

PRACTICAL QR A/G O

Hessenberg reduction

```

function gehrd!(A)
    """Reduced square matrix A to upper Hessenberg form"""
    n = size(A,1)
    for k=1:n-2
        # Compute Householder reflection for column k
        beta, v = house(A[k+1:n,k])
        # Apply the reflection on the left
        apply_left_householder!(A, k+1, k, beta, v)
        # Apply the reflection on the right
        apply_right_householder!(A, row, col, beta, v) _right_householder!(A, n, k+1, beta, v)
    end
    Apply a Householder reflection to the right of matrix `A`.

    `row` is the ending row index to apply the transform.
    `col` is the starting column index. `beta` and `v` are the
    parameters for the Householder reflection.
    """
function apply_right_householder!(A, row, col, beta, v)
    n = size(A,1)
    Av = zeros(n)
    lv = length(v)
    # Apply transform to the right
    # Av = beta * A * v
    for j=col:col+lv-1
        for i=1:row
            Av[i] += v[j-col+1] * A[i,j]
        end
    end
    for i=1:row
        Av[i] *= beta
    end
    # A - beta (Av) v^T
    for j=col:col+lv-1, i=1:row
        A[i,j] -= Av[i] * v[j-col+1]
    end
end

```

Resulting A is
upper Hessenberg

```

    _right_householder!(A, row, col, beta, v)
    Click to collapse the range. _householder!(A, row, col, beta, v)

    Apply a Householder reflection to the left of matrix `A`.

    `row` is the starting row index to apply the transform.
    `col` is the starting column index. `beta` and `v` are the
    parameters for the Householder reflection.
    """
function apply_left_householder!(A, row, col, beta, v)
    n = size(A,1)
    vA = zeros(n)
    lv = length(v)
    # Apply transform to the left
    # vA = beta * v^T * A
    for j=col:n
        for i=row:row+lv-1
            vA[j] += v[i-row+1] * A[i,j]
        end
        vA[j] *= beta
    end
    # A - beta v (v^T A)
    for j=col:n, i=row:row+lv-1
        A[i,j] -= v[i-row+1] * vA[j]
    end
end

```

PRACTICAL QR ALGO

```

function gees!(A) ← A is assumed to be upper Hessenberg
    n = size(A,1)
    if n==1
        return A[1,1]
    end
    D = zeros(Complex{Float64},n)

    # Tolerance for deflation
    tol = eps(Float64)

    q = n # Size of the matrix we are currently working with
    iter = 1 # Counter to detect convergence failure
    iter_per_evalue = 0 # Used to trigger an exceptional shift

    reduce_eps!(A, tol) # Zero out small entries

    while q > 0

        if iter > 10*n
            @'Code failed to converge'
        end

        deflation = true # Were we able to deflate the matrix?

        while deflation
            @'Test for deflation and record eigenvalues if converged'

            end

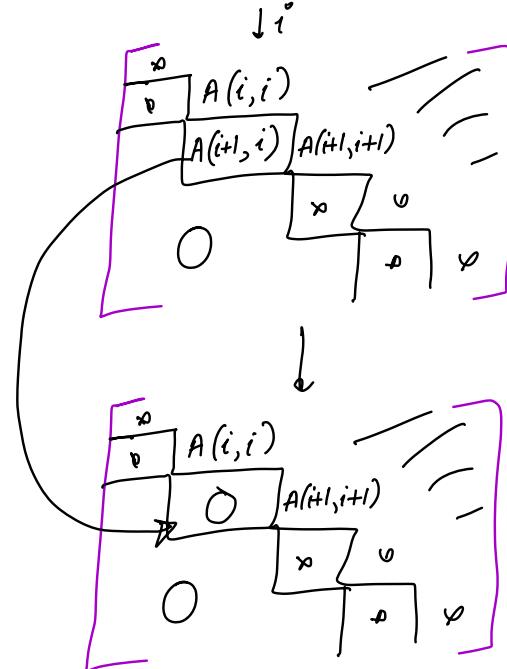
            # If q <= 2 we compute the eigenvalues at the next
            # iteration.
            if q >= 3
                @'Perform Francis QR step'
            end
        end
    end
end

