ECE 604, Lecture 36

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1 Computational Electromagnetics and Numerical Methods

Numerical methods exploit the blinding speed of modern digital computers to perform calculations, and hence to solve large system of equations. These equations are partial differential equations or integral equations. When these methods are applied to solving Maxwell's equations and related equations, the field is known as **computational electromagnetics**.

Maxwell's equations are a form of partial differential equations (PDE). Boundary conditions can be stipulated for these PDE's, and the solution can be sought by solving a boundary value problem (BVP). In solving PDE's the field in every point in space is solved for.

On the other hand, the Green's function method can be used to convert a PDE into an integral equation (IE). Then the fields are expressed in terms of the sources, and the sources are the unknowns to be solved. Sources in IEs are supported by a finite part of space, whereas fields from PDEs permeate all of space. Therefore, sources in IEs are easier to solve for compared to fields in PDEs.

1.1 Examples of Differential Equations

An example of differential equations written in terms of sources are the scalar wave equation:

$$\left(\nabla^2 + k^2\right)\phi(\mathbf{r}) = Q(\mathbf{r}), \tag{1.1}$$

An example of vector differential equation for vector electromagnetic field is

$$\nabla \times \overline{\boldsymbol{\mu}}^{-1} \cdot \nabla \times \mathbf{E}(\mathbf{r}) - \omega^2 \overline{\boldsymbol{\epsilon}} \cdot \mathbf{E}(\mathbf{r}) = i\omega \mathbf{J}(\mathbf{r}) \tag{1.2}$$

These equations are linear equations. They have one commonality, i.e., they can be abstractly written as

$$\mathscr{L}f = g \tag{1.3}$$

where $\mathscr{L}$ is the differential operator, and f is the unknown, and g is the driving source. Differential equations, or partial differential equations have to be solved with boundary conditions. Otherwise, there is no unique solution to these equations.

In the case of the scalar wave equation (1.4), $\mathscr{L} = (\nabla^2 + k^2)$ is a differential operator. In the case of the electromagnetic vector wave equation (1.2), $\mathscr{L} = (\nabla \times \overline{\boldsymbol{\mu}}^{-1} \cdot \nabla \times) - \omega^2 \overline{\boldsymbol{\epsilon}} \cdot$. Furthermore, f will be $\phi(\mathbf{r})$ for the scalar wave equation, while it will be $\mathbf{E}(\mathbf{r})$ in the case of vector wave equation for an electromagnetic system. The g on the right-hand side can represent Q in (1.4) or $i\omega \mathbf{J}(\mathbf{r})$ in (1.2).

1.2 Examples of Integral Equations

This course is replete with PDE's, but we have not come across too many integral equations. Therefore, we shall illustrate the derivation of some integral equations. Since the acoustic wave problem is homomorphic to the electromagnetic wave problem, we will illustrate the derivation of integral equation of scattering using acoustic wave equation.[1]

    The surface integral equation method is rather popular in a number of applications, because it employs a homogeneous-medium Green's function which is simple in form, and the unknowns are on a surface rather than in a volume. In this section, the surface integral equations[2] for scalar and will be studied first. Then, the volume integral equation will be discussed next.

1.2.1 Surface Integral Equations

In an integral equation, the unknown to be sought is embedded in an integral. An integral equation can be viewed as an operator equation as well, just as are differential equations. We shall see how such integral equations with only surface integrals are derived, using the scalar wave equation.
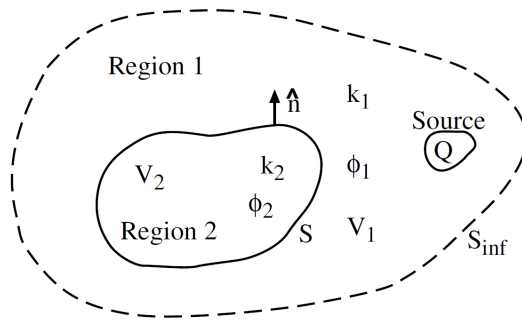

Figure 1: A two-region problem can be solved with a surface integral equation.

