Introduction to Arnoldi method

SF2524 - Matrix Computations for Large-scale Systems

Main eigenvalue algorithms in this course

- Fundamental eigenvalue techniques (Lecture 1)
- Arnoldi method (Lecture 2-3).
- QR-method (Lecture 9-10).

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  Typically suitable when
  - we are interested in a small number of eigenvalues,
  - the matrix is large and sparse
  - Solvable size on current desktop $m \sim 10^6$ (depending on structure)
- QR-method (Lecture 9-10).
  Typically suitable when
  - we want to compute all eigenvalues,
  - the matrix does not have any particular easy structure.
  - Solvable size on current desktop $m \sim 1000$.

Agenda lecture 2

- Introduction to Arnoldi method
- Gram-Schmidt - efficiency and roundoff errors
- Derivation of Arnoldi method
- (Next lecture: Convergence characterization)

Idea of Arnoldi method (slide 1/3)

Eigenvalue problem

$$Ax = \lambda x.$$

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are called *Ritz pairs*.

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- approximates eigenvalues of A "well" if

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Justification of Arnoldi method

- Use Rayleigh-Ritz on $Q = (q_1, \dots, q_m)$ and $Q^T Q = I$, where

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- Arnoldi method is a "clever" procedure to construct $H_m = Q^T AQ$.
- "Clever": We expand Q with one row in each iteration
  $\Rightarrow$ Iterate until we are happy.

Arnoldi method graphically

Graphical illustration of algorithm:

$$Q = \begin{bmatrix} q_1 & q_2 & q_3 & q_4 \end{bmatrix}$$

$$\boxed{} \qquad = H$$

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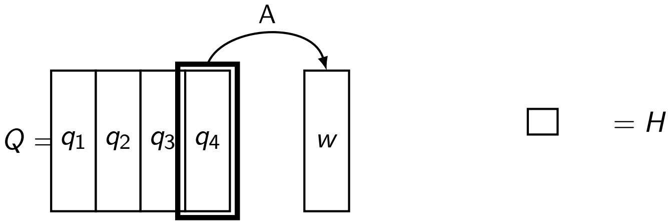

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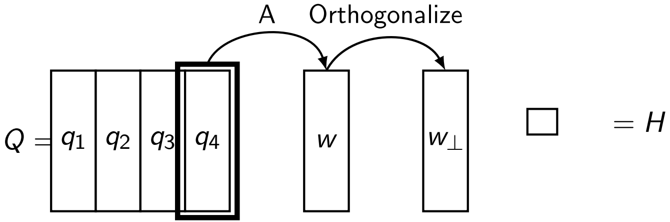

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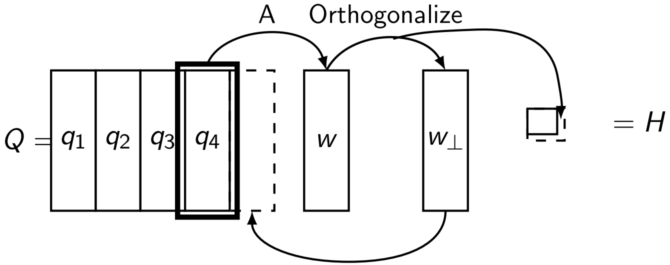

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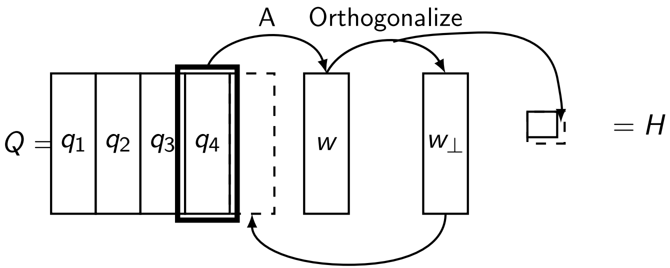

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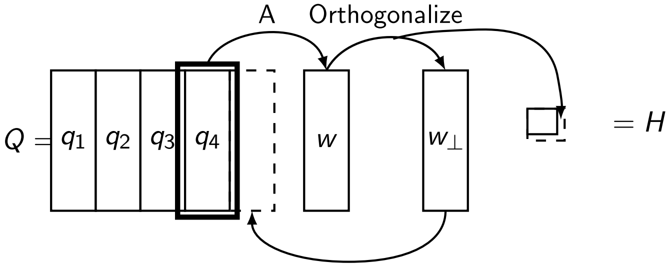

