1 Four special matrices

1. Toeplitz matrix

A Toeplitz matrix or diagonal-constant matrix, named after Otto Toeplitz, is a matrix in which each descending diagonal from left to right is constant. For instance:

$$\begin{bmatrix} a & b & c & d & e \\ f & a & b & c & d \\ g & f & a & b & c \\ h & g & f & a & b \\ i & h & g & f & a \end{bmatrix}$$

2. Circulant matrix

a circulant matrix is a special kind of Toeplitz matrix where each row vector is rotated one element to the right relative to the preceding row vector. For instance:

$$C = egin{bmatrix} c_1 & c_2 & c_3 & \dots & c_n \ c_n & c_1 & c_2 & & c_{n-1} \ c_{n-1} & c_n & c_1 & & c_{n-2} \ dots & & \ddots & dots \ c_2 & c_3 & c_4 & \dots & c_1 \ \end{bmatrix}$$

In numerical analysis, circulant matrices are important because they are diagonalized by a discrete Fourier transform, and hence linear equations that contain them may be quickly solved using a fast Fourier transform.

3. Change T_{11} in Toeplitz matrix

Here we've a free variable in Toeplitz matrix T at position T_{11} .

4. Change T_{11} and T_{nn} in Toeplitz matrix

Here we've two free variables in Toeplitz matrix T at position T_{11} and T_{nn} .

2 Differential eqns and Difference eqns

Part 1. Notation of high order derivative

For n-th derivative, the notation is $\frac{d^n y}{dx^n}$ or $\frac{d^n f(x)}{dx^n}$. Sample of meaning of this notation: $\frac{d^2 y}{dx^2} = \frac{d}{dx} \left(\frac{dy}{dx} \right)$.

Part 2. First order difference

To calculate first order discrete derivative (difference) of u(x), we have three choices: forward, backward and centered:

forward
$$\Delta_F$$
: $u'(x) \approx \frac{u(x+h)-u(x)}{h}$
backward Δ_B : $u'x) \approx \frac{u(x)-u(x-h)}{h}$
centered $(\frac{forward-backward}{2})$ Δ_C : $u'(x) \approx \frac{u(x+h)-u(x-h)}{2h}$

We would like use centered difference for first order difference. The reason comes from the loss of accuracy:

First, recall Taylor series:

$$f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f'''(a)}{3!}(x-a)^3 + \cdots$$

Second, from Taylor series, we have:

$$u(x+h) = u(x) + hu'(x) + \frac{h^2}{2!}u''(x) + \frac{h^3}{3!}u'''(x) + \cdots$$
$$u(x-h) = u(x) - hu'(x) + \frac{h^2}{2!}u''(x) - \frac{h^3}{3!}u'''(x) + \cdots$$

Finally, inserting u(x+h), u(x-h) in three kind of differences, $\Delta_F = \Delta_B \approx u'(x) + o(h)$, $\Delta_C \approx u'(x) + o(h^2)$.

Part 3. Second order difference

The best way to calculate second order discrete derivative (difference) is $u''(x) \approx \frac{-u(x+h)+2u(x)-u(x-h)}{h^2}$, or h with 1 such that $u''(x) \approx -u(x+1)+2u(x)-u(x-1)$. You may wonder where this form comes from. This form is $\Delta_F\Delta_B(=\Delta_B\Delta_F)$, which is better than $\Delta_C\Delta_C$.

Having $\Delta(\Delta u(x)) = -u(x+1) + 2u(x) - u(x-1)$, we can write multi $\Delta(\Delta u(x))$ in matrix form. Here is a funny thing to see in the matrix form

$$\Delta = \begin{bmatrix} 1 & 2 & -1 & & \\ & 1 & 2 & -1 & \\ & & 1 & 2 & -1 \end{bmatrix} \begin{bmatrix} u(i-2) \\ u(i-1) \\ u(i) \\ u(i+1) \\ u(i+2) \end{bmatrix}$$

Above is the second order difference of u(x) at five points with gap 1. You can insert the five point with any function g. If the function is a linear/quadratic function, Δ is a vector with all element being 0/a constant! You can check this. The reason behind the funny thing is that Δ is second order discrete derivative. Also note that the matrix composed of 1, 2, -1 is a Toeplitz matrix.

