Iterative methods for large sparse eigenvalue problems

1.1 *Basic methods*

- Power method (power iteration) summarized in Algorithm 1
- Inverse iteration summarized in Algorithm 2
- Rayleigh quotient iteration summarized in Algorithm 3

Read about these methods in TB pages 202-209.

Note that Rayleigh qoutient iteration can also be used for non-symmetric matrices, although it is presented only for symmetric matrices in TB.

```
Output: Eigenpair approximation (w, λ̃)
Input: A starting vector v with ‖v‖ = 1
for n = 1,2,... do
    w = Av
    v = w/‖w‖
    λ̃ = v^T Av
end
```

Algorithm 1: Power method (Power iteration).

```
Output: Eigenpair approximation (w, λ̃)
Input: A starting vector v with ‖v‖ = 1 and shift μ
for n = 1,2,... do
    Solve linear system (A − μI)w = v
    v = w/‖w‖
    λ̃ = v^T Av
end
```

Algorithm 2: Inverse iteration

Output: Eigenpair approximation $(w, \tilde{\lambda})$
Input: A starting vector v with $\|v\| = 1$ and shift μ
$\tilde{\lambda} = v^T A v$
for $n = 1, 2, \ldots$ **do**
  Solve linear system $(A - \tilde{\lambda} I)w = v$
  $v = w/\|w\|$
  $\tilde{\lambda} = v^T A v$
end

Algorithm 3: Rayleigh Quotient Iteration

Orthogonal matrices and orthogonalizing vectors

In basic linear algebra, we learn that two vectors $x, y \in \mathbb{R}^n$ are orthogonal when $y^T x = 0$. The concept of orthogonality, and its generalization to matrices is very important in this course. We will use it mostly in different factorizations and decompositions of matrices.

The use of decompositions has been selected as one of the most influential concepts in algorithms in the 20th century: https://www.siam.org/pdf/news/637.pdf In this course we also cover other algorithms in the list of important algorithms.

Orthogonal matrices

We need the concept of orthogonal matrices. Note that we define it not only for square matrices.

Some orthogonalization methods are described in TB Lecture 7. We need orthogonalization for a different purpose and therefore need a different presentation.

Definition 1.2.1 (Orthogonal matrix)**.** *$Q \in \mathbb{R}^{n\times m}$ is called an orthogonal matrix if*

$$Q^T Q = I.$$

For complex matrices, the corresponding property is called unitary: $Q^* Q = I$.

Properties:

(i) The columns of an orthogonal matrix are orthonormal.

(ii) If $n = m$, then $Q^T = Q^{-1}$.

(iii) If $n = m$, then $QQ^T = I$.

Note that (iii) is not satisfied if Q is a rectangular matrix ($n \neq m$). For instance

$$Q = \begin{bmatrix} 0 & 1 \\ 1 & 0 \\ 0 & 0 \end{bmatrix}$$

is an orthogonal matrix since $Q^T Q = I$, but

$$QQ^T = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

Gram-Schmidt procedures

The Gram-Schmidt procedure is often explained as a procedure to orthogonalize vectors, meaning that given vectors stored in a matrix $F = [f_1, \ldots, f_m] \in \mathbb{R}^{n\times m}$ with $n \geq m$ we try to determine $q_1, \ldots, q_n$ such that $q_1, \ldots, q_n$ are orthonormal and

$$\operatorname{span}(f_1, \ldots, f_m) = \operatorname{span}(q_1, \ldots, q_m).$$

Such vectors $q_1, \ldots, q_n$ exist if $f_1, \ldots, f_m$ are linearly independent vectors. Note that the matrix $Q = [q_1, \ldots, q_m] \in \mathbb{R}^{n\times m}$ is orthogonal in the sense of Definition 1.2.1.

You have normally learned about the Gram-Schmidt procedure in basic linear algebra courses. We repeat it in a slightly different notation than normal (using orthogonal matrices). It turns out that the classical Gram-Schmidt is not always satisfactory.

The Gram-Schmidt procedure can be directly derived by inductively applying the following result.

In numerical linear algebra, the Gram-Schmidt procedure directly derived from Lemma 1.2.2 is typically called the *classical* Gram-Schmidt procedure in order to distinguish it from variants we discuss later.

Lemma 1.2.2. *Suppose $Q = [q_1, \ldots, q_m] \in \mathbb{R}^{n\times m}$ is an orthogonal matrix and suppose $b \notin \operatorname{span}(q_1, \ldots, q_m)$. Let*

$$h = Q^T b$$

and

$$z = b - Qh = (I - QQ^T)b. \tag{1.1}$$

The vector $h \in \mathbb{R}^n$ is typically referred to as the Gram-Schmidt coefficients

Let $\beta = \|z\|$ and define

$$q_{m+1} := \frac{z}{\beta} \tag{1.2}$$

Then,

(a) the matrix $[q_1, \ldots, q_{m+1}]$ is an orthogonal matrix;

(b) $b = h_1 q_1 + \cdots + h_m q_m + \beta q_{m+1}$; and

(c) $\operatorname{span}(q_1, \ldots, q_{m+1}) = \operatorname{span}(q_1, \ldots, q_m, b)$.