    Consider a scalar wave equation for a two-region problem as shown in Figure 1. In region 1, the governing equation for the total field is

$$\left(\nabla^2 + k_1^2\right)\phi_1(\mathbf{r}) = Q(\mathbf{r}), \tag{1.4}$$

For simplicity, we will assume that the scatterer is impenetrable, meaning that the field in region 2 is zero. Therefore, we need only define Green's functions for regions 1 to satisfy the following equations:

$$\left(\nabla^2 + k_1^2\right)g_1(\mathbf{r}, \mathbf{r}') = -\delta(\mathbf{r} - \mathbf{r}'), \tag{1.5}$$

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[1]The cases of electromagnetic wave equations can be found in *Chew, Waves and Fields in Inhomogeneous Media*.

[2]These are sometimes called boundary integral equations.

The derivation here is similar to the that of Huygens' principle. On multiplying Equation (1.4) by $g_1(\mathbf{r}, \mathbf{r}')$ and Equation (1.5) by $\phi_1(\mathbf{r})$, subtracting the two resultant equations, and integrating over region 1, we have, for $\mathbf{r}' \in V_1$,

$$\int\limits_{V_1} dV \left[g_1(\mathbf{r}, \mathbf{r}') \nabla^2 \phi_1(\mathbf{r}) - \phi_1(\mathbf{r}) \nabla^2 g_1(\mathbf{r}, \mathbf{r}') \right]$$

$$= \int\limits_{V_1} dV \, g_1(\mathbf{r}, \mathbf{r}') Q(\mathbf{r}) + \phi_1(\mathbf{r}'), \quad \mathbf{r}' \in V_1. \qquad (1.6)$$

Since $\nabla \cdot (g \nabla \phi - \phi \nabla g) = g \nabla^2 \phi - \phi \nabla^2 g$, by applying Gauss' theorem, the volume integral on the left-hand side of (1.6) becomes a surface integral over the surface bounding V_1. Consequently,[3]

$$- \int\limits_{S + S_{inf}} dS \, \hat{n} \cdot \left[g_1(\mathbf{r}, \mathbf{r}') \nabla \phi_1(\mathbf{r}) - \phi_1(\mathbf{r}) \nabla g_1(\mathbf{r}, \mathbf{r}') \right]$$

$$= -\phi_{inc}(\mathbf{r}') + \phi_1(\mathbf{r}'), \quad \mathbf{r}' \in V_1. \qquad (1.7)$$

In the above, we have let

$$\phi_{inc}(\mathbf{r}') = - \int\limits_{V_1} dV \, g_1(\mathbf{r}, \mathbf{r}') Q(\mathbf{r}), \qquad (1.8)$$

since it is the incident field generated by the source $Q(\mathbf{r})$.

Note that up to this point, $g_1(\mathbf{r}, \mathbf{r}')$ is not explicitly specified, as long as it is a solution of (1.5). A simple choice for $g_1(\mathbf{r}, \mathbf{r}')$ that satisfies the radiation condition is

$$g_1(\mathbf{r}, \mathbf{r}') = \frac{e^{ik_1 |\mathbf{r} - \mathbf{r}'|}}{4\pi |\mathbf{r} - \mathbf{r}'|}, \qquad (1.9)$$

which is the unbounded, homogeneous medium scalar Green's function. In this case, $\phi_{inc}(\mathbf{r})$ is the incident field generated by the source $Q(\mathbf{r})$ in the absence of the scatterer. Moreover, the integral over S_{inf} vanishes when $S_{inf} \to \infty$ by virtue of the radiation condition. Then, after swapping $\mathbf{r}$ and $\mathbf{r}'$, we have

$$\phi_1(\mathbf{r}) = \phi_{inc}(\mathbf{r}) - \int\limits_{S} dS' \, \hat{n}' \cdot \left[g_1(\mathbf{r}, \mathbf{r}') \nabla' \phi_1(\mathbf{r}') - \phi_1(\mathbf{r}') \nabla' g_1(\mathbf{r}, \mathbf{r}') \right], \quad \mathbf{r} \in V_1.$$

$$(1.10)$$

But if $\mathbf{r}' \notin V_1$ in (1.6), the second term, $\phi_1(\mathbf{r})$, on the right-hand side of (1.6) would be zero, for $\mathbf{r}'$ would be in V_2 where the integration is not performed.

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[3]The equality of the volume integral on the left-hand side of (1.6) and the surface integral on the left-hand side of (1.7) is also known as Green's theorem.

