# Chapter 6: Numerical Solution of Integral Equations

## 1 A background

Many problems in scientific computing can be written in terms of solving integral equations. Here we look at an example of solving integral equation in Computed Tomography (CT). CT is the first non-invasive radiological method allowing the generation of tomographic images of every part of the human body without superimposition of adjacent structure.

In the CT examination, the x-ray, with intensity $I_0$, is projected onto the object. The intensity of the x-ray behind the object, $I$, is measured. We know that

$$I = I_0\ e^{-u},$$

where $u$ is called the contract scale. For example, if the object is air, then $u = 0$, and if the object is water then $u = 1000$. To be more convenient in application, we rescale the measured intensity such that for the equation

$$Ie^{1000} = I_0\ e^{-u},$$

to hold, we have $u = 0$ for water and we call it water's *attenuation* value. Then, the attenuation value of air is -1000HU. Fat has an attenuation value in the range -100HU $\sim$ -50HU. The kidney's attenuation value is 30HU and the bone's attenuation value is 700HU $\sim$ 3000HU.

By projecting an x-ray onto an object and measuring the intensity of the x-ray behind the object, we can determine the attenuation value or the nature of the object. For example, to determine the attenuation value of a one-dimensional object of length $b - a$, we can project an x-ray of intensity $I_0$ perpendicularly onto the object, placed on the interval $t \in [a,\ b]$. Then we can measure the intensity of the recipient x-ray behind the bar, represented by $I(s)$ at location $s$, for $s \in [a,\ b]$. Let $u(t)$, for $t \in [a,\ b]$, represent the attenuation value of the bar at position $t$. Then the following equation describes the relation between the intensity of the projecting x-ray and the intensity of the recipient x-ray

$$I(s) = I_0 e^{-\int_a^b K(s-t)u(t)dt}, \quad \forall s \in [a\ b],$$

where $K(s - t)$ is a given convolution kernel, e.g., $K(s - t) = e^{-\alpha|s-t|}$, where $\alpha > 0$. To solve for $u(t)$, the contract scale of the object, we need to solve the following integral equation

$$\int_a^b K(s-t)u(t)dt = \log(I_o/I(s)), \quad \forall s \in [a\ b].$$

A general *Fredholm integral equation of the first kind* is of the form

$$\int_a^b K(s,t)u(t)dt = f(s), \quad \forall s \in [c,d], \tag{1}$$

where the function $f(s)$ and the kernel $K(s,t)$ are known, and the function $u(t)$ needs to be determined. We note that the ranges of $t$ and $s$ may be different.

The integral equation (1) also arises from the *image processing* problems. Assume the function $u(t)$ represents a curve (an image) on the interval $[a,b]$. Let the integral kernel $K(s,t)$ be of the form $e^{-\alpha|s-t|}$, with $\alpha > 0$, for example, here for example $s \in [a,b]$ as well. Then the function $f(s) = \int_a^b K(s,t)u(t)dt$ represents a blurred image of $u(t)$. We often call the kernel $K(s,t)$ as the blurring operator. If we are given a blurred image $f(s)$ and the blurring operator $K(s,t)$, to determine the original image $u(t)$ is reduced to solving the integral equation (1).

Solving the integral equation (1) is also called an inverse problem. It is a very ill-conditioned problem, which means that a small perturbation in the input, e.g., in $f(s)$, can result a large oscillation in the solution $u(t)$. This is a result of the following *Riemann-Lebesgue Lemma*

$$\lim_{n\to\infty} \int_a^b K(s,t)\sin(nt)dt = 0,$$

which implies that an arbitrarily high-frequency oscillation of $u$ may have very little effect on $f$. Or we can also say that a high-frequency oscillation is an annihilator of the kernel $K(s,t)$.

