I.1.(b) Newton-type methods

Approximate Newton method
Version 1: *Newton correction formula*

Objective:

given an approximate eigenpair (μ, z) of A, where $\mu = z^H A z$ and $\|z\|_2 = 1$, find an improved approximation $(\mu + \eta, z + v)$ with the constraint $v \perp z$ (i.e., $v^H z = 0$).

Newton correction formula. Let $(\mu + \eta, z + v)$ be an exact eigenpair of A

$$A(z + v) = (\mu + \eta)(z + v).$$

Then by the first-order approximation, we have the correction equation

$$(A - \mu I)v - \eta z = -r \quad \text{and} \quad z^H v = 0, \tag{1}$$

where r is the residual vector

$$r = Az - \mu z.$$

In matrix form, we have

$$\begin{bmatrix} A-\mu I & -z \\ z^H & 0 \end{bmatrix} \begin{bmatrix} v \\ \eta \end{bmatrix} = \begin{bmatrix} -r \\ 0 \end{bmatrix}$$

By the block elimination, we have the triangular system

$$\begin{bmatrix} A-\mu I & -z \\ 0 & z^H(A-\mu I)^{-1}z \end{bmatrix} \begin{bmatrix} v \\ \eta \end{bmatrix} = \begin{bmatrix} -r \\ z^H(A-\mu I)^{-1}r \end{bmatrix}$$

Hence, we have the following **Newton correction formula**

$$\eta = \frac{z^H(A-\mu I)^{-1}r}{z^H(A-\mu I)^{-1}z} \tag{2}$$

$$(A-\mu I)v = -r + \eta z \tag{3}$$

Approximate Newton method
Version 2: *Newton correction equation*

Alternative to the Newton correction formula: use a projection formulation.

Let us rewrite the correction equation (1) as

$$(A - \mu I)v = -r + \eta z \quad \text{and} \quad z^H v = 0. \tag{4}$$

Let

$$P = I - zz^H$$

be the orthogonal projector onto the orthogonal complement of z. Then

1. $Pz = 0$,
2. $Pv = v$,
3. $Pr = r$.

Consequently, (4) can be written as the following form, referred to as **Newton correction equation**:

$$P(A - \mu I)Pv = -r \quad \text{and} \quad v \perp z.$$

or

$$(I - zz^H)(A - \mu I)(I - zz^H)v = -r \quad \text{and} \quad v \perp z. \tag{5}$$

Equivalence

Theorem. v satisfies (2) and (3) if and only if v satisfies (5).

Proof:

- We have already shown that if v satisfies (2) and (3), then v satisfies (5).
- Suppose v satisfies (5). Then

  $$(A-\mu I)(I-zz^H)v = -r + zz^H(A-\mu I)(I-zz^H)v = -r+\alpha z$$

  and

  $$v = -(A-\mu I)^{-1}r + \alpha(A-\mu I)^{-1}z.$$

  Since $z^H v = 0$, we have

  $$\alpha = \frac{z^H(A-\mu I)^{-1}r}{z^H(A-\mu I)^{-1}z} = \eta.$$

  Thus v satisfies (2) and (3).

Remark:

Although the Newton correction equation (5) does not give the correction vector v explicitly, it offers an opportunity to apply an iterative method with preconditioing, for example preconditioned GMRES, to solve the correction equation, which in turn we need only to compute the matrix-vector product $P(A - \mu I)Py$, where y is an arbitrary vector.

Jacobi-Davidson method = Newton correction equation + RR

Basic Jacobi-Davidson method: compute only one eigenpair whose eigenvalue is near a focal point τ.

1. $V = v$; normalized starting vector, $\|v\|_2 = 1$.
2. for $k = 1, 2, \ldots, k_{\max}$
3. Using V compute a Ritz pair (μ, z) such that μ is near τ;
4. $r = Az - \mu z$;
5. if r is sufficiently small, return (μ, z), exit;
6. choose a shift κ near τ or μ;
7. solve the correction equation
   $$(I - zz^H)(A - \kappa I)(I - zz^H)v = -r \text{ and } v^H z = 0;$$
8. orthonormalize v with respect to V;
9. $V = \begin{bmatrix} V & v \end{bmatrix}$;
10. end for
11. signal nonconvergence.

Remarks:

- The algorithm has two parameters: τ and κ.
  - τ is the center of a focal region in which we wish to find an eigenpair, and
  - κ is generally chosen equal to τ or μ.

    If it is inexpensive to vary κ, then it can be shown that by choosing $\kappa = \mu$, the algorithm converges quadatically.

- **Solving the correction equation *exactly***

$$(I - zz^H)(A - \kappa I)(I - zz^H)v = -r \quad \text{and} \quad v, r \perp z$$

By $v \perp z$, we have

$$(I - zz^H)(A - \kappa I)v = -r,$$

or

$$(A - \kappa I)v = -r + zz^H(A - \kappa I)v.$$

$$v = -\underbrace{(A - \kappa I)^{-1}r}_{x} + \underbrace{(A - \kappa I)^{-1}z}_{f}\,\underbrace{z^H(A - \kappa I)v}_{a} \equiv -x + fa.$$

By $v \perp z$ again, we have

$$0 = z^H v = -z^H(A - \kappa I)^{-1}r + z^H(A - \kappa I)^{-1}zz^H(A - \kappa I)v.$$

Then we can solve the following equation for "a";

$$z^H\,\underbrace{(A - \kappa I)^{-1}z}_{f}\,\underbrace{(z^H(A - \kappa I)v)}_{a} = z^H\,\underbrace{(A - \kappa I)^{-1}r}_{x}\,.$$

In summary, the correction equation can be solved as follows:

1. Compute $f = (A - \kappa I)^{-1}z$;
2. Compute $c = z^H f$;
3. Solve $(A - \kappa I)x = r$ for x;
4. Compute $b = z^H x$;
5. $a = b/c$ for a;
6. $v = -x + fa$.