A typo was corrected in statement (b) on 2016-11-04

Proof. Proof of (b): This is a direct consequence of (1.1) and (1.2). Proof of (a): Note that

$$[q_1, \ldots, q_{m+1}]^T [q_1, \ldots, q_{m+1}] = [Q, q_{m+1}]^T [Q, q_{m+1}] = \begin{bmatrix} Q^T Q & Q^T q_{m+1} \\ q_{m+1}^T Q & q_{m+1}^T q_{m+1} \end{bmatrix}$$

The conclusion (a) follows from the fact that $Q^T Q = I$,

$$Q^T q_{m+1} = Q^T (I - QQ^T) b = 0$$

and $q_{m+1}^T q_{m+1} = 1$.
Proof of (c): In this course we will several times use the general property that if two rectangular matrices $W \in \mathbb{R}^{n\times m}$ and $V \in \mathbb{R}^{n\times m}$ are related by

$$W = VP \tag{1.3}$$

for some non-singular matrix $P \in \mathbb{R}^{m\times m}$, then then $\operatorname{span}(W) = \operatorname{span}(V)$. If we select P as

$$P = \begin{bmatrix} I & h \\ 0 & \|z\| \end{bmatrix}$$

then (1.3) is satisfied with $V = [Q, q_{m+1}]$ and $W = [Q, b]$. $\square$

Classical Gram-Schmidt example

```
>> Q=(1/sqrt(2))*[1 -1; 1 1; 0 0; 0 0];
>> Q'*Q   % Check if Q is orthogonal
ans =
    1.0000         0
         0    1.0000
>> b=randn(4,1);
>> h=Q'*b;             % Compute Gram-Schmidt coefficients
>> z=b-Q*h;            % Compute "orthogonal complement"
>> beta=norm(z);
>> q_new=z/beta;
>> Q_new=[Q,q_new];    % Construct new Q-matrix
>> Q_new'*Q_new        % Check that Q_new is orthogonal
ans =
    1.0000         0         0
         0    1.0000         0
         0         0    1.0000
>> norm(Q_new*[eye(2), h; zeros(1,2), norm(z)]-[Q,b])
>> P=[eye(2), h; zeros(1,2), beta];
>> norm(Q_new*P-[Q,b])  % Check that span(Q_new)=span([Q,b])
ans =
   1.1444e-16
```

Although the above example suggests that classical Gram-Schmidt works, it will in general not be satisfactory in our context. It turns out that the classical Gram-Schmidt is very sensitive to round-off errors in certain situations.

We now investigate what happens if we have an error in the computation of the Gram-Schmidt coefficients. In other words, we assume that h is approximated by

In practice, we have round-off errors in every floating point operation and a complete round-off error analysis is quite cumbersome. In our simplified analysis we assume that no error is intruduced in the computation of z and $\tilde{q}_{m+1}$. In particular, no additional round-off error is introduced in (1.5) and (1.6).

$$\tilde{h} = \begin{bmatrix} (1+\varepsilon_1)h_1 \\ \vdots \\ (1+\varepsilon_m)h_m \end{bmatrix} = \left(\begin{bmatrix} 1 & & \\ & \ddots & \\ & & 1 \end{bmatrix} + \underbrace{\begin{bmatrix} \varepsilon_1 & & \\ & \ddots & \\ & & \varepsilon_m \end{bmatrix}}_{\Lambda_\varepsilon}\right) Q^T b \qquad (1.4)$$

where $\varepsilon_1,\ldots,\varepsilon_m$ are a small number introduced by the inexact evaluation of Q^Tb, typically of order of the same order of magnitude ϵ_{mach}. Our approximation of z satisfies

$$\tilde{z} = b - Q\tilde{h} = b - Q\Lambda_\varepsilon Q^T b(1+\varepsilon) = z - Q\Lambda_\varepsilon Q^T b \qquad (1.5)$$

such that

$$\tilde{q}_{m+1} = \frac{1}{\|\tilde{z}\|}\tilde{z} = \frac{1}{\|z - Q\Lambda_\varepsilon Q^T b\|}\tilde{z} = \frac{1}{\sqrt{(z-Q\Lambda_\varepsilon Q^T b)^T(z-Q\Lambda_\varepsilon Q^T b)}}\tilde{z} =$$
$$\frac{1}{\sqrt{(z-Q\Lambda_\varepsilon Q^T b)^T(z-Q\Lambda_\varepsilon Q^T b)}}\tilde{z} = \frac{1}{\sqrt{\|z\|^2 + \|\Lambda_\varepsilon\|^2\|QQ^Tb\|^2}}\tilde{z} =$$
$$\tilde{z}(\tfrac{1}{\|z\|} + \mathcal{O}(\varepsilon^2)), \qquad (1.6)$$