```

```

function reduce_eps!(A, tol)
    # Zero out all small entries on the sub-diagonal
    n = size(A,1)
    for i=1:n-1
        if abs(A[i+1,i]) < tol * (abs(A[i,i])+abs(A[i+1,i+1]))
            A[i+1,i] = 0
        end
    end
end

```



PRACTICAL QR AIGO

```

function gees!(A)
    n = size(A,1)
    if n==1
        return A[1,1]
    end
    D = zeros(Complex{Float64},n)

    # Tolerance for deflation
    tol = eps(Float64)

    q = n # Size of the matrix we are currently working with
    iter = 1 # Counter to detect convergence failure
    iter_per_value = 0 # Used to trigger an exceptional shift

    reduce_eps!(A, tol) # Zero out small entries

    while q > 0

        if iter > 10*n
            @'Code failed to converge'
        end

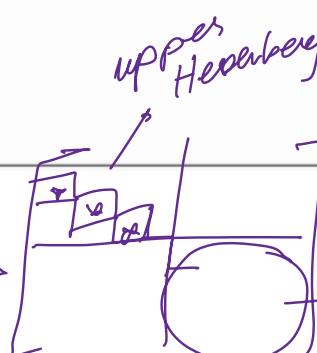
        deflation = true # Were we able to deflate the matrix?

        while deflation
            @'Test for deflation and record eigenvalues if converged'
            end

            # If q <= 2 we compute the eigenvalues at the next
            # iteration.
            if q >= 3
                @'Perform Francis QR step'
            end
        end
    end
end

```

This loop finds



```

# Definition of @"Test for deflation and record eigenvalues if converged"
deflation = false
@"Test deflation for the last 2x2 block"
@"Test deflation for the last 1x1 block"

```

The 2×2 block case is as follows:

```

# Definition of @"Test deflation for the last 2x2 block"
if q <= 2 || A[q-1,q-2] == 0
    if q >= 2
        # The last 2x2 block has converged
        deflation = true # Deflating now
        # Compute the eigenvalues
        a = A[q-1,q-1]; b = A[q-1,q]; c = A[q,q-1];
        d = A[q,q]
        htr = (a+d)/2; dis = (a-d)^2/4 + b*c
        if dis > 0 # Pair of real eigenvalues
            D[q-1] = htr - sqrt(dis)
            D[q] = htr + sqrt(dis)
        else # Complex conjugate eigenvalues
            D[q-1] = htr - sqrt(-dis)*im
            D[q] = htr + sqrt(-dis)*im
        end
        # Reduce the size of the matrix
        q -= 2
        if q>=1
            A = A[1:q,1:q]
        end
    end
end
if q==0
    return D
end

```

In the 1×1 case, we perform similar operations:

```

# Definition of @"Test deflation for the last 1x1 block"
if q <= 1 || A[q,q-1] == 0
    deflation = true
    D[q] = A[q,q]
    q -= 1
    if q>=1
        A = A[1:q,1:q]
    end

