Matrix Diagonalization: What Are We Trying to Do?

Power Method + Gram–Schmidt Orthogonalization

The entire lab in plain words: We are given a small 6×6 matrix. Our C++ program must discover its *six eigenvalues* and *six eigenvectors*, one pair at a time. We then use those results to rebuild the original matrix and calculate its inverse. **We are learning how a numerical algorithm works, not just asking a library to diagonalize a matrix.**

1. What is an eigenvalue? What is an eigenvector?

When a matrix A multiplies an ordinary vector, it can change both the vector's length and direction. Some special vectors do not change their *line of direction* (they may reverse direction). They satisfy

$$\boxed{A\mathbf{x} = \lambda\mathbf{x}}$$

- $\mathbf{x}$ is an **eigenvector**: a special direction.
- λ is an **eigenvalue**: the factor by which the matrix stretches, shrinks, or reverses that vector.

Tiny example: $\begin{pmatrix} 3 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 3 \begin{pmatrix} 1 \\ 0 \end{pmatrix}$. The vector $(1, 0)^T$ is an eigenvector and its eigenvalue is 3.

2. Where does our particular matrix come from?

In physics, the **second derivative** describes curvature (for example in wave and Schrödinger equations). On a grid, we approximate it using the values at three neighboring points:

$$\left.\frac{d^2 f}{dx^2}\right|_{x_i} \approx \frac{f_{i-1} - 2f_i + f_{i+1}}{\Delta^2}, \qquad \Delta = 1.$$

The three coefficients are therefore $1, -2, 1$. This gives the rule: -2 on the main diagonal, 1 just above and below it, and 0 elsewhere. For the assignment, $n = 6$:

$$A = \begin{pmatrix} -2 & 1 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 1 & -2 \end{pmatrix}$$

This is a **symmetric tridiagonal matrix**. Symmetric means $A^T = A$; its eigenvectors can be chosen perpendicular to one another.

3. Our first two programming tasks

Task 1: Store A as a normal C++ 2D array. **Task 2:** Print it and check every entry.

```
const int n = 6;
double A[n][n];
for (int i = 0; i < n; ++i)
  for (int j = 0; j < n; ++j)
    A[i][j] = (i == j) ? -2.0 : (abs(i-j) == 1 ? 1.0 : 0.0);
```

Input parameters: $n = 6$ (matrix size), $itmax = 150$ (maximum iterations per eigenpair), $\varepsilon = 10^{-8}$ (requested precision), and $\Delta = 1$ (grid spacing). The 6×6 matrix is small, so a sparse-storage format such as CSR is unnecessary.

How Do We Find All Six Eigenpairs?

First: the Power Method. Then: Gram–Schmidt.

4. Power Method: find one special direction

Intuition: Start with an ordinary vector and repeatedly multiply it by A. After each multiplication, scale it back to length 1. Usually, the direction settles toward the eigenvector whose eigenvalue has the **largest absolute value**.

One iteration (with a normalized vector $\mathbf{x}^{(t)}$):

$$\underbrace{\mathbf{y} = A\mathbf{x}^{(t)}}_{\text{multiply}} \quad \longrightarrow \quad \underbrace{\mathbf{x}^{(t+1)} = \frac{\mathbf{y}}{\|\mathbf{y}\|}}_{\text{normalize}}$$

Estimate the eigenvalue with the **Rayleigh quotient**:

$$\lambda^{(t+1)} = \frac{(\mathbf{x}^{(t+1)})^T A\mathbf{x}^{(t+1)}}{(\mathbf{x}^{(t+1)})^T\mathbf{x}^{(t+1)}}.$$

Here $\|\mathbf{y}\| = \sqrt{\sum_i y_i^2}$ is the vector length. After normalization, the denominator is 1.

Easy 2×2 demonstration (only to understand the method):

$$B = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}, \qquad \mathbf{x}^{(0)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad B\mathbf{x}^{(0)} = \begin{pmatrix} 2 \\ 1 \end{pmatrix}.$$

Further multiplications give directions $(5,4)^T, (14,13)^T, \ldots$, approaching $(1,1)^T$. Therefore the dominant eigenvalue is 3, because $B(1,1)^T = 3(1,1)^T$. Our actual lab uses the *six-by-six matrix from page 1*, not B.

5. Gram–Schmidt: do not find the same vector again

If we restart the Power Method with a new random vector, we usually converge to the **same dominant eigenvector**. To find another one, we must remove the part parallel to every eigenvector already found.

$$\boxed{\mathbf{y}_\perp = \mathbf{y} - \sum_{j=1}^{k-1} (\mathbf{x}_j^T\mathbf{y})\,\mathbf{x}_j}$$

The previously found $\mathbf{x}_j$ must be normalized. The dot product $\mathbf{x}_j^T\mathbf{y}$ measures how much of $\mathbf{y}$ points along $\mathbf{x}_j$; subtracting that amount makes the new vector perpendicular.