where $\varepsilon = \|\Lambda_\varepsilon\|$. The approximation of the new vector is

$$\tilde{q}_{m+1} = (z - Q\Lambda_\varepsilon Q^T b)(\frac{1}{\|z\|} + \mathcal{O}(\varepsilon^2)) = \frac{z}{\|z\|} - \frac{1}{\|z\|}Q\Lambda_\varepsilon Q^T b + \mathcal{O}(\varepsilon^2) \qquad (1.7)$$

In this first-order estimation, we see that the error is small if

$$\frac{\|Q\Lambda_\varepsilon Q^T b\|}{\|z\|} = \frac{\|\Lambda_\varepsilon Q^T b\|}{\|z\|} \leq \varepsilon\frac{\|Q^T b\|}{\|z\|}$$

is small.

A bad situation can easily be identified, since we can construct a situation where $\|z\|$ is small but Q^Tb is not: Suppose $b = q + \delta e$ where $q = Qd$ and $e \perp Q$ and $\|e\| = 1$. A direct computation leads to

$$\|\tilde{q}_{m+1} - \frac{z}{\|z\|}\| \leq \frac{|\varepsilon|}{|\delta|}\|Qd\| + \mathcal{O}(\varepsilon^2).$$

which suggests that the round-off error is proportional to $|\varepsilon|/|\delta|$.

Conclusion of error analysis of classical Gram-Schmidt method. The Gram-Schmidt procedure is likely to have a large round-off error if the vector b almost lies in the subspace $\text{span}(Q)$.

Modified Gram-Schmidt

In this course we consider two variations of Gram-Schmidt which aim to improve the floating-point arithmetic problems described above.

We now derive the algorithm called *the modified Gram-Schmidt procedure* from the classical Gram-Schmidt procedure. For theoretical purposes we express the classical Gram-Schmidt in for-loops:

The modified Gram-Schmidt procedure is equivalent to the classical Gram-Schmidt procedure in exact arithmetic, but different floating-point arithmetic.

```
for i=1:m
  h(i)=Q(:,i)'*b;
```



```
end
z=b;
for i=1:m
  z=z-h(i)*Q(:,i)
end
```

Note that at iteration i of the second loop, we only need `h(i)` computed at the ith iteration the first loop such that we can merge the two loops:

```
z=b;
for i=1:m
  h(i)=Q(:,i)'*b;
  z=z-h(i)*Q(:,i);
end
beta=norm(z);
```

In the first step inside the for-loop, the vector `z` can be explicitly expressed as:

- Iteration $i = 1$: $z = b$
- Iteration $i = 2$: $z = b - h_1 q_1$
- $\vdots$
- Iteration $i = m$: $z = b - h_1 q_1 - \cdots - h_m q_{m-1}$

Now recall that the vectors $q_1, \ldots, q_m$ are assumed to be orthogonal. The following identies can be directly identified.

- Iteration $i = 1$: $q_i^T z = q_i^T b$
- Iteration $i = 2$: $q_i^T z = q_2^T (b - h_1 q_1) = q_2^T b - h_1 q_2^T q_1 = q_i^T b$
- $\vdots$
- Iteration $i = m$: $q_i^T z = q_m^T b - h_1 q_m^T q_1 - \cdots - h_m q_m^T q_{m-1} = q_m^T b = q_i^T b$

Note that for every iteration we have $q_i^T z = q_i^T b$. Therefore, we can replace `Q(:,i)'*b` with `Q(:,i)'*z` in the for-loop. This is what we call the modified Gram-Schmidt method.

```
z=b;
for i=1:m
  h(i)=Q(:,i)'*z;
  z=z-h(i)*Q(:,i)
end
```

Although modified Gram-Schmidt yields a different result in floating point arithmetic, it is not always clear that the result is better. In fact, theoretical understanding for this is still disputed by some scientists. You will investigate this in practice by for a specific situation in the homeworks.

Caution regarding terminology: In this course we consider $Q \in^{n\times m}$ as an orthogonal matrix and want to orthogonalize b which result in algorithms above. In some literature (such as TB) Gram-Schmidt procedures are described for orthogonalizing an entire matrix $A \in \mathbb{R}^{n\times(m+1)}$.