## 2 Discrete problem

To solve the integral equation (1) numerically, we first cut the interval $[c,d]$ by discrete points $s_i$, $i = 1,2,...,n$. We require (1) hold at each point $s_i$, i.e., we require

$$\int_a^b K(s_i,t)u(t)dt = f(s_i), \quad i = 1,2,...,n.$$

We approximate the integral on the left side of the above equation by certain numerical quadrature rules,

$$\int_a^b K(s_i,t)u(t)dt \approx \sum_{j=1}^n w_j K(s_i,t_j)u(t_j) \approx \sum_{j=1}^n w_j K(s_i,t_j)u_j,$$

by using the function values $u(t_j)$, $j = 1,2,..,n$. Here $t_j$, $j = 1,2,..,n$, represents a partition of the integral interval $[a,b]$. Since the function values $u(t_j)$ are unknown, we approximate them by $u_j$, $j = 1,2,..,n$. The approximation values $u_j$ are determined such

that

$$\sum_{j=1}^{n} w_j K(s_i, t_j) u_j = f(s_i), \quad i = 1, 2, ..., n.$$

This can be written in the form of a system of linear equations

$$A\mathbf{x} = \mathbf{b},$$

where

$$\mathbf{b} = \begin{bmatrix} f(s_1) \\ f(s_2) \\ \vdots \\ f(s_n) \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix},$$

and $A$ is the matrix containing $w_j K(s_i, t_j)$ at its $ij$–entry.

This system of linear equations is a discrete version of the integral equation (1). $A$ is essentially a discretization of the blurring operator $K(s, t)$. In such applications, $A$ can become very numerically singular, i.e., its minimum singular value can be very close to zero. As a result, the system of linear equations can become very ill-conditioned. We call such problems *ill posed* problems.

# 3 Numerical methods for solving ill posed problems

## 3.1 Singular value decomposition

Given any $n$ by $n$ matrix $A$, there always exist orthogonal matrices $U$ and $V$, and a diagonal matrix $\Sigma$ with diagonal entries $\sigma_1 \geq \sigma_2 \geq ... \geq \sigma_n \geq 0$, such that

$$A = U\Sigma V^T = [\mathbf{u}_1\ \mathbf{u}_2\ \ldots\ \mathbf{u}_n] \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_n \end{bmatrix} [\mathbf{v}_1\ \mathbf{v}_2\ \ldots\ \mathbf{v}_n]^T = \sum_{i=1}^{n} \sigma_i \mathbf{u}_i \mathbf{v}_i^T,$$

where $\mathbf{u}_i$ and $\mathbf{v}_i$, $i = 1, 2, \ldots, n$, are the column vectors of $U$ and $V$, respectively. We call this the Singular Value Decomposition (SVD) of $A$. Here $U$ and $V$ are orthogonal matrices, i.e., $UU^T = I$ and $VV^T = I$.

The singularity of the matrix $A$, i.e., the rank of $A$, can be determined by its SVD. If all the singular values of $A$ are nonzero, then $A$ is invertible (non-singular) and the rank of $A$ is $n$. If any singular values of $A$ equal zero, then $A$ is singular, and the rank of $A$ equals the number of nonzero singular values of $A$.

The range of $A$ is spanned by the columns in $U$, corresponding to the nonzero singular values. If $A$ is invertible, then the columns of $U$ form an orthonormal basis of the range of $A$.

Define

$$A_k = \sum_{i=1}^{k} \sigma_i \mathbf{u}_i \mathbf{v}_i^T,$$

for $k = 1, 2, \ldots$, which represents the sum of the first $k$ terms in the singular value decomposition of $A$. Then we can see that

$$A - A_k = \sum_{i=k+1}^{n} \sigma_i \mathbf{u}_i \mathbf{v}_i^T = U \begin{bmatrix} 0 & & & & & \\ & \ddots & & & & \\ & & 0 & & & \\ & & & \sigma_{k+1} & & \\ & & & & \ddots & \\ & & & & & \sigma_n \end{bmatrix} V^T$$

and as a result $\|A - A_k\|_2 = \sigma_{k+1}$. Therefore $A_k$ can be used as an approximation to the original matrix $A$, and the approximation becomes more accurate as $k$ increases.

