



Computational Physics (PHYS6350)

Lecture 5: Linear algebra and matrices: Part II

- Matrix inversion
- Tri- and band-diagonal systems
- QR decomposition
- Eigenvalue problem

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Course materials: <https://github.com/vlvovch/PHYS6350-ComputationalPhysics>

Matrix inversion

Inverse of matrix \mathbf{A} , if it exists, satisfies

$$\mathbf{A}\mathbf{A}^{-1} = \mathbf{I}.$$

Let us denote the columns of the inverse matrix \mathbf{A}^{-1} by \mathbf{x}_k , i.e. $\mathbf{A}^{-1} = (\mathbf{x}_1, \dots, \mathbf{x}_n)$

The vectors \mathbf{x}_k satisfy the following N systems of non-linear equations

$$\mathbf{A}\mathbf{x}_k = \mathbf{v}_k, \quad k = 1 \dots N$$

where $\mathbf{v}_{k,j} = \delta_{kj}$

Since the matrix \mathbf{A} is always the same, these systems can be efficiently solved with LU-decomposition to find all \mathbf{x}_k and thus the inverse matrix \mathbf{A}^{-1}

Complexity: 1 LU-decomposition $O(N^3)$
+ N backsubstitutions [each one is $O(N^2)$]
~ **$O(N^3)$ overall**

Matrix inversion

```
def matrix_inverse_with_ludecomp(A):  
    # First step: LU decomposition of matrix A  
    L, U, row_map = lu_decomp_partialpivot(A)  
    N = len(row_map)  
  
    Ainv = A.copy()  
    for c in range(N):  
        v = np.zeros(N, float)  
        v[c] = 1.  
        x = solve_using_lu_partialpivot(L,U,row_map,v)  
        Ainv[:,c] = x  
  
    return Ainv
```

```
A = np.array([[ 0,  1,  4,  1 ],  
              [ 3,  4, -1, -1 ],  
              [ 1, -4,  1,  5 ],  
              [ 2, -2,  1,  3 ]],float)
```

```
Ainv = matrix_inverse_with_ludecomp(A)  
print("A*A^{-1} = \n", tabulate(A.dot(Ainv)))
```

A*A⁻¹ =

-----	-----	-----	-----
1	-5.55112e-17	1.11022e-16	-1.11022e-16
-2.77556e-17	1	-1.11022e-16	3.33067e-16
2.77556e-17	5.55112e-17	1	4.44089e-16
-2.77556e-17	-5.55112e-17	-5.55112e-16	1
-----	-----	-----	-----

Tridiagonal systems

Tridiagonal system of equation is a special case when the matrix \mathbf{A} is tridiagonal

$$\mathbf{A} = \begin{pmatrix} d_1 & u_1 & & & 0 \\ l_2 & d_2 & u_2 & & \\ & l_3 & \ddots & \ddots & \\ 0 & & \ddots & \ddots & u_{n-1} \\ & & & l_n & d_n \end{pmatrix}$$

Tridiagonal systems of linear equations often appear in physics, e.g.

- Nearest-neighbor interaction (linear chain of springs)
- Finite differences applied to partial differential equations (heat equation)

$$\frac{\partial u(t, x)}{\partial t} = \alpha \frac{\partial^2 u(t, x)}{\partial x^2} \quad \longrightarrow \quad \begin{pmatrix} \frac{\partial u_1(t)}{\partial t} \\ \frac{\partial u_2(t)}{\partial t} \\ \vdots \\ \frac{\partial u_N(t)}{\partial t} \end{pmatrix} = \frac{\alpha}{\Delta x} \begin{pmatrix} -2 & 1 & 0 & \dots & 0 \\ 1 & -2 & 1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & & 1 & -2 & 1 \\ 0 & \dots & 0 & 1 & -2 \end{pmatrix} \begin{pmatrix} u_1(t) \\ u_2(t) \\ \vdots \\ u_N(t) \end{pmatrix}$$

Solving tridiagonal systems

$$\mathbf{A} = \begin{pmatrix} d_1 & u_1 & & 0 \\ l_2 & d_2 & u_2 & \\ & l_3 & \ddots & \ddots \\ 0 & & \ddots & \ddots & u_{n-1} \\ & & & l_n & d_n \end{pmatrix}$$

Tridiagonal system can be solved in linear time $[O(N)]$ with Gaussian elimination and