Double Gram-Schmidt

The next approach to improve the classical Gram-Schmidt procedure is very naive. Since we know that round-off errors will make the vector $z = b - Qh$ to not be orthogonal in practice, we can try to make it orthogonal by applying classical Gram-Schmidt again. This is what is called repeated Gram-Schmidt, or the special case double Gram-Schmidt.

```
>>  h=Q'*b;
>>  z=b-Q*h;
>>  g=Q'*z;
>>  z=z-Q*g
>>  h=h+g;
>>  beta=norm(z);
```

A typo was corrected here on 2016-11-07

Krylov methods

We now consider the space spanned by the iterates of the power method. This is called a Krylov subspace

$$\mathcal{K}_m(A,b) := \operatorname{span}(b, Ab, A^2b, \dots, A^{m-1}b).$$

Due to rounding error issues, the Krylov subspace is usually not computed from $[b, Ab, A^2b, \dots, A^{m-1}b]$, but rather represented with an orthogonal basis of $\mathcal{K}_m(A,b)$. The Arnoldi method can be seen as method to compute an orthogonal bais of a Krylov subspace. More precisely, the Arnoldi method is a method which generates an orthogonal matrix $Q_m \in \mathbb{C}^{n\times m}$ such that

$$AQ_m = Q_{m+1}\underline{H}_m$$

where $\underline{H}_m \in \mathbb{R}^{(m+1)\times m}$ and $Q_{m+1} = [Q_m, q_{m+1}]$. The matrix $\underline{H}_m$ is a so-called Hessenberg matrix, which means that it is an zero elements below the first lower off-diagonal:

$$\underline{H}_m = \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & 0 & \times & \times \\ 0 & 0 & 0 & 0 & 0 & \times \end{bmatrix}$$

The Arnoldi method can be used to compute many quantites. In the context of eigenvalue computations, we take the eigenvalues of $H_m \in \mathbb{C}^{m\times m}$ as eigenvalue approximations.

Arnoldi's method for eigenvalue problems is also discussed in TB pages 251–264.

The Arnoldi method

Output: Eigenpair approximations
Input: The matrix A and vector b.
$q_1 = b/\|b\|$, H_0 =empty matrix
for $n = 1, 2, \ldots$ **do**
  Compute $x = Aq_n$
  Orthogonalize x against $q_1, \ldots, q_n$ by computing $h \in \mathbb{C}^n$ and $x_\perp \mathbb{C}^m$ such that $Q^T x_\perp = 0$ and

$$x_\perp = x - Qh.$$

  Let $\beta = \|x_\perp\|$
  Let $q_{n+1} = x_\perp/\beta$
  Let

$$\underline{H}_n = \begin{bmatrix} \underline{H}_{n-1} & h \\ 0 & \beta \end{bmatrix}$$

end

Algorithm 4: Arnoldi's method for eigenvalue problems.

The Lanczos method

Specialization of Arnoldi's method for symmetric matrices.

The Lanczos iteration is also described in TB pages 276-278.

Output: Eigenpair approximations
Input: The matrix A and vector b.
b =arbitrary, $q_1 = b/\|b\|$, H_0 =empty matrix
for $n = 1, 2, \ldots$ **do**
  v=Aq$_n$
  $\alpha_n = q_n^T v$
  v=v-$\beta_{n-1}q_{n-1} - \alpha_n q_n$
  $\beta_n = \|v\|$
  q$_{n+1} = v/\beta_n$
end

Convergence of Arnoldi's method for eigenvalue problems

Recall that, unless it breaks down, k steps of the Arnoldi method generates an orthogonal basis of a Krylov subspace, represented by a matrix $Q = (q_1, \ldots, q_k) \in \mathbb{C}^{n \times k}$ such that $Q^*Q = I$ and

$$\text{span}(q_1, \ldots, q_k) = \mathcal{K}_k(A, b) := \text{span}(b, Ab, \ldots, A^{k-1}b).$$

The eigenvalue approximations (called Ritz values) are subsequently found from the eigenvalues of

$$H = Q^*AQ.$$

The matrix $H \in \mathbb{C}^{k\times k}$ is a Hessenberg matrix and can be generated as a by-product of the Arnoldi method. We call a pair (μ, Qv) a Ritz pair and Qv a Ritz vector, if v and μ safisfy

$$Hv = \mu v.$$

Bound for subspace-eigenvector angle

As a first indicator of the convergence we will characterize the following quantity

$$\text{error in eigenvector } x_i \sim \|(I - QQ^*)x_i\| \tag{1.8}$$

Recall: $Q \in \mathbb{C}^{n\times k}$ is an orthogonal matrix which means that $Q^*Q = I \in \mathbb{C}^{k\times k}$. However, $I \neq QQ^* \in \mathbb{C}^{n\times n}$.

where

$$Ax_i = \lambda_i x_i.$$

It is very natural to associate the accuracy of the eigenvector with this quantity from a geometric perspective. The indicator in the right-hand side of (1.8) is called (the norm of) the orthogonal complement of the projection of x_i onto the space spanned by Q and it can be interpreted as the sine of the canonical angle between the Krylov subspace and an eigenvector. For the moment, we will only justify this indicator with this geometric reasoning and the following observation:

Lemma 1.4.1. *Suppoe (λ_i, x_i) is an eigenpair A. If the Krylov subspace contains the eigenvector ($x_i \in \mathcal{K}_k(A, b)$), then the indicator vanishes$\|(I - QQ^*)x_i\| = 0$ and there is at least one Ritz value μ such that $\mu = \lambda_i$.*

The Arnoldi method produces an exact approximation if the Krylov subspace contains an eigenvector, or equivalently the indicator is zero.