Part 3. Differential equations

For example,
$$-\frac{d^2u}{dx^2} = 1$$
, $\frac{du}{dx}(0) = 0$, $u(1) = 0$.

This is very easy to calculate.

3 Solving a Linear System

Part 1. Four matrix decompositions

All these four decompositions are covered in 18.06 Linear Algebra.

Elimination: A = LU and A = LDU

Orthogonalization: A = QR

Eigenvalues: $A = S\Lambda S^{-1}$

Singular values: $A = U\Sigma V^T$

Supplement:

For a matrix $A = BDB^T$, where D is a diagonal matrix, A is symmetric, since $A^T = BD^TB^T = BDB^T = A$. Then LDU decomposition on A, we get $A = LDL^T$.

Part 2.

More detail is needed.

For AX = I, we know $X = A^{-1}$. The deep insight is that columns of A^{-1} are responses to n impulses (columns of I).

4 Delta function day

Part 1. Definition of Delta function

The Dirac delta can be loosely thought of as a function on the real line which is zero everywhere except at the origin, where it is infinite,

$$\delta(x) = \begin{cases} +\infty, & x = 0 \\ 0, & x \neq 0 \end{cases}$$

and which is also constrained to satisfy the identity, $\int_{-\infty}^{\infty} \delta(x) dx = 1$

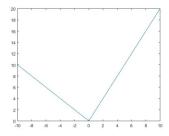
$$\int_{-\infty}^{\infty} \delta(x) \, dx = 1$$

Part 2. Delta function and differential eqns

For example,

$$\begin{cases} -\frac{d^2u}{dx} = \delta(x-a), where \ 0 < a < 1 \\ u(0) = 0 \\ u(1) = 0 \end{cases}$$
 (1)

To get the solution of u(x), first let's see what equation (1) means. (1) tells us that u(x) consists two lines, and there is a turning point, because only in this way can we get (1), for instance(not the solution for (1), (2), (3):)



But we have a better way to decompose the picture above as u(x) = -R(x - x)a)+C+Dx, where R(x) is Ramp function. There are many equivalent definitions of Ramp function, here are two of them.

$$R(x):=\begin{cases} x, & x\geq 0;\\ 0, & x<0 \end{cases}$$
 The convenience of $u(x)=-R(x-a)+C+Dx$ is that we can easily insert

equations (2) and (3) to get C and D.

Part 3. Boundary in differential eqns

We name equations (2) and (3) as boundaries in the differential eqns in part 2. Boundaries as u(x) = a and u'(x) = a are called fixed boundary and free boundary.

You can see that if we have at least one fixed boundaries, we can get only one solution. If the two boundaries are both free boundaries, we have numerous solutions.

5 & 6 & 7 Eigenvalues & positive definite

Covered in 18.06 Linear Algebra.

8 Springs and masses; the main framework

Suppose, as below, here are 4 springs and 3 masses. The force comes from the ith spring is $w_i = c_i e_i$, where c_i is the constant for spring i, e_i is the elongation in spring i. And the displacement for the ith mass is u_i .



It's easy to show $e_1 = u_1$, $e_2 = u_2 - u_1$, and so on. And $w_1 = c_1 e_1$, $w_2 = c_2 e_2$, and so on. Write these equations in matrix form:

$$\begin{bmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \end{bmatrix} = \begin{bmatrix} 1 \\ -1 & 1 \\ & -1 & 1 \\ & & -1 & 1 \\ & & & -1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix}$$

$$\begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix} \begin{bmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \end{bmatrix}$$

And this is a stable(balance) state, from high school. We know $w1 - w2 = m_1g$, $w2 - w3 = m_2g$ and $w3 - w4 = m_3g$. Denote m_ig as f_i and write these equations in matrix form:

$$\begin{bmatrix} 1 & -1 & & & \\ & 1 & -1 & & \\ & & 1 & -1 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix}$$

Write these matrix equations shorter: e = Au, w = Ce, and $f = A^Tw$. Here the two Toeplitz matrix are transpose of each other, which is **not** a coincidence.