1. **Gaussian elimination:** at each step need to subtract only one row below the current one, and at most two elements
2. **Backsubstitution:** subtract only single element from the upper superdiagonal

$$\begin{aligned} x_n &= \tilde{v}_n, \\ x_k &= \tilde{v}_k - \tilde{u}_k x_{k+1}, \quad k = 1 \dots N - 1. \end{aligned}$$

Solving tridiagonal systems

```
# Solve tridiagonal system of linear equations
# d: vector of diagonal elements
# l: vector of elements on the lower subdiagonal
# u: vector of elements on the upper superdiagonal
# v0: right-hand-side vector
def linsolve_tridiagonal(d, l, u, v0):
    # Initialization
    N = len(v0)
    a = d.copy() # Current diagonal elements
    b = u.copy() # Current upper diagonal elements
    v = v0.copy()

    # Gaussian elimination
    for r in range(N):
        if (a[r] == 0.):
            print("Diagonal element is zero! Cannot solve")
            return None
        b[r] /= a[r]
        v[r] /= a[r]
        a[r] = 1.
        if (r < N - 1):
            a[r + 1] -= l[r+1] * b[r]
            v[r + 1] -= l[r+1] * v[r]

    # Backsubstitution
    x = np.empty(N, float)
    x[N - 1] = v[N - 1]
    for r in range(N-2, -1, -1):
        x[r] = v[r] - b[r] * x[r + 1]

    return x
```

Test for a random tridiagonal matrix

```
def random_tridiagonal(n):
    A = np.random.rand(n, n)
    for r in range(n):
        for c in range(0, r-1):
            A[r][c] = 0.
        for c in range(r + 2, n):
            A[r][c] = 0.
    return A
```

```
n = 8
A = random_tridiagonal(n)
print("A =\n", tabulate(A))
v = np.random.rand(n)
x = linsolve_tridiagonal(*(get_tridiagonal(A)), v)
print(" x = ", x)
print("Ax = ", A.dot(x))
print(" v = ", v)
```

```
A =
-----
0.258085  0.365256  0          0          0          0          0          0
0.598828  0.60432  0.0777664  0          0          0          0          0
0          0.839862  0.209281  0.418171  0          0          0          0
0          0          0.730628  0.406732  0.789413  0          0          0
0          0          0          0.597044  0.627719  0.575418  0          0
0          0          0          0          0.639515  0.293871  0.737697  0
0          0          0          0          0          0.74846  0.477541  0.704847
0          0          0          0          0          0          0.00826684  0.109495
-----
x = [ 2.2288744 -0.6670926 -5.72667763  5.03759801  3.51116171 -7.41798625
      1.22249979  8.40485586]
Ax = [0.33158055 0.48623086 0.34782961 0.63663712 0.94324165 0.96734828
      0.9558695  0.93039484]
v = [0.33158055 0.48623086 0.34782961 0.63663712 0.94324165 0.96734828
      0.9558695  0.93039484]
```

Band-diagonal systems

Band-diagonal system: in each row

- at most m_{lower} non-zero elements to the left of the main diagonal
- at most m_{upper} non-zero elements to the right of the main diagonal

$$\mathbf{A} = \begin{pmatrix} d_1 & u_{1,1} & u_{2,1} & & & & \\ l_{1,2} & d_2 & u_{1,2} & u_{2,2} & & & 0 \\ l_{2,3} & l_{1,3} & d_3 & u_{1,3} & u_{2,3} & & \\ & l_{2,4} & l_{1,4} & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots & u_{1,n-2} & u_{2,n-2} \\ & 0 & & \ddots & \ddots & \ddots & u_{1,n-1} \\ & & & & l_{2,n} & l_{1,n} & d_n \end{pmatrix}$$

Generalization of tridiagonal systems ($m_{\text{lower}} = m_{\text{upper}} = 1$)

- k -nearest-neighbor interaction (linear chain of springs)
- High-order finite difference applied to partial differential equations (heat equation)

Solving band-diagonal systems

$$\mathbf{A} = \begin{pmatrix} d_1 & u_{1,1} & u_{2,1} & & & & \\ l_{1,2} & d_2 & u_{1,2} & u_{2,2} & & & 0 \\ l_{2,3} & l_{1,3} & d_3 & u_{1,3} & u_{2,3} & & \\ & l_{2,4} & l_{1,4} & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots & u_{1,n-2} & u_{2,n-2} \\ & 0 & & \ddots & \ddots & \ddots & u_{1,n-1} \\ & & & & l_{2,n} & l_{1,n} & d_n \end{pmatrix}$$