```

```

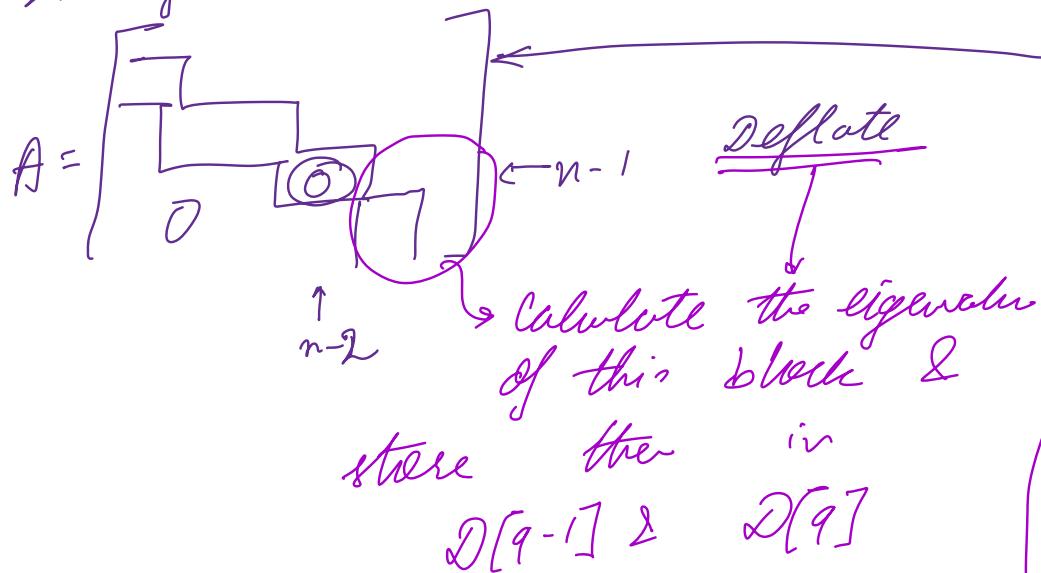
if q==0
    return D
end
if deflation
    iter_per_value = 0 # Reset the counter
end

```

largest quasi-triangular block.

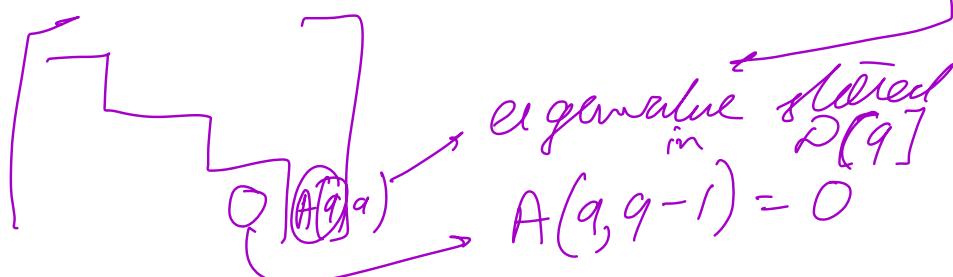
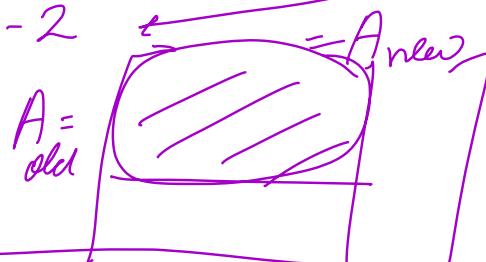
see below

Start from $q = n$.



Reduce $q = q - 2$

& change



PRACTICAL QR ALGO

```
# Definition of @"Test for deflation and record eigenvalues if converged"
deflation = false
@"Test deflation for the last 2x2 block"
@"Test deflation for the last 1x1 block"
```

The 2×2 block case is as follows:

```
# Definition of @"Test deflation for the last 2x2 block"
if q <= 2 || A[q-1,q-2] == 0
    if q >= 2
        # The last 2x2 block has converged
        deflation = true # Deflating now
        # Compute the eigenvalues
        a = A[q-1,q-1]; b = A[q-1,q]; c = A[q,q-1];
        d = A[q,q]
        htr = (a+d)/2; dis = (a-d)^2/4 + b*c
        if dis > 0 # Pair of real eigenvalues
            D[q-1] = htr - sqrt(dis)
            D[q] = htr + sqrt(dis)
        else # Complex conjugate eigenvalues
            D[q-1] = htr - sqrt(-dis)*im
            D[q] = htr + sqrt(-dis)*im
        end
        # Reduce the size of the matrix
        q -= 2
        if q >= 1
            A = A[1:q,1:q]
        end
    end
end
if q==0
    return D
end
```