Finally, $f = A^T C A u$. We call $K = A^T C A$ as **stiffness matrix**. It's easy to calculate u in f = K u, because K is a very good matrix, symmetric, positive definite. In 18.085, the constant c for a spring, or other material, is always positive, so K is positive definite. In somewhere else, c may be negative, which enables us to do some cool things, but beyonds area of 18.085.

We call $\frac{1}{2}e^TCe$ as the **energy** of this system. It's just the sum of energy on each spring, i.e., $\frac{1}{2}e^TCe = \sum \frac{1}{2}c_ie_i^2$.

For $K = A^T C A$, if we do the calculation with multiplying column in A^T , C and every row in A, non-zero elements in every resulting matrix are $\pm c_i$. In this way, we know how much every spring contributes to K. This is what **ADINA** do, covered later.

9 Oscillation

Part 1. Question of oscillation

Like previous section, 3 springs and 2 masses as below. Our formula is

$$M\frac{d^2u}{dt^2} + Ku = 0 (1)$$

and initial conditions u(0), $\frac{du}{dt}(0)$, where M is a diagonal matrix, $M_{ii} = m_i$ (weight), u is displacement of these masses, t is time, $K = A^T C A$ comes from the previous section.



Equation (1) makes sense that $\frac{d^2u}{dt^2}$ is acceleration, making it essentially

Newton's second law. Write equation (1) in detail:

$$\begin{bmatrix} m_1 \\ m_2 \end{bmatrix} \begin{bmatrix} u_1'' \\ u_2'' \end{bmatrix} + \begin{bmatrix} c_1 + c_2 & -c_2 \\ -c_2 & c_2 + c_3 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = 0$$

Part 2. Solve by eigenvectors

The solution for (1) is shaped like $u(t) = \sum_i a_i(\cos w^i t) x^i + b_i(\sin w^i t) x^i$, where x^i is the *i*th constant vector. Inserting u(t) in (1), we get $Kx = w^2 Mx$, or better $M^{-1}Kx = w^2 x$. You see that x and w^2 are eigenvector and eigenvalue of $M^{-1}K$. And M^{-1} can be calculated in a sudden since M is a diagonal matrix. Now we only need a_i and b_i to get the complete solution, which can be done with the initial conditions.

Part 3. Solve by difference

Here we change the derivative $\frac{d^2u}{dt^2}$ with second order difference.

10~&~11 Finite differences in time $\&~{\rm Least~squares}$

Part 1. Finite differences in time

For $\frac{du}{dt} = Au$, from 2.2 we have three methods to replace derivative with difference, which are equivalent to:

Forward Euler $\frac{u_{n+1}-u_n}{\Delta t} = Au_n$

Backward Euler $\frac{u_{n+1}-u_n}{\Delta t}=Au_{n+1}$

Trapezoidal rule $\frac{u_{n+1}-u_n}{\Delta t} = \frac{1}{2}(Au_{n+1}+Au_n)$

For the Trapezoidal rule, it's equivalent to $u_{n+1} = (I - \frac{\Delta t}{2}A)^{-1}(I + \frac{\Delta t}{2}A)u_n$, where $G = (I - \frac{\Delta t}{2}A)^{-1}(I + \frac{\Delta t}{2}A)$ is the growth matrix, and $eig(G) = \frac{1 + \frac{\Delta t}{2}eig(A)}{1 - \frac{\Delta t}{2}eig(A)}$.

Part 2. Least squares (part1)

This is covered in 18.06 Linear Algebra.

12 Graphs and networks

Part 1. Graph

As below, 4 nodes and 5 edges.



We can use **incidence** matrix A to describe the graph, where each row stands for a edge, each column stands for a node, and -1 for start, 1 for end.

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

 A^TA equals to degree matrix subtracts adjacency matrix. Degree matrix D is a diagonal matrix, where D_{ii} is how many edges node i connects. Adjacency matrix W is a n(# nodes)*n matrix, where $W_{ij} = 1$ or 0 stands for there is/isn't an edge between node i and j.

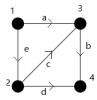
Part 2. Network

I will cover this part in the next section.

13 Kirchhoff's Current Law(KCL)

The same graph in section 12. We can view each edge as an directed electric current. The **Kirchhoff's Current Law** is that for every node, the sum of current is 0. For example, for node 3, a + b + c = 0. The **Kirchhoff's voltage**

Law is that: the directed sum of the electrical potential differences (voltage) around any closed network is zero.