Therefore, we can write (1.10) as

$$\left. \begin{array}{l} \text{if } \mathbf{r} \in V_1, \quad \phi_1(\mathbf{r}) \\ \text{if } \mathbf{r} \in V_2, \quad 0 \end{array} \right\} = \phi_{inc}(\mathbf{r}) - \int_S dS' \, \hat{n}' \cdot [g_1(\mathbf{r}, \mathbf{r}')\nabla'\phi_1(\mathbf{r}') - \phi_1(\mathbf{r}')\nabla'g_1(\mathbf{r}, \mathbf{r}')].$$

$$(1.11)$$

The above equation is evocative of Huygens' principle. It says that when the observation point $\mathbf{r}$ is in V_1, then the total field $\phi_1(\mathbf{r})$ consists of the incident field, $\phi_{inc}(\mathbf{r})$, and the contribution of field due to surface sources on S. But if the observation point is in V_2, then the surface sources on S generate a field that exactly cancels the incident field $\phi_{inc}(\mathbf{r})$, making the total field in region 2 zero. This fact is the core of the **extinction theorem** as shown in Figure 2 (see Born and Wolf 1980).

In (1.11), $\hat{n} \cdot \nabla\phi_1(\mathbf{r})$ and $\phi_1(\mathbf{r})$ act as surface sources. Moreover, they are impressed on S, creating a field in region 2 that cancels exactly the incident field in region 2 (see Figure 2).
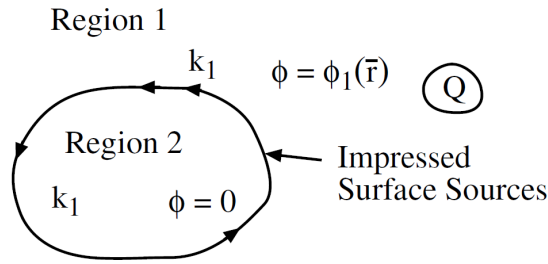

Figure 2: The illustration of the extinction theorem.

Applying the extinction theorem, integral equations can now be derived. So, using the lower parts of Equations (1.11), we have

$$\phi_{inc}(\mathbf{r}) = \int_S dS' \, \hat{n}' \cdot [g_1(\mathbf{r}, \mathbf{r}')\nabla'\phi_1(\mathbf{r}') - \phi_1(\mathbf{r}')\nabla'g_1(\mathbf{r}, \mathbf{r}')], \quad \mathbf{r} \in V_2,$$

$$(1.12)$$

The integral equations above still has two independent unknowns, ϕ_1 and $\hat{n} \cdot \nabla\phi_1$. Next, boundary conditions can be used to eliminate one of these two unknowns.

An acoustic scatterer which is impenetrable either has a hard surface boundary condition where normal velocity is zero, or it has soft surface where the pressure is zero (also called a pressure release surface). Since the force or the velocity of the particle is proportional to the $\nabla\phi$, a hard surface will have $\hat{n} \cdot \nabla\phi_1 = 0$, or a homogeneous Neumann boundary condition, while a soft surface will have

$\phi_1 = 0$, a homogeneous Dirichlet boundary condition.

$$\phi_{inc}(\mathbf{r}) = \int\limits_S dS' \, \hat{n}' \cdot [g_1(\mathbf{r}, \mathbf{r}')\nabla'\phi_1(\mathbf{r}')], \quad \mathbf{r} \in V_2, \quad \text{soft boundary condition}$$

(1.13)

$$\phi_{inc}(\mathbf{r}) = -\int\limits_S dS' \, \phi_1(\mathbf{r}')\nabla' g_1(\mathbf{r}, \mathbf{r}'], \quad \mathbf{r} \in V_2, \quad \text{hard boundary condition}$$

(1.14)

More complicated surface integral equations (SIEs) for penetrable scatterers, as well as vector surface integral equations for the electromagnetics cases are derived in *Chew, Waves and Fields in Inhomogeneous Media*. Also, there is another class of integral equations called volume integral equations (VIEs). They are derived in WFIM.

Nevertheless, all the integral equations can be unified under one notation:

$$\mathscr{L}f = g \tag{1.15}$$

This is similar to the differential equation case. The difference is that the unknown f represents the source of the problem, while g is the incident field impinging on the scatterer or object. Furthermore, f does not need to satisfy any boundary condition, since the field radiated via the Green's function satisfies the radiation condition.