In the 1×1 case, we perform similar operations:

```
# Definition of @"Test deflation for the last 1x1 block"
if q <= 1 || A[q,q-1] == 0
    deflation = true
    D[q] = A[q,q]
    q -= 1
    if q >= 1
        A = A[1:q,1:q]
    end
```

```
if q==0
    return D
end
if deflation
    iter_per_value = 0 # Reset the counter
end
```

```

function gees!(A)
    n = size(A,1)
    if n==1
        return A[1,1]
    end
    D = zeros(Complex{Float64},n)

    # Tolerance for deflation
    tol = eps(Float64)

    q = n # Size of the matrix we are currently working with
    iter = 1 # Counter to detect convergence failure
    iter_per_evalue = 0 # Used to trigger an exceptional shift

    reduce_eps!(A, tol) # Zero out small entries

    while q > 0

        if iter > 10*n
            @'Code failed to converge'
        end

        deflation = true # Were we able to deflate the matrix?

        while deflation
            @'Test for deflation and record eigenvalues if converged'

            end

            # If q <= 2 we compute the eigenvalues at the next
            # iteration.
            if q >= 3
                @'Perform Francis QR step'
            end
        end
    end
end

```

```

# Definition of @"Perform Francis QR step"
# Searching for the smallest unreduced sub-block
p = q
while p > 1 && A[p,p-1] != 0
    p -= 1
end

# If the unreduced sub-block has size 2 or less, we move on
# to the next iteration.
if q-p+1 >= 3
    B = A[p:q,p:q] # Extract sub-block
    exceptional_shift = ((iter_per_evalue%5) == 0 &&
                           iter_per_evalue>0)
    # Francis QR step
    gees_single_step!(B, exceptional_shift)
    # Reduce matrix
    reduce_eps!(B, tol)
    A[p:q,p:q] = B # Copy the resulting matrix back
    iter += 1 # Increment iteration counter
    iter_per_evalue += 1 # Counter for exceptional_shift
end

```

Say after possible deflation.

$A_{\text{after deflation}}$ (smaller size)

9×9

non-zero

(otherwise would have been deflated)

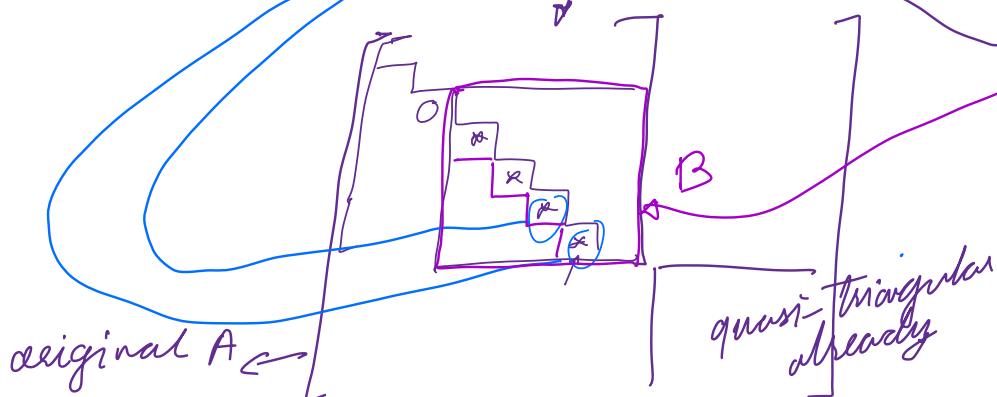
P reduced by $P = P^{-1}$

If $q-p+1 > 3$ then A
do Francis step

Otherwise do not do
Francis step. Deflate
in the next step.

So after Francis step we
do not reduce q.

