

Let $V^{(k)}$ be the set of subspace vectors at step k and assume $V^{(k)T} V^{(k)} = I$
 Let $A = A^T$

We want to solve $(A - \lambda I)^{-1} B = X$ which is equivalent to

$$(A - \lambda I) X = B$$

Let $W^{(k)} = A V^{(k)}$

① solve the equation in the subspace. The subspace projected equation is

$$V^T (A - \lambda I) P_V X = V^T B \quad \text{where} \quad P_V = V V^T \quad (\text{dropping } (k) \text{ for now})$$

$$V^T (A - \lambda I) V V^T X = V^T B$$

$$(W^T V - \lambda I) V^T X = V^T B \Rightarrow (a - \lambda I) x = b$$

where $a = W^T V$, $x = V^T X$, $b = V^T B$

a is a $k \times k$ matrix, where k is the size of the Krylov space so you can solve this by using a normal dense algorithm like `np.linalg.solve()`

Once you have x , then you generate $X^{(k)}$, then guess the full space with

$$X^{(k+1)} = V^{(k)} x$$

Now notice that at convergence, this should satisfy

$$(A - \lambda I) V x - B = 0$$

$$\Rightarrow W x - \lambda x - B = 0$$

So we can define the residual

$$r^{(k)} = W^{(k)} x - \lambda V^{(k)} x - B$$

The algorithm stops when $|r^{(k)}|$ is below a threshold. If it is not converged then just like the normal Davidson, the new vector comes from

$$(\text{diag}(A) - \lambda I)^{-1} r^{(k)} = v$$

Then you just orthogonalize v and add it to $V^{(k+1)}$