Assume that $A$ is a nonsingular matrix (even though it can be very ill-conditioned), then all the singular values of $A$ are positive and

$$A^{-1} = \left(U \Sigma V^T\right)^{-1} = V \Sigma^{-1} U^T = \sum_{i=1}^{n} \sigma_i^{-1} \mathbf{v}_i \mathbf{u}_i^T.$$

Therefore the solution to the linear system $A\mathbf{x} = \mathbf{b}$ is

$$\mathbf{x} = A^{-1}\mathbf{b} = \sum_{i=1}^{n} \sigma_i^{-1} \mathbf{v}_i \mathbf{u}_i^T \mathbf{b} = \sum_{i=1}^{n} \frac{\mathbf{u}_i^T \mathbf{b}}{\sigma_i} \mathbf{v}_i,$$

which is a linear combination of $\mathbf{v}_i$, with coefficients determined by the inner products $\mathbf{u}_i^T \mathbf{b}$ and the singular values $\sigma_i$. If a singular value $\sigma_i$ is very close to zero, then any error in computing $\mathbf{u}_i^T \mathbf{b}$, e.g., the rounding error, will be amplified enormously, which will make the obtained numerical results not accurate at all.

In fact, in most applications of integral equations, the matrix $A$ is very ill-conditioned and then its singular values $\sigma_k$ will become very close to zero when $k$ increases. In this case, to obtain a meaningful numerical solution of the ill-posed problem, we need to stop the summation before $\sigma_i$ becomes too small, e.g., before $\sigma_i$ falls below a prescribed tolerance value $\varepsilon$. We take the following truncated sum

$$\mathbf{x}_{truncate} = \sum_{i=1}^{k} \frac{\mathbf{u}_i^T \mathbf{b}}{\sigma_i} \mathbf{v}_i,$$

where $\sigma_{k+1} < \varepsilon < \sigma_k$, as an approximate solution. We call this the approximate solution obtained from the truncated singular value decomposition.

### 3.2 Tikhonov regularization

Another approach of solving ill-posed problems is the Tikhonov regularization.

We note that the solution to the system of linear equations $A\mathbf{x} = \mathbf{b}$ is equivalent to the following minimization problem

$$\min_{\mathbf{x}} \|\mathbf{b} - A\mathbf{x}\|_2^2.$$

But we know that the above minimization problem will lead to an unstable solution due to the ill conditioning of $A$ as discussed above. The magnitude of $\mathbf{x}$ can become unrealistically large. To control the magnitude of $\mathbf{x}$ in the solution, we can consider solving the following minimization problem

$$\min_{\mathbf{x}} \{\|\mathbf{b} - A\mathbf{x}\|_2^2 + \mu\|\mathbf{x}\|^2\},$$

where $\mu$ is a chosen positive parameter, called *penalty* parameter. We can see that at the minimizer, the norm of $\mathbf{x}$ cannot be too large, which is an alternative to the truncation of the sum in the singular value decomposition.

Let us first show that the minimization problem has a unique solution. Let us denote the objective function by $f(\mathbf{x})$ and we have

$$f(\mathbf{x}) = (\mathbf{b} - A\mathbf{x})^T(\mathbf{b} - A\mathbf{x}) + \mu\mathbf{x}^T\mathbf{x} = \mathbf{b}^T\mathbf{b} + \mathbf{x}^T(A^TA + \mu I)\mathbf{x} - 2\mathbf{x}^TA^T\mathbf{b}.$$

and

$$\nabla f(\mathbf{x}) = -2A^T\mathbf{b} + 2(A^TA + \mu I)\mathbf{x}, \qquad \nabla^2 f(\mathbf{x}) = 2(A^TA + \mu I).$$

Since the Hessian matrix of the objective function is always positive definite, we know that the minimization problem has a global minimum which satisfies $\nabla f(\mathbf{x}) = 0$, i.e.,

$$(A^TA + \mu I)\mathbf{x} = A^T\mathbf{b}.$$

Therefore one approach of using the Tikhonov regularization is to solve this normal equation. Another way to derive this normal equation is to write the above minimization problem with penalty term as the following linear least squares problem

$$\min_x \left\| \begin{bmatrix} \mathbf{b} - A\mathbf{x} \\ -\sqrt{\mu}\mathbf{x} \end{bmatrix} \right\|_2^2, \quad \text{i.e.,} \quad \min_x \left\| \begin{bmatrix} \mathbf{b} \\ 0 \end{bmatrix} - \begin{bmatrix} A \\ \sqrt{\mu}I \end{bmatrix} \mathbf{x} \right\|_2^2.$$