In words:

- Suppose the Krylov subspace contains the eigenvector ($x_i \in \mathcal{K}_k(A, b)$). Then, there exists a vector $z \in \mathbb{C}^k$ such that $x_i = Qz$. Moreover, this is an eigenvector of H such that the Arnoldi method will generate an exact eigenvalue of A. Moreover, the indicator is $\|(I - QQ^*)x_i\| = \|(I - QQ^*)Qz\| = 0$.
- If, similar to above, $x_i \approx x \in \mathcal{K}_k(A, b)$, we expect the indicator to be small and an eigenvalue of H also to be close λ_i.

The indicator can be bounded as follows, where we assume diagonalizability of the matrix.

Theorem 1.4.2. *Suppose $A \in \mathbb{C}^{n\times n}$ is diagonalizable and let the matrix $X = (x_1, \ldots, x_n) \in \mathbb{C}^{n\times n}$ and diagonal matrix $\Lambda \in \mathbb{C}^{n\times n}$ be the Jordan decomposition such that*

$$A = X\Lambda X^{-1}.$$

Suppose $\alpha_1, \ldots, \alpha_n \in \mathbb{C}\backslash\{0\}$ are such that

$$b = \alpha_1 x_1 + \cdots + \alpha_n x_n \tag{1.9}$$

Recall: The eigenvectors of a diagonalizable matrix form a basis of $\mathbb{C}^n$.

and

$$\varepsilon_i^{(m)} := \min_{\substack{p\in P_{m-1}\\ p(\lambda_i)=1}} \max(|p(\lambda_1)|,\ldots,|p(\lambda_{i-1})|,|p(\lambda_{i+1})|,\ldots,|p(\lambda_n)|)$$

where P_n denotes polynomials of degree n. Suppose the Arnoldi method does not break down when applied to A and started with b. Let $Q\in\mathbb{C}^{n\times m}$ be the orthogonal basis generated after m iterations. Then,

$$\|(I-QQ^*)x_i\| \le \xi_i\varepsilon_i^{(m)}, \tag{1.10}$$

where

$$\xi_i = \sum_{\substack{j=1\\ j\neq i}}^{n} \frac{|\alpha_j|}{|\alpha_i|}.$$

The indicator can be bounded by a product consisting of two scalar values: $\varepsilon_i^{(m)}$ which only depends on the eigenvalues and iteration number; and ξ_i only depending on the starting vector and eigenvectors.

Proof. The proof consists of three steps.

1. Consider any vector $u\in\mathbb{C}^n$. Then

$$\min_{z\in\mathbb{C}^m} \|u-Qz\|_2$$

is a linear least squares problem with a solution given by the normal equations $Q^*u = Q^*Qz$. Hence, $z=Q^*u$. This implies that (for any vector u) we have

$$\min_{z\in\mathbb{C}^m} \|u-Qz\|_2 = \|u-QQ^*u\| = \|(I-QQ^*)u\|$$

2. Although we ultimately want to bound the left-hand side of (1.10), the proof is simplified by considerations of a scaling the left-hand side of (1.10) with α_i as follows:

$$\begin{aligned}\|(I-QQ^*)\alpha_i x_i\| &= \min_{z\in\mathbb{C}^m}\|\alpha_i x_i - Qz\| \\ &= \min_{y\in\mathcal{K}_m(A,b)}\|\alpha_i x_i - y\|\end{aligned}$$

Apply step 1 reversely with $u=\alpha_i x_i$

Now note that the space $\mathcal{K}_m(A,b)$ can be characterized with polynomials. It is easy to verify that $y\in\mathcal{K}_m(A,b)$ is equivalent to the existance of a polynomial $p\in P_{m-1}$ such that $y=p(A)b$. Consequently,

$$\|(I-QQ^*)\alpha_i x_i\| = \min_{p\in P_{m-1}}\|\alpha_i x_i - p(A)b\|.$$

3. The final step consists of inserting the expansion of b in terms of eigenvectors (1.9) and applying appropriate bounds:

