In general, we are looking to fit single contracted Gaussian-type functions by a sums of contracted and uncontracted Gaussian-type functions (i.e. split-valence basis sets). In the simplest possible case, H_2, the minimal basis set is described by a single s-type contracted Gaussian-type function, and we are fitting this function using only split-valence basis sets made up of s-type functions (in any case, basis functions of different angular momentum will have zero overlap by symmetry, except perhaps the s-type component of Cartesian d-functions):

$$\phi_{\mathrm{MBS}}(\mathbf{r}) = \sum_{j=1}^{n} c_{1,j}\ e^{-\alpha_{1,j} r^2} \tag{1}$$

$$\phi_{\mathrm{CBS}}(\mathbf{r}) = \sum_{k=1}^{N} C_k \sum_{i=1}^{n_k} c_{k,i}\ e^{-\alpha_{k,i} r^2} \tag{2}$$

Here, N represents the number of contracted basis functions per atom and n is the number of primitive Gaussian-type functions per shell. We will use i and j as primitive basis function indices and k and l as contracted basis function indices.

In other words, we want to determine what values of C_l to choose so that ϕ_{CBS} most closely reproduces ϕ_{MBS}. The pre-determined contraction coefficients $c_{1,j}$ and $c_{k,i}$ are chosen so that each subshell in the split-valence basis is normalized.

Minimizing the integrated squared difference between ϕ_{MBS} and ϕ_{CBS}, R^2, with respect to changes in contraction coefficients C_k:

$$\begin{aligned}
R^2 &= \int \left(\phi_{\mathrm{MBS}}(\mathbf{r}) - \phi_{\mathrm{CBS}}(\mathbf{r})\right)^2 d\mathbf{r} \\
&= 1 + \int \phi_{\mathrm{CBS}}(\mathbf{r})\phi_{\mathrm{CBS}}(\mathbf{r}) d\mathbf{r} - 2\int \phi_{\mathrm{MBS}}(\mathbf{r})\phi_{\mathrm{CBS}}(\mathbf{r}) d\mathbf{r} \\
&= 1 + \sum_{k=1}^{N}\sum_{l=1}^{N} C_k C_l \sum_{i=1}^{n_k}\sum_{j=1}^{n_l} c_{k,i} c_{l,j} \int e^{-(\alpha_{k,i}+\alpha_{l,j}) r^2} d\mathbf{r} \\
&\quad - 2\sum_{k=1}^{N} C_k \sum_{i=1}^{n_k}\sum_{j=1}^{n} c_{k,i} c_{1,j} \int e^{-(\alpha_{k,i}+\alpha_{1,j}) r^2} d\mathbf{r}
\end{aligned} \tag{3}$$

Defining some handy intermediate quantities:

$$S_{k,l} = \sum_{i=1}^{n_k}\sum_{j=1}^{n_l} c_{k,i}\ c_{l,j} \left(\frac{\pi}{\alpha_{k,i}+\alpha_{l,j}}\right)^{3/2} \tag{4}$$

$$T_k = \sum_{i=1}^{n_k}\sum_{j=1}^{n} c_{k,i}\ c_{1,j} \left(\frac{\pi}{\alpha_{k,i}+\alpha_{1,j}}\right)^{3/2} \tag{5}$$

Note: $S_{k,k} = 1$ by intermediate normalization of subshells.

$$\begin{aligned} R^2 &= 1 + \sum_{k=1}^{N} \sum_{l=1}^{N} C_k C_l S_{k,l} - 2 \sum_{k=1}^{N} C_k T_k \\ &= 1 + \sum_{k=1}^{N} \sum_{l \neq k}^{N} C_k C_l S_{k,l} + \sum_{k=1}^{N} C_k^2 - 2 \sum_{k=1}^{N} C_k T_k \end{aligned} \tag{6}$$

Minimize R^2 by requiring partial derivatives with respect to C_k to be zero:

$$\frac{dR^2}{dC_k} = \sum_{l \neq k}^{N} C_l S_{k,l} + 2C_k - 2T_k = 0 \tag{7}$$

In matrix form,

$$\vec{\mathbf{A}}\mathbf{x} = \mathbf{b} \tag{8}$$

where $\mathbf{x}$ is the unknown coefficient vector and:

$$\begin{aligned} A_{k,l} &= (S_{k,l} + S_{l,k}) \text{ if } k \neq l \\ &= 2S_{k,k} \text{ otherwise} \end{aligned} \tag{9}$$

$$b_k = 2T_k \tag{10}$$

Even more simply,

$$A_{k,l} = 2S_{k,l} \tag{11}$$

$$b_k = 2T_k \tag{12}$$

And, in fact, we don't even have to bother with the factor of two, as it will cancel on both sides of the matrix equation:

$$A_{k,l} = S_{k,l} \tag{13}$$

$$b_k = T_k \tag{14}$$