Tiny example: If $\mathbf{x}_1 = (1,1)^T/\sqrt{2}$ and $\mathbf{y} = (1,0)^T$, then

$$\mathbf{y}_\perp = (1,0)^T - \tfrac{1}{2}(1,1)^T = (\tfrac{1}{2}, -\tfrac{1}{2})^T, \quad \frac{\mathbf{y}_\perp}{\|\mathbf{y}_\perp\|} = \frac{(1,-1)^T}{\sqrt{2}}.$$

The new vector is perpendicular to $\mathbf{x}_1$; their dot product is zero.

6. The combined iteration for our 6×6 matrix

1. Find the first normalized eigenvector using the Power Method; save it as $\mathbf{x}_1$.
2. For the next eigenvector, choose a new trial vector and make it perpendicular to all saved eigenvectors using Gram–Schmidt.
3. In **every iteration**, calculate $A\mathbf{x}$, remove the directions of the earlier eigenvectors, normalize, and calculate the new eigenvalue estimate.
4. Save each eigenvalue estimate to a file. Stop at convergence or at $itmax = 150$. Repeat until all six eigenpairs are found.

Important: Use $|\lambda^{(t)} - \lambda^{(t-1)}| < 10^{-8}$ as one convergence test, and also check the **residual** $\|A\mathbf{x} - \lambda\mathbf{x}\|$ (ideally $< 10^{-8}$). If the projected vector has nearly zero length, start from a different trial vector. If 150 iterations are insufficient, report that clearly rather than claiming convergence.

What Must Our Program Deliver?

Reconstruct A, calculate A^{-1}, and check the result.

7. Expected eigenvalues: use these to check your program

The following are the six eigenvalues of our assignment's matrix, ordered by decreasing absolute value (the order in which the basic Power Method usually finds them):

Pair	Eigenvalue	Pair	Eigenvalue
1	−3.8019377358	4	−1.5549581321
2	−3.2469796037	5	−0.7530203963
3	−2.4450418679	6	−0.1980622642

Every eigenpair must satisfy $A\mathbf{x}_k \approx \lambda_k \mathbf{x}_k$, with $\|\mathbf{x}_k\| = 1$.

8. Task 4a: rebuild the original matrix

After we have all the eigenpairs, each eigenvector contributes a small matrix called an *outer product*, $\mathbf{x}_k \mathbf{x}_k^T$. Multiply this matrix by its eigenvalue and add all six contributions:

$$\boxed{A_{\text{num}} = \sum_{k=1}^{6} \lambda_k \, \mathbf{x}_k \mathbf{x}_k^T \;\approx\; A.}$$

Why does this work? Because our symmetric matrix has six orthonormal eigenvectors. If Q has these vectors as its columns and D contains the eigenvalues on its diagonal, then

$$Q^T Q = I, \qquad Q^T A Q = D, \qquad A = Q D Q^T.$$

The sum above is simply the component-by-component form of QDQ^T.

9. Task 4b: build the inverse matrix

For the inverse, use the **same eigenvectors** and replace each eigenvalue by its reciprocal:

$$\boxed{A_{\text{num}}^{-1} = \sum_{k=1}^{6} \frac{1}{\lambda_k} \, \mathbf{x}_k \mathbf{x}_k^T \;\approx\; A^{-1}.}$$

This is possible because none of the six eigenvalues is zero. The exact inverse, for comparison, is

$$A^{-1} = -\frac{1}{7} \begin{pmatrix} 6 & 5 & 4 & 3 & 2 & 1 \\ 5 & 10 & 8 & 6 & 4 & 2 \\ 4 & 8 & 12 & 9 & 6 & 3 \\ 3 & 6 & 9 & 12 & 8 & 4 \\ 2 & 4 & 6 & 8 & 10 & 5 \\ 1 & 2 & 3 & 4 & 5 & 6 \end{pmatrix}.$$

Numerical results may contain very small rounding errors: A_{num} and A_{num}^{-1} need not match the exact values digit for digit.

10. Files to save and tests to show

Suggested output files

- `eigenvalue_1.txt` through `eigenvalue_6.txt`: iteration number and eigenvalue estimate.
- `reconstructed_A.txt`: the calculated 6×6 matrix A_{num}.
- `inverse_A.txt`: the calculated 6×6 inverse matrix.

Numerical checks

- Eigenpairs: $\|A\mathbf{x}_k - \lambda_k \mathbf{x}_k\| \approx 0$.
- Orthogonality: $\mathbf{x}_i^T \mathbf{x}_j \approx \delta_{ij}$.
- Reconstruction: $A_{\text{num}} \approx A$.
- Inverse: $A\, A_{\text{num}}^{-1} \approx I$.

The big picture: Power iteration finds special directions; Gram–Schmidt keeps them different. Together, the six eigenpairs let us reconstruct A and A^{-1} - a key technique behind many physics calculations.