KCL here in matrix form it's $A^Tw = 0$ if there is no additional current source, where w is current, A is comes from section 12. w = Ce, where C is constant, reciprocal of resistance, **conductance**. If there is no battery on edges, e = Au, where u is electric potential, otherwise e = b - Au, where b is battery source. So finally we can write these equations in just one or two equations:

- i. One equation: $A^TCAu = A^TCb f$, called **displacement method**.
- ii. Two equations: $C^{-1}w + Au = b$ and $A^Tw = f$, called **mixed method**.

14 Exam Review

15 & 16 Trusses and A^TCA

A truss with 5 bars and 5 nodes(pins), every node have horizontal displacement u^H and vertical displacement u^V . We have Au=0.

17 & 18 Finite elements in 1D

Part 1. The transpose of A = d/dx

For A = d/dx, $A^T = A^* = -d/dx$. A concrete proof will be given later. A

rough proof is that:

$$A = \begin{bmatrix} 1 & & & & \\ -1 & 1 & & & \\ & -1 & 1 & & \\ & & -1 & 1 \end{bmatrix} A^{T} = \begin{bmatrix} 1 & -1 & & & \\ & 1 & -1 & & \\ & & 1 & -1 & \\ & & & 1 \end{bmatrix}$$

Look at A and A^T , from section 2, A is first order (backward) difference, and A^T is minus first order (forward) difference.

Part 2. Inner product on functions & concrete proof for $A^T = A^* = -d/dx$

For vectors, the inner product is defined as $a \cdot b = a^T b = \sum_i a_i b_i$. For functions, the idea of inner product of functions comes from $\sum_i a_i b_i$ that $(e, w) = \int e(x)w(x)dx$. Functions are orthogonal when (e, w) = 0.

 $(Au)^Tw=u^T(A^Tw)$ holds for vectors, where A=d/dx. To generalize it to functions, $(Au)^Tw$ becomes $\int \frac{du}{dx}w(x)dx$, $u^T(A^Tw)$ becomes $\int u(x)(\frac{d}{dx})^Tw(x)dx$. We don't like the transpose sign in the integration, so use **integration by parts** in calculus on $\int \frac{du}{dx}w(x)dx$:

$$\int \frac{du}{dx} w(x) dx = \int u(x) (-\frac{dw}{dx} dx) + [u(x)w(x)]_{x=lower\ bound}^{x=higher\ bound}$$
 So when $[u(x)w(x)]_{x=lower\ bound}^{x=higher\ bound} = 0$, you see the left side is $(Au)^Tw$, the

right side is $u^T(A^Tw)$, where $A^T = -d/dx$! This is the concrete proof of $A^T = A^* = -d/dx$.

Part 3. Weak form

The strong form of differential equation is $-\frac{d}{dx}(c\frac{du}{dx}) = f(x)$. The weak form is multiplying (chosen, so known)test function v(x) at both side, which does inner product:

$$\int c(x) \frac{du}{dx} \frac{dv}{dx} dx = \int f(x)v(x) dx$$

You may wonder where is the minus sign. The minus sign disappeared because $(d/dx)^T = -d/dx$ in inner product as discussed in part 1 and 2, or explicitly: $\int f(x)v(x)dx = \int -\frac{d}{dx}(c\frac{du}{dx})v(x)dx = \int c(x)\frac{du}{dx}\frac{dv}{dx}dx - [c(x)\frac{du}{dx}v(x)]_{x=lower}^{x=higher}\frac{bound}{bound}$

I think, the reason why we use test function here is that we can't deal with the strong form directly since there is $\frac{d}{dx}$ in $-\frac{d}{dx}(c\frac{du}{dx}) = f(x)$.