The program returns to S
and does deflation if
the Francis step was
successful in reducing
the bottom corner sub-diagonal
elements?



```

function gees!(A)
    n = size(A,1)
    if n==1
        return A[1,1]
    end
    D = zeros(Complex{Float64},n)

    # Tolerance for deflation
    tol = eps(Float64)

    q = n # Size of the matrix we are currently working with
    iter = 1 # Counter to detect convergence failure
    iter_per_evalue = 0 # Used to trigger an exceptional shift

    reduce_eps!(A, tol) # Zero out small entries

    while q > 0
        if iter > 10*n
            @'Code failed to converge'
        end

        deflation = true # Were we able to deflate the matrix?
        while deflation
            @'Test for deflation and record eigenvalues if converged'
        end
    end

    # If q <= 2 we compute the eigenvalues at the next
    # iteration.
    if q >= 3
        @'Perform Francis QR step'
    end
end

```

```

# Definition of @"Perform Francis QR step"
# Searching for the smallest unreduced sub-block
p = q
while p > 1 && A[p,p-1] != 0
    p -= 1
end

# If the unreduced sub-block has size 2 or less, we move on
# to the next iteration.
if q-p+1 >= 3
    B = A[p:q,p:q] # Extract sub-block
    exceptional_shift = ((iter_per_evalue%5) == 0 &&
                          iter_per_evalue>0)
    # Francis QR step
    gees_single_step!(B, exceptional_shift)
    # Reduce matrix
    reduce_eps!(B, tol)
    A[p:q,p:q] = B # Copy the resulting matrix back
    iter += 1 # Increment iteration counter
    iter_per_evalue += 1 # Counter for exceptional_shift
end

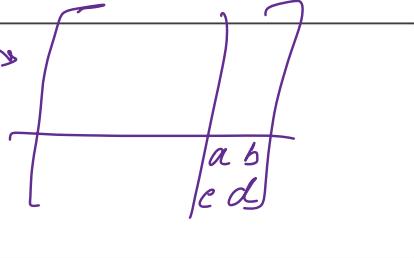
```

FRANCIS Step

```

function double_shift_st(A)
    a = A[1,1]
    b = A[1,2]
    c = A[2,1]
    d = A[2,2]
    s = a+d      # sum
    t = a*d - b*c # product
    return s,t
end

```



```

function gees_single_step!(A, exceptional_shift)
    n = size(A,1); tol = 0.01
    # This tolerance is used to test for early convergence of the last
    # 2x2 or 1x1 block.

```

Which shift should we apply?
`if abs(A[n-1,n-2]) < tol * (abs(A[n-2,n-2]) + abs(A[n-1,n-1])) || ! (abs(A[n,n-1]) < tol * (abs(A[n-1,n-1]) + abs(A[n,n])))`
If either (double-shift test) == true
or (single-shift test) == false, do a double shift:
`s, t = double_shift_st(A[n-1:n,n-1:n])`

```

else # Single shift should be used
    s = 2*A[n,n]
    t = A[n,n]^2
end

```

```

if exceptional_shift
    @'Exceptional shift'
end

```

@'Apply the Francis QR step'

```

# Definition of @"Apply the Francis QR step"
# Assembling the first column
v = [ A[1,1]*A[1,1] + A[1,2]*A[2,1] - s*A[1,1] + t;
      A[2,1]*(A[1,1]+A[2,2]-s);
      A[2,1]*A[3,2] ]

```

```

beta, v = house(v)

```

```

apply_left_householder!(A, 1, 1, beta, v)
apply_right_householder!(A, min(4,n), 1, beta, v)

```

```

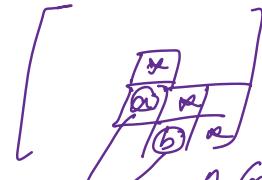
for k=2:n-1
    beta, v = house(A[k:min(k+2,n),k-1])
    apply_left_householder!(A, k, k-1, beta, v)
    apply_right_householder!(A, min(k+3,n), k, beta, v)
end

```

Whether to apply a double or a single - shift

Heuristic

1) Is the last 2×2 block converging



$A(n-1, n-2)$

$\text{abs}(A(n-1, n-2)) < \text{tol} * (\text{abs}(A(n-2, n-2) + \text{abs}(A(n-1, n-1)))$
OR
 $\text{abs}(A(n, n-1)) > \text{tol} * (\text{abs}(A(n-1, n-1) + \text{abs}(A(n, n)))$

Idea: If a is big we should do single - shift

If b is small we should do single - shift

If a is small or b is large we do double - shift.

