3.10 Schmidts orthonormalization procedure

Having a set of linearly independent vectors $\vec{v}_i$, there exists a simple straight forward, but time consuming procedure to create an orthonormal set of vectors $\vec{e}_i$.

(i) Calculate

$$\vec{e}_1 = \frac{\vec{v}_1}{|\vec{v}_1|} ,$$

set $i = 2$.

(ii) Calculate

$$\vec{b}_i = \vec{v}_i - \sum_{j=1}^{i-1} \langle \vec{v}_i \, | \vec{e}_j \rangle \, \vec{e}_j .$$

(iii) Calculate

$$\vec{e}_i = \frac{\vec{b}_i}{|\vec{b}_i|} ,$$

increase i by 1 and continue at item (ii) until all basic vectors have been calculated.

Since the vectors $\vec{v}_i$ are linearly independent, non of the calculated vectors $\vec{b}_i$ will get zero. By dividing each resulting vector $\vec{b}_i$ by it's length $\vec{e}_i$ are normal and by the procedure of subtracting all parallel components one enforces

$$\langle \vec{e}_i | \, \vec{e}_j \rangle = \delta_{i,j} .$$

Different sets of orthonormal vectors $\vec{e}_i$ will result when changing the order of the vectors $\vec{v}_i$ for subtracting.
For a non orthonormal set of base vectors one can either use this orthonormalization procedure which allows afterward to apply the simple Eq. (3.11) or use directly Eq. (3.8). Sometimes there is a small advantage when using the first approach: If a fit is not good enough one can just calculate more projections and add more fitting functions without recalculating the first fitting coefficients. This does not work for the more general Eq. (3.8) where the matrix inversion has to be repeated fully when adding more fitting functions, i.e. base vectors.