2   Subspace Projection Methods

Several operator equations have been derived in the previous sections. They are all of the form

$$\mathscr{L}f = g \tag{2.1}$$

2.1   Function as a Vector

In the above, f is a functional vector which is the analogy of the vector $\mathbf{f}$ in matrix theory or linear algebra. In linear algebra, the vector $\mathbf{f}$ is of length N in an N dimensional space. It can be indexed by a set of countable index, say i, and we can described such a vector with N numbers such as $f_i, i = 1, \ldots, N$ explicitly. This is shown in Figure 3(a).

A function $f(x)$, however, can be thought of as being indexed by x in the 1D case. However, the index in this case is a continuum, and countably infinite. Hence, it corresponds to a vector of infinite dimension and it lives in an infinite dimensional space.[4]

To make such functions economical in storage, for instance, we replace the function $f(x)$ by its sampled values at N locations, such that $f(x_i)$, $i = $

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[4]When these functions are square integrable, these infinite dimensional spaces are called Hilbert spaces.

$1, \ldots, N$. Then the values of the function in between the stored points $f(x_i)$ can be obtained by interpolation. Therefore, a function vector $f(x)$, even though it is infinite dimensional, can be approximated by a finite length vector, $\mathbf{f}$. This concept is illustrated in Figure 3(b) and (c). This concept can be generalized to a function of 3D space $f(\mathbf{r})$. If $\mathbf{r}$ is sampled over a 3D volume, it can provide an index to a vector $f_i = f(\mathbf{r}_i)$, and hence, $f(\mathbf{r})$ can be thought of as a vector as well.
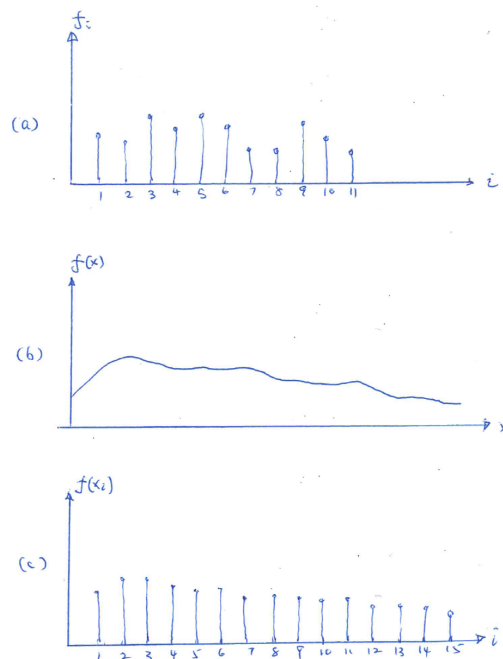

Figure 3: A function can be thought of as a vector.

2.2 Operator as a Map

An operator like $\mathscr{L}$ above can be thought of as a map or a transformation. It maps a function f defined in a Hilbert space V to g defined in another Hilbert space W. Mathematically, this is written as

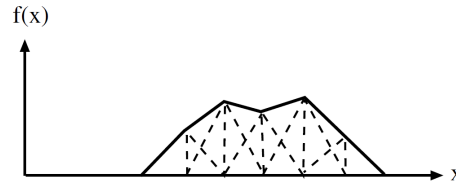$$\mathscr{L} : V \to W \tag{2.2}$$

Indicating that $\mathscr{L}$ is a map of vectors in the space V to the space W. Here, V is also called the domain space (or domain) of $\mathscr{L}$ while W is the range space (or range) of $\mathscr{L}$.

## 2.3 Approximating Operator Equations with Matrix Equations

One main task of numerical method is first to approximate an operator equation $\mathscr{L}f = g$ by a matrix equation $\overline{\mathbf{L}} \cdot \mathbf{f} = \mathbf{g}$. To convert the above, we first let

$$f \cong \sum_{n=1}^{N} a_n f_n = g \tag{2.3}$$

In the above, $f_n, n, \ldots, N$ are known functions called basis functions. Now, a_n's are the new unknowns to be sought. Also the above is an approximation, and the accuracy of the approximation depends very much on the original function f. A set of very popular basis functions are functions that form a piece-wise linear interpolation of the function from its nodes. These basis functions are shown in Figure 4.

(a) One Dimension

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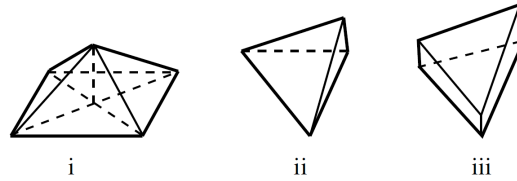
(b) Two Dimensions

Figure 4: Examples of basis function in (a) one dimension, (b) two dimension. Each of these functions are define over a finite domain. Hence, they are also called sub-domain basis functions.