s, t computation for double shift

Using the old notation (from the notes)

$$M_{E_1} = \begin{bmatrix} x \\ y \\ z \\ 0 \\ \vdots \\ 0 \end{bmatrix} \quad \left\{ \begin{bmatrix} h_{11} & h_{12} & \dots \\ h_{21} & h_{22} & \dots \\ \vdots & \vdots & \ddots \\ 0 & h_{32} & \dots \end{bmatrix} - \alpha_1 I \right\}$$

$$x = h_{11}^2 + h_{12} h_{21} - (\alpha_1 + \alpha_2) h_{11} + \alpha_1 \alpha_2$$

$$y = h_{21} (h_{11} + h_{22} - (\alpha_1 + \alpha_2))$$

$$z = h_{21} h_{32}$$

Here

$$V = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

s, t for single shift

$$s = 2d, t = d^2$$

If $\alpha_1 = \alpha_2 [= d]$ \rightarrow current guess.

$$x = h_{11}^2 + h_{12} h_{21} - (2d) h_{11} + d^2$$

$$z = \dots$$

```
function double_shift_st(A)
    a = A[1,1]
    b = A[1,2]
    c = A[2,1]
    d = A[2,2]
    s = a+d # sum
    t = a*d - b*c # product
    return s,t
end
```

$$\begin{aligned} \lambda I - \begin{bmatrix} a & b \\ c & d \end{bmatrix} &= (\lambda - a)(\lambda - d) - cb \\ &= \lambda^2 - (\underbrace{a+d)}_s \lambda + \underbrace{ad - cb}_t \end{aligned}$$

$$\boxed{\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} a & b \\ c & d \end{bmatrix}}$$

```

# Definition of @"Apply the Francis QR step"
# Assembling the first column
v = [ A[1,1]*A[1,1] + A[1,2]*A[2,1] - s*A[1,1] + t;
      A[2,1]*(A[1,1]+A[2,2]-s);
      A[2,1]*A[3,2] ]
.
beta, v = house(v)

apply_left_householder!( A, 1, 1, beta, v)
apply_right_householder!(A, min(4,n), 1, beta, v)

for k=2:n-1
  beta, v = house(A[k:min(k+2,n),k-1])
  apply_left_householder!( A, k, k-1, beta, v)
  apply_right_householder!(A, min(k+3,n), k, beta, v)
end

.....
Click to collapse the range. _householder!(A, row, col, beta, v)

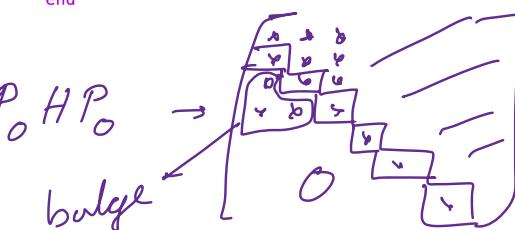
Apply a Householder reflection to the left of matrix `A`.

`row` is the starting row index to apply the transform.
`col` is the starting column index. `beta` and `v` are the
parameters for the Householder reflection.
.....

function apply_left_householder!(A, row, col, beta, v)
  n = size(A,1)
  vA = zeros(n)
  lv = length(v)
  # Apply transform to the left
  # vA = beta * v^T * A
  for j=col:n
    for i=row:row+lv-1
      vA[j] += v[i-row+1] * A[i,j]
    end
    vA[j] *= beta
  end
  # A - beta v (v^T A)
  for j=col:n, i=row:row+lv-1
    A[i,j] -= v[i-row+1] * vA[j]
  end
end

```

Q. Where did the $QR = H - \mu I$
 $H = RQ + \mu I$ step go?



$$\begin{aligned}
 & P_{n-1} \cdots P_1 (P_0 H P_0) P_1 \cdots P_{n-2} \\
 & = \left[\begin{array}{cccc} & & & \\ & & & \\ & & & \\ & & & \end{array} \right] \xrightarrow{\text{hopefully low values}}
 \end{aligned}$$