Solving band-diagonal system proceeds also through Gaussian elimination

- At each step one has to normalize $m_{\text{upper}} + 1$ elements in the current row, then subtract the current row from at most m_{lower} rows below it. $O(N \times m_{\text{upper}} \times m_{\text{lower}})$
- Backsubstitution step: in each row subtract up to m_{upper} elements to the right from the main diagonal. $O(N \times m_{\text{upper}})$

Overall complexity: $O(N \times m_{\text{upper}} \times m_{\text{lower}})$

Solving band-diagonal systems

```
# Solving linear system of banded equations
# d: diagonal elements of the banded matrix
# l: lower non-zero diagonals of the banded matrix
# u: upper non-zero diagonals of the banded matrix
# v0: r.h.s. vector
def linsolve_banded(d, l, u, v0):
    # Initialization
    v = v0.copy()
    N = len(v)
    mlower = len(l)
    mupper = len(u)

    a = d.copy() # Diagonal elements
    dup = u.copy() # Upper diagonal elements
    dlow = l.copy() # Lower diagonal elements

    # Gaussian elimination
    for r in range(N):
        # Divide row r by diagonal element
        div = a[r]
        if (div == 0.):
            print("Diagonal element is zero! Cannot solve the system with simple")
            return None
        for c in range(r+1, min(r + mupper + 1, N)):
            dup[c-r-1, r] /= div
        a[r] /= div
        v[r] /= div

        # Now subtract this row from the lower rows
        # We do not need to go through all the rows
        # but only up to a certain row depending
        # on the number of non-zero elements to right and left of the main diagonal
        max_row = min(r + mlower, N - 1)

        # First the vector
        for r2 in range(r+1, max_row + 1):
            v[r2] -= dlow[r2 - r - 1, r2] * v[r]

        # Then the matrix rows
        for c in range(r + 1, min(r + mupper + 1, N)):
            for r2 in range(r+1, max_row + 1):
                if (c == r2):
                    a[r2] -= dlow[r2 - r - 1, r2] * dup[c-r-1, r]
                elif (c < r2 and r2 - c - 1 < mlower):
                    dlow[r2 - c - 1, r2] -= dlow[r2 - r - 1, r2] * dup[c-r-1, r]
                elif (c > r2 and c - r2 - 1 < mupper):
                    dup[c - r2 - 1, r2] -= dlow[r2 - r - 1, r2] * dup[c-r-1, r]

    # Backsubstitution
    x = np.empty(N, float)
    for r in range(N-1, -1, -1):
        x[r] = v[r]
        for c in range(r+1, min(r + mupper + 1, N)):
            x[r] -= dup[c - r - 1, r] * x[c]

    return x
```

```
def random_banded(n, mlower, mupper):
    A = np.random.rand(n, n)
    for r in range(n):
        for c in range(0, r-mlower):
            A[r][c] = 0.
        for c in range(r + mupper + 1, n):
            A[r][c] = 0.
    return A
```

```
n = 10
mupper = 4
mlower = 3
A = random_banded(n, mlower, mupper)
print("A =\n", tabulate(A))
v = np.random.rand(n)
x = linsolve_banded(* (get_banded(A, mlower, mupper)), v)
print(" x = ", x)
print("Ax = ", A.dot(x))
print(" v = ", v)
```

```
A =
-----
0.398214  0.972929  0.249665  0.0841269  0.667612  0          0          0          0          0
0.668918  0.27899  0.98081  0.311536  0.395787  0.250914  0          0          0          0
0.103901  0.955985  0.591015  0.178139  0.194452  0.565519  0.207813  0          0          0
0.094764  0.417524  0.401467  0.507737  0.198962  0.872389  0.999096  0.0251162  0          0
0          0.624273  0.727381  0.409819  0.859236  0.00593723  0.68357  0.707848  0.427377  0
0          0          0.304125  0.768458  0.03066  0.322861  0.123774  0.0664194  0.775458  0.117592
0          0          0          0.294081  0.698817  0.82127  0.43601  0.743528  0.107041  0.917906
0          0          0          0          0.642317  0.763591  0.0719641  0.752717  0.223502  0.607639
0          0          0          0          0          0.18334  0.0233041  0.0637123  0.95644  0.420615
0          0          0          0          0          0          0.698929  0.919066  0.824737  0.521482
-----
x = [-0.28014041  0.17110358  1.10225327 -1.21247032  0.14011191  0.26755524
      0.024373  -0.04051962  0.83538165  0.223171 ]
Ax = [0.32164853  0.68630553  0.75354435  0.15641687  0.87865905  0.1685409
      0.23585233  0.58787029  0.93990131  0.78514492]
v = [0.32164853  0.68630553  0.75354435  0.15641687  0.87865905  0.1685409
      0.23585233  0.58787029  0.93990131  0.78514492]
```