Upon substituting (2.3) into (2.1), we obtain

$$\sum_{n=1}^{N} a_n \mathscr{L} f_n = g \tag{2.4}$$

Then, multiplying (2.4) by w_m and integrate over the space that $w_m(\mathbf{r})$ is defined, then we have

$$\sum_{n=1}^{N} a_n \langle w_m, \mathscr{L} f_n \rangle = \langle w_m, g \rangle, m = 1, \ldots, N \tag{2.5}$$

In the above, the inner product is defined as

$$\langle f_1, f_2 \rangle = \int d\mathbf{r} f_1(\mathbf{r}) f_2(\mathbf{r}) \tag{2.6}$$

where the integration is over the support of the functions, or the space over which the functions are defined. For PDEs these functions are defined over a 3D space, while in SIEs, these functions are defined over a surface. In a 1D problems, these functions are defined over a 1D space.

The functions $w_m, m = 1, \ldots, N$ is known as the weighting functions or testing functions. The testing functions should be chosen so that they can approximate well a function that lives in the range space W of the operator $\mathscr{L}$. Such set of testing functions lives in the dual space of the range space. For example, if f_r lives in the range space of the operator $\mathscr{L}$, the set of function f_d, such that the inner product $\langle f_d, f_r \rangle$ exists, forms the dual space of W.

The above is a matrix equation of the form

$$\overline{\mathbf{L}} \cdot \mathbf{a} = \mathbf{g} \tag{2.7}$$

where

$$\begin{aligned} \left[\overline{\mathbf{L}} \right]_{mn} &= \langle w_m, \mathscr{L} f_n \rangle \\ [\mathbf{a}]_n = a_n, [\mathbf{g}]_m &= \langle w_m, g \rangle \end{aligned} \tag{2.8}$$

What has effectively happened here is that given an operator $\mathscr{L}$ that maps a function that lives in an infinite dimensional Hilbert space V, to another function that lives in another infinite dimensional Hilbert space W, via the operator equation $\mathscr{L} f = g$, we have approximated the Hilbert spaces with finite dimensional spaces (subspaces), and finally, obtain a finite dimensional matrix equation that is the representation of the original infinite dimensional operator equation.

In the above, $\overline{\mathbf{L}}$ is the matrix representation of the operator $\mathscr{L}$ in the subspaces, and $\mathbf{a}$ and $\mathbf{g}$ are the vector representations in their respective subspaces.

When such a method is applied to integral equations, it is usually called the method of moments (MOM). (Surface integral equations are also called boundary integral equations (BIEs) in other fields.) But when this method is applied to solve PDEs, it is called the finite element method (FEM).

2.4   Mesh Generation

In order to approximate a function defined on an arbitrary shaped surface or volume by sum of basis functions, it is best to mesh (tessellate) the surface and volume by meshes. In 2D, all shapes can be tessellated by union of triangles, while a 3D volume can be mesh (tessellated) by union of tetrahedrons. Such meshes are used not only in CEM, but in other fields such as solid mechanics. Hence, there are many commercial software available to generate sophisticated meshes.

When a surface is curved, or of arbitrary shape, it can be meshed by union of triangles as shown in Figure 5. When a volume is of arbitrary shape of a volume

is around an arbitrary shape object, it can be meshed by tetrahedrons as shown in Figure 6. Then basis functions are defined to interpolate the field between nodal values or values defined on the edges of a triangle or a tetrahedron.
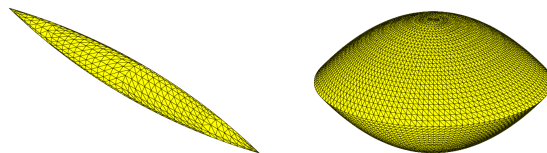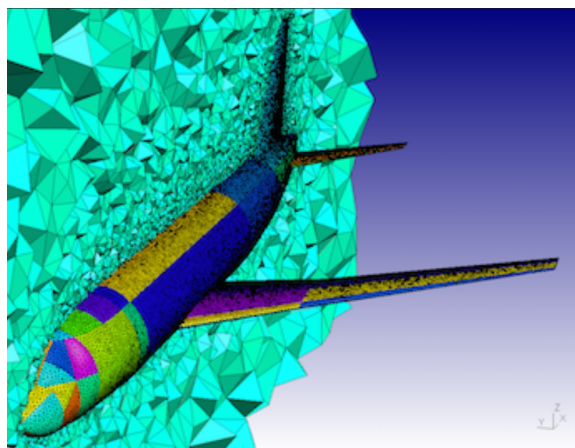

