangle$$

Using the Gaussian contraction formula:

$$G_c(x; \alpha_c, X_c) G_b(x; \alpha_b, X_b) = \exp\left(-\frac{\alpha_c \alpha_b}{(\alpha_c + \alpha_b)} (X_c - X_b)^2\right) \exp(-\gamma_{cb}(x - X_{cb})^2)$$

Where:

$$X_{cb} = \frac{(\alpha_c X_c + \alpha_b X_b)}{(\alpha_c + \alpha_b)}$$

$$\gamma_{cb} = \alpha_c + \alpha_b$$

Then express the middle GTO in terms of the center of the contraction of GTOs c and b:

$$(x - X_c)^{nx_c} = (x - X_{cb} + X_{cb} - X_c)^{nx_c} = \sum_{k=0}^{nx_c} C_{nx_c}^k (x - X_{cb})^{nx_c - k} (X_{cb} - X_c)^k$$

So:

$$\begin{aligned} &(x - X_c)^{nx_c} G_c(x; \alpha_c, X_c)(x - X_b)^{nx_b} G_b(x; \alpha_b, X_b) \\ &\quad = \sum_{k=0}^{nx_c} C_{nx_c}^k (X_{cb} - X_c)^k \exp\left(-\frac{\alpha_c \alpha_b}{(\alpha_c + \alpha_b)} (X_c - X_b)^2\right) (x \\ &\quad - X_{cb})^{nx_c - k} \exp(-\gamma_{cb}(x - X_{cb})^2) \end{aligned}$$

Then:

$$I_{acb} = \langle (x - X_a)^{nx_a} G_a(x;\alpha_a, X_a) | (x - X_c)^{nx_c} G_c(x;\alpha_c, X_c) | (x - X_b)^{nx_b} G_b(x;\alpha_b, X_b) \rangle$$
$$= \exp\left(-\frac{\alpha_c \alpha_b}{(\alpha_c + \alpha_b)} (X_c - X_b)^2\right) \sum_{k=0}^{nx_c} C_{nx_c}^k (X_{cb}$$
$$- X_c)^k \langle (x - X_a)^{nx_a} G_a(x;\alpha_a, X_a) | (x - X_{cb})^{nx_c - k} G_{cb}(x;\gamma_{cb}, X_{cb}) \rangle$$
$$= \exp\left(-\frac{\alpha_c \alpha_b}{(\alpha_c + \alpha_b)} (X_c - X_b)^2\right) \sum_{k=0}^{nx_c} C_{nx_c}^k (X_{cb} - X_c)^k S_{a,cb}^{(k)}$$

Now compute the derivatives:

$$S_{a,cb}^{(k)} = \langle (x - X_a)^{nx_a} G_a(x;\alpha_a, X_a) | (x - X_{cb})^{nx_c - k} G_{cb}(x;\gamma_{cb}, X_{cb}) \rangle$$

$\frac{dS_{a,cb}^{(k)}}{dX_a}$ - directly

$\frac{dS_{a,cb}^{(k)}}{dX_c} = \frac{dS_{a,cb}^{(k)}}{dX_{cb}} \frac{dX_{cb}}{dX_c} = \frac{\alpha_c}{\gamma_{cb}} \frac{dS_{a,cb}^{(k)}}{dX_{cb}}$,

$\frac{dS_{a,cb}^{(k)}}{dX_b} = \frac{dS_{a,cb}^{(k)}}{dX_{cb}} \frac{dX_{cb}}{dX_b} = \frac{\alpha_b}{\gamma_{cb}} \frac{dS_{a,cb}^{(k)}}{dX_{cb}}$.

$$\frac{dI_{abc}}{dX_a} = \exp\left(-\frac{\alpha_c \alpha_b}{(\alpha_c + \alpha_b)} (X_c - X_b)^2\right) \sum_{k=0}^{nx_c} C_{nx_c}^k (X_{cb} - X_c)^k \ \frac{dS_{a,cb}^{(k)}}{dX_a}$$

$$\frac{dI_{abc}}{dX_c} = -\frac{2\alpha_c \alpha_b}{(\alpha_c + \alpha_b)} (X_c - X_b) I_{abc}$$
$$+ \exp\left(-\frac{\alpha_c \alpha_b}{(\alpha_c + \alpha_b)} (X_c - X_b)^2\right) \sum_{k=0}^{nx_c} C_{nx_c}^k \Bigg[k (X_{cb} - X_c)^{k-1} \ \left(\frac{\alpha_c}{\gamma_{cb}} - 1\right) S_{a,cb}^{(k)}$$
$$+ (X_{cb} - X_c)^k \frac{dS_{a,cb}^{(k)}}{dX_{cb}} \frac{\alpha_c}{\gamma_{cb}} \Bigg]$$

$$\frac{dI_{abc}}{dX_b} = \frac{2\alpha_c \alpha_b}{(\alpha_c + \alpha_b)} (X_c - X_b) I_{abc}$$
$$+ \exp\left(-\frac{\alpha_c \alpha_b}{(\alpha_c + \alpha_b)} (X_c - X_b)^2\right) \sum_{k=0}^{nx_c} C_{nx_c}^k \Bigg[k (X_{cb} - X_c)^{k-1} \frac{\alpha_b}{\gamma_{cb}} S_{a,cb}^{(k)}$$
$$+ (X_{cb} - X_c)^k \frac{dS_{a,cb}^{(k)}}{dX_{cb}} \frac{\alpha_b}{\gamma_{cb}} \Bigg]$$