Then the above normal equation is just the normal equation solving this linear least squares problem. This linear least squares problem can also be solved by using the SVD. Denote the singular value decomposition of $A$ by

$$A = U\Sigma V^T,$$

i.e.,

$$A\mathbf{v}_i = \sigma_i\mathbf{u}_i, \quad i = 1, 2, ..., n,$$

where $\mathbf{u}_i$ and $\mathbf{v}_i$, $i = 1, 2, \ldots, n$, are the column vectors of $U$ and $V$, and $\sigma_1 \geq \sigma_2 \geq ... \geq \sigma_n > 0$ are the singular values. Here $U$, $V$, and $\Sigma$ are all $n \times n$ matrices. Then we can derive the SVD of the coefficient matrix in the linear least squares problem by observing that

$$\begin{bmatrix} A \\ \sqrt{\mu} I \end{bmatrix} \mathbf{v}_i = \begin{bmatrix} \sigma_i \mathbf{u}_i \\ \sqrt{\mu} \mathbf{v}_i \end{bmatrix} = \sqrt{\sigma_i^2 + \mu} \begin{bmatrix} \frac{\sigma_i}{\sqrt{\sigma_i^2+\mu}} \mathbf{u}_i \\ \frac{\sqrt{\mu}}{\sqrt{\sigma_i^2+\mu}} \mathbf{v}_i \end{bmatrix}, \quad i = 1, 2, ..., n,$$

which defines the reduced singular value decomposition

$$\begin{bmatrix} A \\ \sqrt{\mu} I \end{bmatrix} = \widehat{U} \, \widehat{\Sigma} \, V^T,$$

where $\widehat{U}$ is a $2n \times n$ matrix with $n$ orthonormal columns, $\widehat{\Sigma}$ is a $n \times n$ diagonal matrix containing the singular values $\sqrt{\sigma_i^2 + \mu}$ on its diagonal, $V$ is the same $n \times n$ orthogonal matrix as in the singular value decomposition of $A$. The columns of $\widehat{U}$ form an orthonormal basis of the range of the coeeficient matrix.

Thus the solution to the linear least squares problem can be determined by

$$\widehat{U}^T \left( \begin{bmatrix} \mathbf{b} \\ 0 \end{bmatrix} - \begin{bmatrix} A \\ \sqrt{\mu} I \end{bmatrix} \mathbf{x} \right) = \widehat{U}^T \left( \begin{bmatrix} \mathbf{b} \\ 0 \end{bmatrix} - \widehat{U} \, \widehat{\Sigma} \, V^T \mathbf{x} \right) = \widehat{U}^T \begin{bmatrix} \mathbf{b} \\ 0 \end{bmatrix} - \widehat{\Sigma} \, V^T \mathbf{x} = 0,$$

i.e., the residual is perpendicular to the range of the coefficient matrix. Then we have

$$\begin{aligned} \mathbf{x} &= V \, \widehat{\Sigma}^{-1} \, \widehat{U}^T \begin{bmatrix} \mathbf{b} \\ 0 \end{bmatrix} = [\mathbf{v}_1 \; \mathbf{v}_2 \; \ldots \; \mathbf{v}_n] \left( \frac{1}{\sqrt{\sigma_i^2 + \mu}} \right)_{n \times n} \begin{bmatrix} \frac{\sigma_1 \mathbf{u}_1^T \mathbf{b}}{\sqrt{\sigma_1^2+\mu}} \\ \vdots \\ \frac{\sigma_n \mathbf{u}_n^T \mathbf{b}}{\sqrt{\sigma_n^2+\mu}} \end{bmatrix} \\ &= \sum_{i=1}^{n} \frac{\sigma_i \mathbf{u}_i^T \mathbf{b}}{\sigma_i^2 + \mu} \, \mathbf{v}_i = \sum_{i=1}^{n} \frac{\mathbf{u}_i^T \mathbf{b}}{\sigma_i + \mu/\sigma_i} \, \mathbf{v}_i, \end{aligned}$$

which is also a linear combination of $\mathbf{v}_i$, with coefficients determined by the inner products $\mathbf{u}_i^T \mathbf{b}$ and the singular values $\sigma_i$. Here we count all the terms in the summation, instead of doing the truncated sum. The denominator in the coefficients contains $\mu/\sigma_i$ to avoid division by a value close to zero, for $\sigma_i$ close to zero.