Part 4. Galerkin's method

The **Galerkin's method** is to discretize the weak form. First, substitute u(x) in weak form with $U(x) = \sum_{1,2,\dots,n} U_i \phi_i(x)$, where U_i is unknown number and $\phi_i(x)$ is chosen(so known) trail function. (I feel this substitution quite a bit likes variational inference.) Second, choose n test functions V_i . For each V_i , inserting it to weak form, get

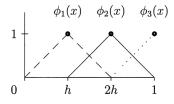
$$\int c(x) \left(\sum_{j=1,\dots,n} U_j \frac{d\phi_j}{dx}\right) \frac{dV_i}{dx} = \int f(x) V_i(x) dx$$

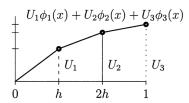
For all V_i , we can write the equation above in matrix form that KU = F, where $K_{ij} = \int c(x) \frac{dV_i}{dx} \frac{d\phi_j}{dx} dx$, $U = [U_1, U_2, \cdots, U_n]^T$, $F_i = \int f(x)V_i(x)dx$. The finite element method(FEM) approximation is $\sum U_i \phi_i(x)$ for u(x).

Frequently, test function V_i is the same as trail function ϕ_i , then $K_{ij} = K_{ji}$.

Part 5. Linear finite element

In linear finite element, the ϕ_i , $U(x) = \sum U_i \phi_i(x)$ look like below





19 Quadratic/cubic elements

23 & 24 Laplace's equation

Part 1. Laplace's equation and its solutions

Laplace's equation is $u_{xx} + u_{yy} = 0$. And magically, the solutions to this

equation always come in pairs that u(x, y) and s(x, y). The pairs come from f(x + iy), where u(x, y) = Re[f(x + iy)] and s(x, y) = Im[f(x + iy)].

Let's see some simple examples. Let $f(x+iy)=(x+iy)^n$, then the (u(x,y),s(x,y)) pair is $(x,y),(x^2-y^2,2xy),(x^3-3xy^2,3x^2y-y^3),\cdots$. You can check this is correct easily. A nice thing here is that if replace x,y with $r\cos\theta,r\sin\theta$, which is in polar coordinate, the solutions can be nicely written as $u_n=r^n\cos n\theta,s_n=r^n\sin n\theta$, see part 4.

What I think the most magical thing for Laplace's equation is that u(x,y) and s(x,y) are perpendicular at the cross point! See explanation in part 3. For example, for $u(x,y) = x^2 - y^2$ and s(x,y) = 2xy, let s(x,y) = 1, then for $u(x,y) = 1,2,3,\cdots$, there are many cross points of u(x,y) and s(x,y). At every cross point, u(x,y) and s(x,y) are perpendicular! It maybe hard to check this example with pencil and paper, but you can check u(x,y) = x and s(x,y) = y easily. What makes me think it magical is that because of the perpendicular, it acts as gradient descent! If we know the field of gradient u(x,y), we don't need gradient descent anymore, we can get gradient's whole trace u(x,y) at once!

Part 2. Analytic function and harmonic function

We know that any superposition of solutions to a linear equation (here Laplace's equation) is again a solution. For the example above, we have $f(x + iy) = f(z) = \sum_{n=0}^{\infty} c_n z^n$, called **analytic function**, the solutions in pair are u(x, y) = Re[f(x+iy)] and s(x,y) = Im[f(x+iy)], called **harmonic function**.

Part 3. The Cauchy-Riemann Equation

For f(x+iy), we have $\frac{\partial^2 f(x+iy)}{\partial x \partial y} = \frac{\partial^2 f(x+iy)}{\partial y \partial x}$, resulting $\frac{\partial}{\partial y} f(x+iy) = i \frac{\partial}{\partial x} f(x+iy)$ because $\frac{\partial^2 f(x+iy)}{\partial x \partial y} = \frac{\partial}{\partial y} \frac{\partial f(x+iy)}{\partial x} = \frac{\partial}{\partial y} \frac{\partial f(x+iy)}{\partial z} \frac{\partial z}{\partial x} = \frac{\partial}{\partial y} \frac{\partial f(x+iy)}{\partial z}$, and $\frac{\partial^2 f(x+iy)}{\partial x \partial y} = \frac{\partial}{\partial x} \frac{\partial f(x+iy)}{\partial z} = \frac{\partial}{\partial x} \frac{\partial f(x+iy)}{\partial z} \frac{\partial z}{\partial y} = \frac{\partial}{\partial x} \frac{\partial f(x+iy)}{\partial z} i$.