Since x_i eigenvector, $p(A)x_i = p(\lambda_i)x_i$

For any two sets $S\subset Z$:

$$\begin{aligned}
\|(I-QQ^*)\alpha_i x_i\| &= \min_{p\in P_{m-1}} \|\alpha_i x_i - p(A)\sum_{j=1}^n \alpha_j x_j\| \\
&= \min_{p\in P_{m-1}} \left\| \alpha_i x_i - \sum_{j=1}^n \alpha_j p(\lambda_j) x_j \right\| \\
&\le \min_{\substack{p\in P_{m-1}\\ p(\lambda_i)=1}} \left\| \alpha_i x_i - \sum_{j=1}^n \alpha_j p(\lambda_j) x_j \right\| \\
&= \min_{\substack{p\in P_{m-1}\\ p(\lambda_i)=1}} \|\alpha_i x_i - \alpha_i x_i - \sum_{\substack{j=1\\ j\neq i}}^n \alpha_j p(\lambda_j) x_j\| \\
&= \min_{\substack{p\in P_{m-1}\\ p(\lambda_i)=1}} \|\sum_{\substack{j=1\\ j\neq i}}^n \alpha_j p(\lambda_j) x_j\| \\
&\le (\sum_{\substack{j=1\\ j\neq i}}^n |\alpha_j|)\cdot \min_{\substack{p\in P_{m-1}\\ p(\lambda_i)=1}} \max_{j\neq i}(|p(\lambda_j)|) \\
&= (\sum_{\substack{j=1\\ j\neq i}}^n |\alpha_j|)\cdot \varepsilon_i^{(m)}
\end{aligned}$$

The conclusion of the theorem is established by dividing the equation by $|\alpha_i|$.

□

Note that $\|b\| = 1$ and $\|x_1\| = \cdots = \|x_n\| = 1$. Hence the coefficients $\alpha_1, \ldots, \alpha_n$ are balanced. In particular they satisfy

$$1 = \|\alpha_1 x_1 + \cdots + \alpha_n x_n\| \le |\alpha_1| + \cdots + |\alpha_n|.$$

and

$$\xi_i = \frac{1}{|\alpha_i|}\sum_{j=1}^n |\alpha_j| - 1 \ge \frac{1}{|\alpha_i|} - 1$$

From this we can easily identify a very good situation and a very bad situation.

- Suppose for all $j \neq i$, $\alpha_j = \delta$ and suppose δ is small. We have that $\xi_i = \frac{(n-1)\delta}{\alpha_i}$. Due to balancing α_i cannot be small. Hence, ξ_i is small, showing fast convergence for this eigenvalue.
- On the other hand, if α_i (the component of the starting vector in the direction of the ith eigenvector) is very small, we have $\xi_i \gg 1$ which implies that the right-hand side of (1.10) is large and we have slow convergence.

This serves as a justification for a more general property.

Rule-of-thumb. Starting vector dependency. The Arnoldi method for eigenvalue problems will "favor" eigenvectors which have large components in the starting vector.

The word "favors" is purposely vague. It should be interpreted as the situation that one observes often in practice, but certainly not always. If we have a particular structure in the matrix or starting vector, we might observe convergence to other eigenvalues.

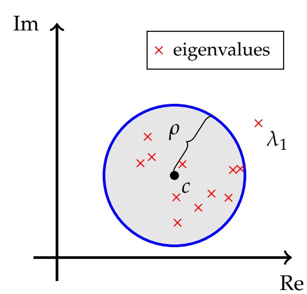
Bounding $\varepsilon_i^{(m)}$

In the characterization of the indicator in Theorem 1.4.2 above we introduced the quantity $\varepsilon_i^{(m)}$. This quantity bounds (up to a constant) the error in eigenvector x_i at iteration m. Although $\varepsilon_i^{(m)}$ is defined through a polynomial optimization problem, which is complicated to solve, it is surprisingly easy to use this to obtain bounds providing qualitative understanding of the convergence of the Arnoldi method for eigenvalue problems. We illustrate the power with a specific bound.

Think: $\varepsilon_i^{(m)}$ measures how "difficult" it is to push down a polynomial in points λ_j, for all $j \neq i$ and maintain $p(\lambda_i) = 1$.

