Lecture Notes For: Numerical Methods for Scientific Computing

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In this document, I have organized different numerical methods that are commonly used for scientific computing.

Chapter 1

System of Linear Equations

1.1 Direct Methods

1.1.1 LU Decomposition

1.1.2 RQ Decomposition

1.1.3 Guassian Elimination

1.1.4 Tridiagonal Matrix

1.1.5 Approximate Method

We want to solve the following system of equations:

$$\boldsymbol{A}x = b$$

.

We set the matrix $\boldsymbol{A}$ to be: $\boldsymbol{A} = \boldsymbol{S} - \boldsymbol{T}$, in which $\boldsymbol{S}$ and $\boldsymbol{T}$ are the some matrices which are chosed in a smart way!. Let's plug in the new value of $\boldsymbol{A}$ in the system of linear equations:

$$\begin{aligned}
(\boldsymbol{S} - \boldsymbol{T})x &= b \\
\boldsymbol{S}x &= \boldsymbol{T}x + b \\
x &= \boldsymbol{S}^{-1}(\boldsymbol{T}x + b) = \boldsymbol{S}^{-1}\boldsymbol{T}x + \boldsymbol{S}^{-1}b
\end{aligned}$$

So we will have:

$$\boxed{x = \boldsymbol{S}^{-1}\boldsymbol{T}x + \boldsymbol{S}^{-1}b} \tag{1.1.1}$$

Now let's plug in an initial guess x_0 in RHS of the the equation 1.1.1 and name it x_1. Then we can do this repeatedly to get the following equations:

$$
\begin{aligned}
x_1 &= \boldsymbol{S}^{-1}\boldsymbol{T}x_0 + \boldsymbol{S}^{-1}b \\
x_2 &= \boldsymbol{S}^{-1}\boldsymbol{T}x_1 + \boldsymbol{S}^{-1}b \\
&\vdots \\
x_n &= \boldsymbol{S}^{-1}\boldsymbol{T}x_{n-1} + \boldsymbol{S}^{-1}b
\end{aligned}
$$

To see if we have get closer to the actual solution of the system of equations, let's asume that the actual solution is x. So let's define the following errors:

$$
\begin{aligned}
\epsilon_0 &= x - x_0 \\
\epsilon_1 &= x - x_1 \\
\epsilon_2 &= x - x_2 \\
&\vdots \\
\epsilon_n &= x - x_n
\end{aligned}
$$

By pluggin in $x_0 = x - \epsilon_0$ in equation 1.1.1 we will get:

$$
\begin{aligned}
x_1 &= \boldsymbol{S}^{-1}\boldsymbol{T}(x - \epsilon_0) + \boldsymbol{S}^{-1}b \\
&= \underbrace{\boldsymbol{S}^{-1}\boldsymbol{T}x + \boldsymbol{S}^{-1}b}_{x} - \boldsymbol{S}^{-1}\boldsymbol{T}\epsilon_0 \\
&= x - \boldsymbol{S}^{-1}\boldsymbol{T}\epsilon_0 = x - \epsilon_1 \\
&\Rightarrow \boxed{\epsilon_1 = \boldsymbol{S}^{-1}\boldsymbol{T}}
\end{aligned}
$$

Using the same logic we will get:

$$\epsilon_n = (\boldsymbol{S}^{-1}\boldsymbol{T})^n \tag{1.1.2}$$

So using this iterative method to find the approximate solution of the system of the linear equations, we will converge to the actual solution if the largest eigenvalue of the matrix $\boldsymbol{S}^{-1}\boldsymbol{T}$ is smaller than one. Now the only problem is to find the value of $\boldsymbol{S}$ is a clever way such that it meets the convergence criteria and is easy to invert. Note that the time complexity of inverting a matrix is $O(N^3)$. So an inapproporate choice of $\boldsymbol{S}$ will be very costly.

1.1.6 Jacobi Method

One idea for $\boldsymbol{S}$ is the identity matrix $\mathcal{I}$.

$$\boldsymbol{S} = \mathcal{I} = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix} \tag{1.1.3}$$

1.1.7 Guass Seidel Method

S is the lower trianglar matrix

Chapter 2

Matrices

2.1 Eigenvalue and Eigenvectors

2.1.1 Power Method

This is to calculate the largest eigenvalue of a matric