In part 1, we have f(x+iy)=u(x,y)+is(x,y), and plug it here that $\frac{\partial}{\partial y}(u+is)=i\frac{\partial}{\partial x}(u+is)$. Match the real part and imaginary part, then we get the **Cauchy-Riemann Equation**:

$$\frac{\partial u}{\partial x} = \frac{\partial s}{\partial y}$$

$$\frac{\partial u}{\partial y} = -\frac{\partial s}{\partial x}$$

Why are u(x,y) and s(x,y) perpendicular at the cross point in part 1? Plugging the Cauchy-Riemann Equation in $u'(x,y) \cdot s'(x,y)$, which is the dot product of tangent line and equivalently the dot product of direction of u'(x,y) and s'(x,y), $u'(x,y) \cdot s'(x,y) = (\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}) \cdot (\frac{\partial s}{\partial x}, \frac{\partial s}{\partial y}) = (\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}) \cdot (-\frac{\partial u}{\partial y}, \frac{\partial u}{\partial x}) = 0$.

Part 4. Polar coordinate: Laplace's equation in a circle

In part1, we said, if we replace x, y with $r \cos \theta, r \sin \theta$, which is in polar coordinate, the solutions can be nicely written as $u_n = r^n \cos n\theta, s_n = r^n \sin n\theta$. Why?

First, $x + iy = r\cos\theta + ir\sin\theta = r(\cos\theta + i\sin\theta) = re^{i\theta}$.

Then, $(re^{i\theta})^n = re^{in\theta} = r^n(\cos n\theta + i\sin n\theta) = r^n\cos n\theta + ir^n\sin n\theta$.

Finally, u(x, y), s(x, y) are the real and imaginary part that $r^n \cos n\theta$, $r^n \sin n\theta$.

25 & 26 Fast Poisson solvers

Part 1. K in 2D

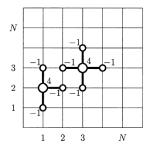
For **Poisson's equation** $-u_{xx} - u_{yy} = f(x, y)$, we can discretize the derivative with second difference and describe it as KU = F. We have seen KU = F in 1-dimension in section 17 & 18. Let's discretize it in a 2-dimension square.

First, discretize the 2D square as meshes with meshwidth h, as below. The Poisson's equation for a molecule centered at position (i, j) (the molecules at the boundary are not take into account) is as below, looks like a filter, aha?

$$4U_{i,j} - U_{i,j-1} - U_{i-1,j} - U_{i+1,j} - U_{i,j+1} = h^2 f(ih, jh)$$

For molecules next to the boundary, the corresponding U is dropped, or concretely, moved to the right side of the equation according to the book.

So we know the corresponding row in K for every molecule. For example, if give the index from left to right and bottom to top, the corresponding (6-th) row in K for (1,2) is $[-1,0,0,0,0,4,-1,0,0,0,-1,\cdots]$ with length of 5^2 .



Part 2. K in 2D with Kronecker product

There exists a way to generate K in 2D with math, **Kronecker product**. The Kronecker product is defined as:

$$\mathbf{A} \otimes \mathbf{B} = \begin{bmatrix} a_{11}\mathbf{B} & \cdots & a_{1n}\mathbf{B} \\ \vdots & \ddots & \vdots \\ a_{m1}\mathbf{B} & \cdots & a_{mn}\mathbf{B} \end{bmatrix}$$

We know the K in 1D should be

$$K_{1D} = \begin{bmatrix} 2 & -1 & & \\ -1 & 2 & -1 & \\ & \cdot & \cdot & \cdot \\ & & -1 & 2 \end{bmatrix}$$

Then K in 2D is

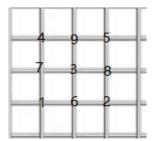
$$K = kron(I, K_{1D}) + kron(K_{1D}, I) = \begin{bmatrix} K_{1D} + 2I & -I \\ -I & K_{1D} + 2I & -I \\ & \cdot & \cdot & \cdot \\ & & -I & K_{1D} + 2I \end{bmatrix}$$

Part 3. Solve Poisson's equation with (elimination and fill-in) or cyclic odd-even reduction

A simple to solve Poisson's equation is elimination. This is straightforward but time-consuming comparing to other good ideas.