Corollary 1.4.3. *Suppose $C(\rho, c) \subset \mathbb{C}$ is a disk centered at $c \in \mathbb{C}$ with radius ρ such that it contains all eigenvalues but λ_1. That is, $\lambda_2, \ldots, \lambda_n \in C(\rho, c)$ and $\lambda_1 \notin C(\rho, c)$. Then,*

$$\varepsilon_1^{(m)} \le \left(\frac{\rho}{|\lambda_1 - c|}\right)^{m-1}.$$



Proof. The proof consists of selecting a particular polynomial in the polynomial optimization problem,

$$\begin{aligned}\varepsilon_1^{(m)} &:= \min_{\substack{p \in P_{m-1}\\ p(\lambda_1)=1}} \max(|p(\lambda_1)|, \ldots, |p(\lambda_{i-1})|, |p(\lambda_{i+1})|, \ldots, |p(\lambda_n)|) \\ &= \max_{j \neq i} |q(\lambda_j)|,\end{aligned}$$

for any $q \in P_{m-1}$ satisfying $q(\lambda_1) = 1$, in particular

$$q(z) = \frac{1}{(\lambda_1 - c)^{m-1}}(z - c)^{m-1}.$$

Hence, from the definition of ρ and c we have that

$$\begin{aligned}\varepsilon_1^{(m)} &\le \max_{i>1} \frac{|\lambda_i - c|^{m-1}}{|\lambda_1 - c|^{m-1}} \\ &\le \frac{\rho^{m-1}}{|\lambda_1 - c|^{m-1}}.\end{aligned}$$

□

The result can be intuitively interpreted as follows. If we can construct a small disc that encloses all eigenvalues but one eigenvalue we expect fast (at least linear geometric) convergence for that eigenvalue. This can be achieved for an eigenvalue which is well separated from the rest of the eigenvalues and also in an outer part of the spectrum. We call this "extreme" isolated eigenvalues.

Rule-of-thumb. Eigenvalue dependency. Arnoldi's method for eigenvalue problems favors convergence to "extreme" isolated eigenvalues.

Note the difference between an "extreme" eigenvalue and the eigenvalues which are largest in modulus (absolute value). The Arnoldi method will favor "extreme" whereas the power method will essentially always converge to the eigenvalue largest in modulus.

An a posteriori theorem

In the previous section we saw a characterization of the error involving the eigenvectors and eigenvalues of the matrix A. The following result provides an explicit characterization of $\|Av - \mu v\|$ where (μ, v) is an approximate eigenpair. It is expressed in terms of quantities computed during the iteration.

A priori vs. a posteriori: Error characterizations can be classified into two types. An *a priori* (latin for "from before") error estimate involves quantities which are known before the algorithm is carried out. An *a posteriori* (latin for "from after") error characterization involves quantites computed during the iteration. Theorem 1.4.2 is an a priori error bound. Theorem 1.4.4 is an (exact) a posteriori error characterization since the right-hand side involves H_k and z which are computed from the iteration.

Theorem 1.4.4. *Suppose Q_k and $\underline{H}_k$ satisfy the Arnoldi relation*

$$AQ_k = Q_{k+1}\underline{H}_k \tag{1.11}$$

where $Q_k \in \mathbb{C}^{n\times k}$ and $Q_{k+1} = [Q_k, q_{k+1}] \in \mathbb{C}^{n\times k}$ are orthogonal matrices. Moreover, suppose (μ, v) is a Ritz pair such that $H_k z = \mu z$ and $v = Q_k z$. Then,

$$\|Av - \mu v\|_2 = |h_{k+1,k}||e_k^T z|. \tag{1.12}$$

Proof. From the fact that (μ, v) is a Ritz pair, we have

$$\begin{aligned} Av - \mu v &= AQ_k z - \mu Q_k z \\ &= (AQ_k - Q_k H_k)z \\ &= h_{k+1,k} q_{k+1} e_k^T z \end{aligned}$$

Use $v = Q_k z$.

Use that since $\underline{H}_k$ is a Hessenberg matrix, (1.11) can be written as $AQ_k = Q_k H_k + h_{k+1,k} q_{k+1} e_k^T$.

The conclusion follows from the fact that $e_k^T z$ is a scalar and q_{k+1} is normalized since Q_{k+1} is orthogonal. More precisely, $\|Av - \mu v\|_2 = |h_{k+1,k}|\|q_{k+1} e_k^T z\| = |h_{k+1,k}|\|q_{k+1}\||e_k^T z| = |h_{k+1,k}||e_k^T z|$. □

The result can be used to study break-down. Break-down corresponds to the situation where we cannot carry out that Gram-Schmidt orthogonalization process since the new vector is contained in the span of previous iterations. It implies that the $y_\perp = 0$ and $\beta = 0$. This implies in turn that $h_{k+1,k} = 0$. Hence, due to (1.12), if we have breakdown the error is already zero and the Ritz pairs are eigenpairs of the original problem.