QR decomposition*

Any real square matrix **A** permits a decomposition

$$\mathbf{A} = \mathbf{Q}\mathbf{R}$$

where

- **Q** is orthogonal, $\mathbf{Q}^{-1}=\mathbf{Q}^T$, and thus, $\mathbf{Q}^T\mathbf{Q} = \mathbf{I}$
- **R** is upper diagonal

There are many algorithms for constructing the QR decomposition:

- from simple Gram-Schmidt process (numerically unstable)
- to more involved methods using Householder transformation or
- Givens rotations.



`numpy.linalg.qr`

*Has nothing to do with QR codes

QR decomposition and systems of linear equations

System of linear equations

$$\mathbf{Ax} = \mathbf{v}.$$

If $\mathbf{A} = \mathbf{QR}$ we can rewrite the system as

$$\mathbf{QRx} = \mathbf{v}.$$

Multiplying each side of the equation by \mathbf{Q}^T , we have

$$\mathbf{Rx} = \mathbf{Q}^T \mathbf{v}.$$

The matrix \mathbf{R} is upper triangular, thus, the system can be solved using backsubstitution.

```
def linsolve_using_qr(Q,R,v):  
    # Initialization  
    N = len(v)  
    # Calculate y = Q^T v  
    y = np.zeros(N,float)  
    for r in range(N):  
        for c in range(N):  
            y[r] += Q[c][r] * v[c]  
  
    # Backsubstitution for R*x = y  
    x = np.empty(N,float)  
    for r in range(N-1,-1,-1):  
        x[r] = y[r]  
        for c in range(r+1,N):  
            x[r] -= R[r][c] * x[c]  
  
        x[r] /= R[r][r]  
    return x
```

```
A = np.array([[ 0,  1,  4,  1 ],  
              [ 3,  4, -1, -1 ],  
              [ 1, -4,  1,  5 ],  
              [ 2, -2,  1,  3 ]],float)  
  
Q, R = np.linalg.qr(A)  
v = np.array([ -4,  3,  9,  7 ],float)  
x = linsolve_using_qr(Q,R,v)  
print('x  =', x)  
print('Ax =', A.dot(x))  
print('v  =', v)
```

Eigenvalue problem

A common matrix problem in physics is the calculation of eigenvalues and eigenvectors of a matrix (e.g. classical and quantum mechanics).

The eigenvalue problem corresponds to the equation

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v}.$$

Here λ are the eigenvalues and \mathbf{v} are the eigenvectors

General approach (not used in practice):

- Eigenvalues are roots of the characteristic polynomial

$$\det(\lambda I - A) = 0$$

- Once λ are found, the eigenvectors can be computed by solving linear system

$$(\mathbf{A} - \lambda\mathbf{I})\mathbf{v} = 0$$

- This approach is impractical: numerically unstable to solve high-degree polynomial roots

Eigenvalue problem

In most cases the matrix \mathbf{A} is either real symmetric or Hermitian (complex numbers).

In this case, for a $N \times N$ matrix there are N eigenvectors $\mathbf{v}_1, \dots, \mathbf{v}_N$ with real eigenvalues $\lambda_1, \dots, \lambda_N$. The eigenvectors are orthogonal, i.e. $\mathbf{v}_i \mathbf{v}_j = \delta_{ij}$ with the appropriate normalization.

The eigenvalue problem can thus be cast as a matrix equation

$$\mathbf{A}\mathbf{V} = \mathbf{V}\mathbf{D}.$$

Here \mathbf{V} is the matrix of eigenvectors, i.e. column k corresponds to the eigenvector \mathbf{v}_k , and \mathbf{D} is a diagonal matrix with entries corresponding to eigenvalues, $\mathbf{D} = \text{diag}(\lambda_1, \dots, \lambda_N)$.

How to solve the matrix equation $\mathbf{A}\mathbf{V} = \mathbf{V}\mathbf{D}$. ?

QR algorithm

QR algorithm is a method of finding eigenvalues and/or eigenvectors based on an iterative procedure.