If we change the index of these molecules as counting every 2 molecules,

we can do elimination faster, because K would be more organized inside. For example, for 3*3 molecules, from left to right and bottom to top, we assign the index as



Part 3. Solve Poisson's equation in 1D with eigenvectors

For K in 1D, it's very special that second order difference, which enables us to find its eigenvectors (y_i) and eigenvalues (λ_i) easily even with pencil and paper. From 18.06, if A is invertible, A and A^{-1} have the same eigenvectors, and the eigenvalues are reciprocal of each other. So we know the eigenvectors and eigenvalues for K^{-1} . So for $Ku=f,\ u=K^{-1}f$. Recall the meaning of eigenvectors in 18.06, we decompose f to eigenvectors' direction as $f=\sum a_iy_i$, then $u=K^{-1}f=\sum \frac{1}{\lambda_i}a_iy_i$, or $u=S\Lambda^{-1}S^{-1}f$ in matrix form where S,Λ are eigenvector and eigenvalue matrix.

For K in 2D, the solution comes from the same idea, but we need help of the Discrete Sine Transform in part 4.

Part 4. The Discrete Sine Transform in 1D

In 1D, column k of the eigenvector matrix S contains the eigenvector y_k . The number $S_{jk}=\sin\frac{jk\pi}{N+1}$ is the jth component of that eigenvector. For our example in part 1 with N+1=6, $\frac{jk\pi}{N+1}$ is always multiple of $\frac{\pi}{6}$. $(\sin\frac{1\pi}{6},\sin\frac{2\pi}{6},\sin\frac{3\pi}{6},\cdots)$ is a list that $(\frac{1}{2},\frac{\sqrt{3}}{2},1,\frac{\sqrt{3}}{2},\frac{1}{2},0,-\frac{1}{2},-\frac{\sqrt{3}}{2},-1,-\frac{\sqrt{3}}{2},-\frac{1}{2},-0,\cdots$ (repeat forever)). The kth column of S(kth eigenvector y_k) just takes every kth number from that list. So for our example, here are the first five eigenvectors:

$$y_1 = \begin{bmatrix} 1/2 \\ \sqrt{3}/2 \\ 1 \\ \sqrt{3}/2 \\ 1/2 \end{bmatrix} \quad y_2 = \begin{bmatrix} \sqrt{3}/2 \\ \sqrt{3}/2 \\ 0 \\ -\sqrt{3}/2 \\ -\sqrt{3}/2 \end{bmatrix} \quad y_3 = \begin{bmatrix} 1 \\ 0 \\ -1 \\ 0 \\ 1 \end{bmatrix} \quad y_4 = \begin{bmatrix} \sqrt{3}/2 \\ -\sqrt{3}/2 \\ 0 \\ \sqrt{3}/2 \\ -\sqrt{3}/2 \end{bmatrix} \quad y_5 = \begin{bmatrix} 1/2 \\ -\sqrt{3}/2 \\ 1 \\ -\sqrt{3}/2 \\ 1/2 \end{bmatrix}$$

Those eigenvectors are orthogonal! This is guaranteed by the symmetry of K. All these eigenvectors have length 3, so $S/\sqrt{3}$ is an orthonormal matrix Q, with $Q^TQ=I$. What's more, for this very special example, S and Q are also symmetric, so $Q^{-1}=Q^T=Q$.

Part 5. Solve Poisson's equation in 2D with eigenvectors

To extend this eigenvalue (Discrete Sine Transform) method to two dimensions, we need the eigenvalues and eigenvectors of K in 2D. The key point is that the N^2 eigenvectors of K in 2D are separable that each eigenvector y_{kl} separates into a product of sines, where (i,j) is for F_{ij} and U_{ij} in Poisson's equation:

the
$$(i,j)$$
 component of y_{kl} is $\sin \frac{ik\pi}{N+1} \sin \frac{jl\pi}{N+1}$