Literature and further reading

The proof and reasoning above is inspired by [5]. Other convergence bounds involving Schur factorizations, that lead to similar qualitative understanding can be found in [6], where also complications of the non-generic cases are discussed. There are also further characterizations of convergence and the connection with potential theory [4]. In the above reasoning we characterized the angle between the subspace and the eigenvector. Although this serves as a very accurate prediction of the error in practice, it does not directly give a rigorous bound on the accuracy of Ritz pair. Several approaches to describe the convergence of Ritz values and Ritz vectors have been done in for instance [2, 3]. There is also considerable research on the effect of rounding errors in Krylov methods. Unlike many other numerical methods, the effect of finite arithmetic can improve the performance of the algorithm. See also the recent summary of the convergence of the Arnoldi method for eigenvalue problems [1]. The a posteriori error estimate in Theorem 1.4.4 is contained in some recent text-books in numerical linear algebra such as [7].

Appendix: Jordan canonical form (JCF)

The Jordan canonical form, also sometimes the Jordan form or the Jordan decomposition, is a transformation that brings the matrix to a certain block diagonal form.

The Jordan canonical form is typically treated in basic linear algebra courses, but also used in the study of stability theory in for instance systems theory and differential equations. We need it several times in the course.

Definition 1.6.1 (Jordan canonical form)**.** *The Jordan decomposition of a matrix $A \in \mathbb{R}^{n\times n}$ is an invertible matrix $X \in \mathbb{R}^{n\times n}$ and a block diagonal matrix*

$$D = \begin{bmatrix} J_1 & & \\ & \ddots & \\ & & J_q \end{bmatrix}$$

where

$$J_i = \begin{bmatrix} \lambda_i & 1 & & \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ & & & \lambda_i \end{bmatrix} \in \mathbb{R}^{n_i\times n_i}$$

such that

$$A = XDX^{-1}.$$

The matrix J_i is called a Jordan block, or sometimes a Jordan matrix.

Example of Jordan decomposition

The Jordan decomposition of

$$A = \begin{bmatrix} 3 & 0 & 0 \\ 0 & 3 & 0 \\ 1 & 0 & 3 \end{bmatrix}$$

is represented by

$$D = \begin{bmatrix} 3 & 1 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 3 \end{bmatrix}, \quad X = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{bmatrix}$$

since $A = XDX^{-1}$. Note that the eigenvalue $\lambda = 3$ has two Jordan blocks, one of size $n_1 = 2$ and one of size $n_2 = 1$.

Theorem 1.6.2 (Existance and uniqueness of Jordan decomposition). *All matrices $A \in \mathbb{R}^{n\times n}$ have a Jordan decomposition. The (unordered) set of Jordan blocks is unique for any given matrix.*

Definition 1.6.3. *If a matrix A has a Jordan decomposition where all Jordan blocks have size one (such that D is a diagonal matrix) the matrix A is called a diagonalizable matrix.*

Lemma 1.6.4. *Suppose A is symmetric. Then A is diagonalizable and the X matrix in the Jordan decomposition can be chosen as an orthogonal matrix.*

Lemma 1.6.5. *If $A \in \mathbb{R}^{n\times n}$ has n distinct eigenvalues, then A is diagonalizable.*

Appendix: Orthogonal matrices and QR factorization

The QR-factorization is a factorization involving an orthogonal matrix Q and an upper triangular matrix R.

Definition 1.7.1 (Orthogonal matrix). *$Q \in \mathbb{R}^{n\times m}$ is called an orthogonal matrix if*

$$Q^T Q = I.$$

For complex matrices, the corresponding property is called unitary: $Q^* Q = I$.

Orthogonal matrices are important in matrix computations, most importantly when the matrix represents a basis of a vector space. Many properties of the vector space are not robust with respect to rounding errors if the basis is not orthogonal.

Properties:

(i) The columns of an orthogonal matrix are orthonormal.

(ii) If $n = m$, then $Q^T = Q^{-1}$.

(iii) If $n = m$, then $QQ^T = I$.

Note that (iii) is not satisfied if Q is a rectangular matrix ($n \neq m$). For instance

$$Q = \begin{bmatrix} 0 & 1 \\ 1 & 0 \\ 0 & 0 \end{bmatrix}$$

is an orthogonal matrix since $Q^T Q = I$, but

$$QQ^T = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

A QR-factorization can be computed with the matlab command `[Q,R]=qr(A)`. It will however in general not return the solution with positive diagonal elements.

Theorem 1.7.2 (Uniqueness of QR-factorization)**.** *For any matrix $A \in \mathbb{R}^{n\times m}$, $n \leq m$ there exists an orthogonal matrix $Q \in \mathbb{R} \in \mathbb{R}^{n\times m}$ and an upper triangular matrix $R \in \mathbb{R}^{m\times m}$ such that*

$$A = QR.$$

Moreover, if A is non-singular, the diagonal elements of R can be chosen positive, and the decomposition where the diagonal elements of R are positive is unique.

The QR-decomposition is the underlying method to solve overdetermined linear systems of equations, for instance with the backslash operator in matlab when the matrices are rectangular. The decomposition can be computed in a finite number of operations with for instance Householder reflectors or Givens rotations, which will be used in this course.

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