1. One starts with matrix $\mathbf{A}_1 = \mathbf{A}$ and calculates its QR decomposition $\mathbf{A}_1 = \mathbf{Q}_1\mathbf{R}_1$
2. The next matrix is computed as $\mathbf{A}_2 = \mathbf{R}_1\mathbf{Q}_1$.
 - This is a similarity transform. Multiplying both sides by $\mathbf{I} = \mathbf{Q}_1^T\mathbf{Q}_1$ and taking into account $\mathbf{A}_1 = \mathbf{Q}_1\mathbf{R}_1$, one gets $\mathbf{A}_2 = \mathbf{Q}_1^T\mathbf{A}_1\mathbf{Q}_1$.
3. The process is repeated as follows,

$$\mathbf{A}_{n+1} = \mathbf{R}_n\mathbf{Q}_n = \mathbf{Q}_n^T\mathbf{A}_n\mathbf{Q}_n.$$

4. Matrix \mathbf{A}_n converges to **diagonal form** in the limit $n \rightarrow \infty$ (for real symmetric \mathbf{A}):

$$\mathbf{A}_\infty = \mathbf{Q}^T\mathbf{A}\mathbf{Q}, \text{ where } \mathbf{Q} = \prod_{k=1}^{\infty} \mathbf{Q}_k \text{ where } \mathbf{Q} \text{ is an orthogonal matrix.}$$

Multiply \mathbf{A}_∞ by \mathbf{Q} from the right: $\mathbf{A}\mathbf{Q} = \mathbf{Q}\mathbf{A}_\infty$

Compare with $\mathbf{A}\mathbf{V} = \mathbf{V}\mathbf{D}$  $\mathbf{Q} = \mathbf{V}$ $\mathbf{A}_\infty = \mathbf{D}$
eigenvector matrix eigenvalue matrix

In practice, the algorithm stops once non-diagonal elements of \mathbf{A}_n are below a certain threshold ϵ .

QR algorithm

```
def eigen_qr_simple(A, iterations=1000):
    Ak = np.copy(A)
    n = len(A[0])
    QQ = np.eye(n)
    for k in range(iterations):
        Q, R = np.linalg.qr(Ak)
        Ak = np.dot(R, Q)
        QQ = np.dot(QQ, Q)
        if k%100 == 0:
            print("A", k, "=")
            print(tabulate(Ak))
            print("\n")
    return Ak, QQ
```

```
n = 5
A = np.random.rand(n, n)
# Make symmetric
for r in range(n):
    for c in range(r):
        A[r][c] = A[c][r]
```

```
# We call the function
AQ = eigen_qr_simple(A)

# Print A' = D
print("A' =\n", tabulate(AQ[0]))
print("Q =\n", tabulate(AQ[1]))

# We compare our results with the official numpy algorithm
print(np.linalg.eig(A))

# Check orthogonality
print("v1*v2 = ", P[:,0].dot(P[:,1]))
```

```
A' =
-----
2.74844 -3.02815e-16 1.6284e-16 -5.32145e-17 2.4959e-16
0 -0.746594 1.15176e-17 4.62374e-17 -1.69369e-17
0 9.02192e-67 -0.643849 -9.85419e-17 1.54078e-16
0 -4.94066e-324 -4.5242e-287 0.331455 -2.97135e-16
0 -4.94066e-324 -7.90505e-323 1.77529e-36 -0.305375
-----

Q = v1 v2 v3 v4 v5
-----
-0.537155 -0.550458 0.199338 0.418962 -0.439541
-0.445186 -0.37513 0.179416 -0.561737 0.559775
-0.483201 0.62303 0.264306 -0.365474 -0.418235
-0.457385 0.126918 -0.871099 0.0886914 0.0894995
-0.265687 0.38987 0.315282 0.606205 0.557247
-----
v1*v2 = -2.513426757818653e-16
```

Linear algebra: Summary

$$\mathbf{Ax} = \mathbf{v}.$$

System of N linear equations

- General case: use LU-decomposition [$O(N^3)$] + forward/back-substitution [$O(N^2)$] $\sim O(N^3)$
- No need to repeat LU-decomposition when \mathbf{v} (but not \mathbf{A}) changes
- Tridiagonal system: Can be solve in linear $O(N)$ time
- Band-diagonal: $O(N \times m_{\text{upper}} \times m_{\text{lower}})$

$$\mathbf{Av} = \lambda \mathbf{v}.$$

Eigenvalue problem

- General case: use QR-decomposition and QR algorithm (iterative)
- Specialized algorithms for sparse matrices (e.g. **Lanczos algorithm**)
final project idea(?)