Figure 5:

Figure 6:

3   Solving Matrix Equation by Optimization

When a matrix system get exceedingly large, it is preferable that a direct inversion of the matrix equation not performed. Direct inversions (e.g., using Gaussian elimination or Kramer's rule) have computational complexity[5] of $O(N^3)$, and requiring storage of $O(N^2)$. Hence, when N is large, other methods have to be sought.

To this end, it is better to convert the solving of a matrix equation into an optimization problem. These methods can be designed so that a much larger system can be solved with a digital computer. Optimization problem results in finding the stationary point of a functional.[6] First, we will figure out how to

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[5]The scaling of computer time with respect to the number of unknowns (degrees of freedom) is known in the computer parlance as computational complexity.

[6]Functional is usually defined as a function of a function. Here, we include a function of a vector to be a functional as well.

find such a functional.

Consider a matrix equation given by

$$\overline{\mathbf{L}} \cdot \mathbf{f} = \mathbf{g} \tag{3.1}$$

For simplicity, we consider $\overline{\mathbf{L}}$ as a symmetric matrix.[7] Then one can define a functional

$$I = \mathbf{f}^t \cdot \overline{\mathbf{L}} \cdot \mathbf{f} - 2\mathbf{f}^t \cdot \mathbf{g} \tag{3.2}$$

Such a functional is called a quadratic functional because it is analogous to $I = Lx^2 - 2xg$, which is quadratic, in its simplest 1D rendition.

Taking the first variation with respect to $\mathbf{f}$, namely, we let $\mathbf{f} = \mathbf{f}_0 + \delta\mathbf{f}$, and find the leading order approximation of the functional. Therefore, one gets

$$\delta I = \delta\mathbf{f}^t \cdot \overline{\mathbf{L}} \cdot \mathbf{f}_0 + \mathbf{f}_0^t \cdot \overline{\mathbf{L}} \cdot \delta\mathbf{f} - 2\delta\mathbf{f}^t \cdot \mathbf{g} \tag{3.3}$$

If $\overline{\mathbf{L}}$ is symmetric, the first two terms are the same, and the above becomes

$$\delta I = 2\delta\mathbf{f}^t \cdot \overline{\mathbf{L}} \cdot \mathbf{f}_0 - 2\delta\mathbf{f}^t \cdot \mathbf{g} \tag{3.4}$$

For $\mathbf{f}_0$ to be the optimal point or the stationary point, then its first variation has to be zero, or that $\delta I = 0$. Thus we conclude that

$$\overline{\mathbf{L}} \cdot \mathbf{f}_0 = \mathbf{g} \tag{3.5}$$

Hence, the optimal point to the functional I is the solution to (3.1)

Such method, when applied to an infinite dimensional Hilbert space problem, is called variational method, but the main ideas are similar. The wonderful idea about such a method is that instead of doing direct inversion, one can search for the optimal point or stationary point of the quadratic functional using gradient search methods.

3.1 Gradient of a Functional

It turns out that the gradient of a quadratic functional can be found quite easily. To do this, it is better to write out functional using index (or indicial, or Einstein) notation. In this notation, the functional I becomes

$$I = \sum_{i,j} f_j L_{ji} f_i - \sum_j 2f_j g_j = f_j L_{ji} f_i - 2f_j g_j \tag{3.6}$$

Also, in this notation, the summation symbol is dropped, and summation over repeated indices is implied in the last equality. To find the gradient in a multi-dimensional space spanned by f_j, one takes the first variation of I with respect to $f_{j'}$ yielding

$$\delta I = 2\delta f_{j'} L_{ij'} f_i - 2\delta f_{j'} g_{j'} \tag{3.7}$$

$$\frac{\partial I}{\partial f_{j'}} = 2L_{ij'} f_i - 2g_{j'} \tag{3.8}$$

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[7]Functional for the asymmetric case can be found in *Chew, Waves and Fields in Inhomogeneous Media*, Chapter 5.