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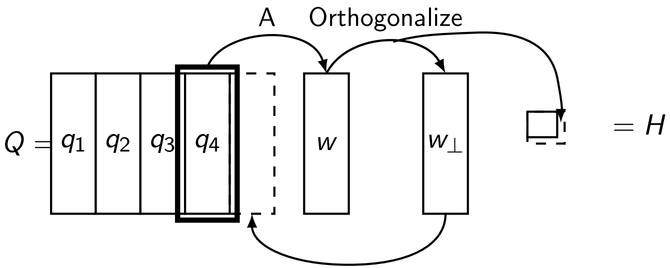

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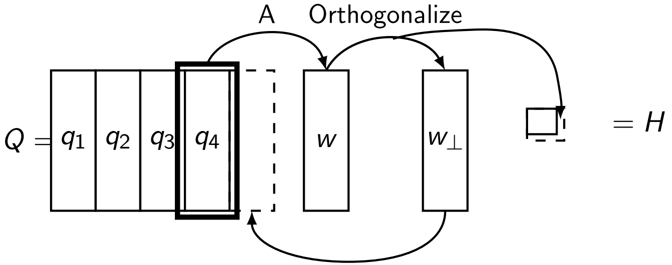

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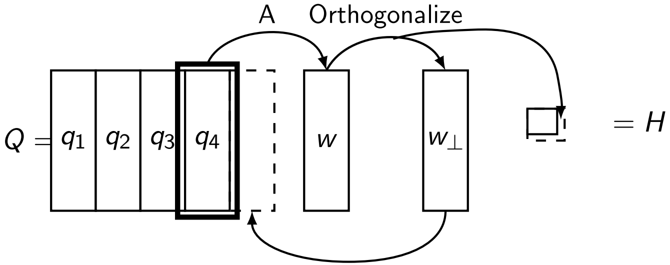

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We will now...

(1) derive a good orthogonalization procedure: variants of Gram-Schmidt,

(2) show that Arnoldi generates a Rayleigh-Ritz approximation,

(3) characterize the convergence (next lecture).

Gram-Schmidt methods (for numerical computations)

in particular for the Arnoldi method

Problem ("easier" problem)

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(a) $Q_{m+1} = [Q_m, q_{m+1}]$ is orthogonal

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

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Solution:

1. Compute a vector y which is orthogonal to Q_k
2. Normalize vector y

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$$\begin{aligned} y &= w - Qh \\ w &= Qh + y = h_1 q_1 + \cdots h_k q_k + \beta q_{k+1} \end{aligned}$$

Classical Gram-Schmidt

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>> beta=norm(y)
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* Show that it often works *

* Show a case where it doesn't work *

* Modified GS on black board *

* Double GS on black board *

```matlab
function [Q,H]=arnoldi(A,b,m)
% [Q,H]=arnoldi(A,b,m)
% A simple implementation of the Arnoldi method.
% The algorithm will return an Arnoldi "factorization":
%   Q*H(1:m+1,1:m)-A*Q(:,1:m)=0
% where Q is an orthogonal basis of the Krylov subspace
% and H a Hessenberg matrix.
%
    n=length(b);;
    Q=zeros(n,m+1);
    Q(:,1)=b/norm(b);
    for k=1:m
        w=A*(Q(:,k)); % Matrix-vector product
                      % with last element
        %%% Orthogonalize w against columns of Q
        % correct sol of HW1.2b
        [h,beta,worth]=hw1_good_gs(Q,w,k);
        %%% Put Gram-Schmidt coefficients into H
        H(1:(k+1),k)=[h;beta];
        %%% normalize
        Q(:,k+1)=worth/beta;
    end
end
```

-:--- arnoldi.m   All L8   (MATLAB +1 yas Abbrev Fill)

Convergence theory of Arnoldi's method for eigenvalue problems

Example of convergence theory of the Arnoldi method for eigenvalue problems:

Theorem (Jia, SIAM J. Matrix. Anal. Appl. 1995)

Let Q_m and H_m be generated by the Arnoldi method and suppose $\lambda_i^{(m)}$ is an eigenvalue of H_m. Assume that $\ell_i = 1$ and the associated value $\|(I - Q_m Q_m^T)x_i\|$ is sufficiently small. Let $P_i^{(m)}$ be the spectral projector associated with $\lambda_i^{(m)}$. Then,

$$|\lambda_i^{(m)} - \lambda_i| \leq \|P_i^{(m)}\| \gamma_m \frac{\|(I - Q_m Q_m^T)x_i\|}{\|Q_m Q_m^T x_i\|} + \mathcal{O}\left(\frac{\|(I - Q_m Q_m^T)x_i\|^2}{\|Q_m Q_m^T x_i\|^2}\right)$$

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The theorem is not a part of the course. In this course we will gain qualitative understanding by bounding

$$\|(I - Q_m Q_m^T)x_i\|.$$