The eigenvalue in two dimensions is the sum $\lambda_k + \lambda_l$ of one-dimensional eigenvalues:

$$\lambda_{kl} = (2 - 2\cos\frac{k\pi}{N+1}) + (2 - 2\cos\frac{l\pi}{N+1})$$

Now the solution of KU=F in 2D comes by a two-dimensional sine transform:

$$F_{ij} = \sum \sum a_{kl} \sin \frac{ik\pi}{N+1} \sin \frac{jl\pi}{N+1}, U_{ij} = \sum \sum \frac{a_{kl}}{\lambda_{kl}} \sin \frac{ik\pi}{N+1} \sin \frac{jl\pi}{N+1}$$

Or extremely in matrix form that for $KU=F,\,U=K^{-1}F=S\Lambda^{-1}S^{-1}F$ because $K=S\Lambda S^{-1}\Leftrightarrow K^{-1}=S\Lambda^{-1}S^{-1}$, which comes from 18.06 that if A is invertible, A and A^{-1} have the same eigenvectors, and the eigenvalues are reciprocal of each other.

28 & 29 Fourier series

Part 1. Fourier sine/cosine series

Fourier sine series:

$$S(x) = b_1 \sin x + b_2 \sin 2x + b_3 \sin 3x + \dots = \sum_{n=1}^{\infty} b_n \sin nx$$

The item $\sin 0x$ is dropped off since it equals to 0, but not for Fourier cosine series. To get the coefficient b_i , first recall orthogonality of these sines that:

$$\int_0^\pi \sin nx \sin kx dx = 0 \text{ if } n \neq k \tag{1}$$

Then we take advantage of that orthogonality that multiply $\sin kx$ on both sides of Fourier sine series, and take integral:

$$\int_0^{\pi} S(x) \sin kx dx = \int_0^{\pi} b_1 \sin x \sin kx dx + \dots + \int_0^{\pi} b_k \sin kx \sin kx dx + \dots$$

Because of orthogonality above, all items in the right side is 0 except $\int_0^{\pi} b_k \sin kx \sin kx dx$, which is $\frac{\pi}{2}$. So:

$$b_k = \frac{2}{\pi} \int_0^{\pi} S(x) \sin kx dx = \frac{1}{\pi} \int_{-\pi}^{\pi} S(x) \sin kx dx$$

, where the last equal sign comes from S(x) = -S(x).

Fourier cosine series is similar to Fourier sine series C(x).

Part 2. Fourier Complete series and Fourier Complex Exponential Series

S(x) + C(x) gives the Fourier Complete Series:

$$F(x) = a_0 + \sum_{n=1}^{\infty} a_n \cos nx + \sum_{n=1}^{\infty} b_n \sin nx$$

The coefficients can be solved similar to Fourier sine series as:

$$a_0 = \frac{1}{2\pi} \int_{-\pi}^{\pi} F(x) dx$$

$$a_k = \frac{1}{\pi} \int_{-\pi}^{\pi} F(x) \cos kx dx$$

$$b_k = \frac{1}{\pi} \int_{-\pi}^{\pi} F(x) \sin kx dx$$

The integral range $[-\pi, \pi]$ comes from that to utilize the orthogonality as equation (1), the range need to be $[-\pi, \pi]$.

Fourier Complex Exponential Series is:

$$F(x) = c_0 + c_1 e^{ix} + c_{-1} e^{ix} + \dots + \dots = \sum_{n=-\infty}^{\infty} c_n e^{inx}$$
, where $i^2 = 1$

The coefficients are given as:

$$c_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} F(x)e^{-inx} dx$$

Part 3. Application: Laplace's Equation in a circle

For Laplace's Equation in a circle, combination of all solutions is:

$$u(r,\theta) = a_0 + a_1 r \cos \theta + b_1 r \sin \theta + a_2 r^2 \cos 2\theta + b_2 r^2 \sin 2\theta + \cdots$$
 (2)

For example, we let r = 1. The coefficients are automatically solved since equation (2) is exactly the Fourier Complete series, in which we can get coefficients easily.

1 Things to do

Pay attention to variational inference and Fourier transform(KCF)!

Function is mapping. Map set x to y, and f (in f(x)) is the rule to map! Functional Analysis

Appro the CNN with a function which can be solved in a sudden. For example, for Lenet, the network is mapping a two-dimension matrix a vector with length 10(0 9). If there exist some basic mapping functions, we can take combinations of them(as f), then approximate the Lenet with f. The approximation process could be easy, we can just compare the output vector, define a loss, then use SGD.