Notice that the remaining equation has one index j' remaining in index notation, meaning that it is a vector equation. We can reconstitute the above using our more familiar matrix notation that

$$\nabla_{\mathbf{f}} I = 2\overline{\mathbf{L}} \cdot \mathbf{f} - 2\mathbf{g} \tag{3.9}$$

The left-hand side is a notation for the gradient of a functional in a multidimensional space defined by $\mathbf{f}$, and the right-hand side is the expression for calculating this gradient. One need only to perform a matrix-vector product to find this gradient. Hence, the computational complexity of finding this gradient is $O(N^2)$ at worst, and $O(N)$ for many sparse matrices. In a gradient search method, such a gradient is calculated repeated until the optimal point is found. Such methods are called iterative methods.

If the optimal point can be found in N_{iter} iterations, then the CPU time scales as $N_{iter} N^{\alpha}$ where $1 < \alpha < 2$. There is a clever gradient search algorithm, called the conjugate gradient method that can find the optimal point in N_{iter} in exact arithmetics. In many gradient search methods, $N_{\text{iter}} \ll N$ resulting in great savings in computer time.

What is more important is that this method does not require the storage of the matrix $\overline{\mathbf{L}}$, but a computer code that produces the vector $\mathbf{g}_o = \overline{\mathbf{L}} \cdot \mathbf{f}$ as an output, with $\mathbf{f}$ as an input. Both $\mathbf{f}$ and $\mathbf{g}_o$ require only $O(N)$ memory storage. Such methods are called matrix-free methods. Even when $\overline{\mathbf{L}}$ is a dense matrix, but is the matrix representation of some Green's function, fast methods now exist to perform the dense matrix-vector product in $O(N \log N)$ operations.[8]

The value I is also called the cost function, and its minimum is sought in the seeking of the solution by gradient search method. Figure 7 shows the contour plot of a cost function in 2D. When the condition number of the matrix $\overline{\mathbf{L}}$ is large (implying that the matrix is ill-conditioned), the contour plot will resembler a deep valley. And hence, the gradient search method will tend to zig-zag along the way as it finds the solution.

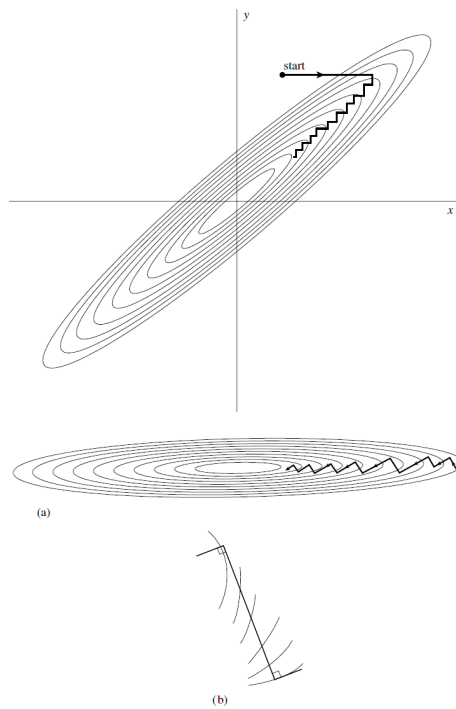[8] Chew et al, *Fast and Efficient Algorithms in CEM.*

Figure 7: Courtesy of Numerical Recipe.

Figure 8 shows a cartoon picture in 2D of the histories of different search paths from a machine-learning example where a cost functional similar to I has to be minimized. Finding the optimal point or the minimum point of a general functional is still a hot topic of research: it is important in artificial intelligence.
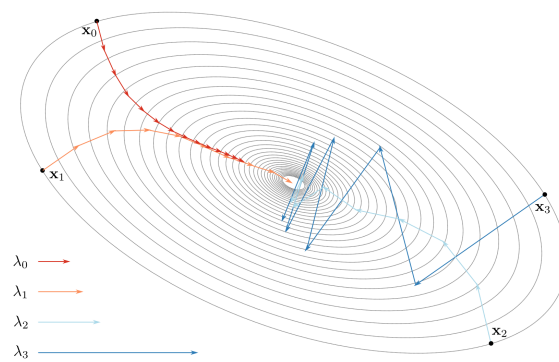

Figure 8: Courtesy of Y. Ioannou.