¶ This course has two themes: How to understand equations, and how to solve them.

Textbook: Strang's CSE

§0.1 One dimensional Problem

Example: Describe the displacement u for a continuous elastic bar hanging vertically. See Figure 3.1.

- *Assume that boundary conditions are $u(0) = 0$ (fixed) and $w(1) = c\frac{du}{dx}(1) = 0$(free). Assume that the point originally at distance x from the top is displaced down to $x + u(x)$.*
- **Hooke's law**: *The internal force w depends on the strain $e = \frac{du}{dx}$ (elongation) and the elastic coefficient c:*

$$w(x) = c\,\frac{du}{dx} \qquad (0 < x < 1)$$

- **Force Balance:** *The equilibrium of our small piece requires that the difference in internal force at two ends of $[x, x+\Delta x]$ to balance the external forces of gravity over $[x, x+\Delta x]$.*

$$\Big(c\frac{du}{dx}\Big)_{x+\Delta x} - \Big(c\frac{du}{dx}\Big)_{x} + f\Delta x = 0 \quad \Leftrightarrow \quad -\frac{d}{dx}\Big(c\frac{du}{dx}\Big) = f$$

Discrete Version (Important in CSE!)

We can view $u \simeq (u(x_1), u(x_2), u(x_3), u(x_4)) := (u_1, u_2, \cdots, u_4)$ where $x_k = k\Delta x = k/4$. Similarly, we view the continuous functions w and e as the vectors $w \simeq (w_0, w_1, w_2, w_3)$ and $e \simeq (e_0, e_1, e_2, e_3)$, respectively. Note that $u_0 = 0$ (fixed) and $w_4 = 0$(free).

- **Stretching:** Approximating $\frac{du}{dx} \approx \frac{u(x+\Delta x)-u(x)}{\Delta x}$,

$$e = \frac{du}{dx} = Au = \frac{1}{\Delta x}\begin{pmatrix} 1 & & & \\ -1 & 1 & & \\ & -1 & 1 & \\ & & -1 & 1 \end{pmatrix} u \quad \text{with} \quad u(0) = 0$$

  A is the derivative $\frac{d}{dx}$ applied to u.

- **Hooke's law:** $w(x) = c(x)e(x) = c(x)\frac{du}{dx} = CAu$ where C is diagonal matrix corresponding to the elastic coefficient c.

- **Force Balance:** $A^T w = -\frac{dw}{dx} = f(x)$ with $w(1) = 0$.

  1. Why is the transpose of $A = \frac{d}{dx}$ given by $A^T = -\frac{d}{dx}$?

$$\underbrace{(Au, w)}_{inner\ pro.} = \underbrace{(Au)^T w}_{strain \times stress} \Delta x \approx \int_0^1 \underbrace{\frac{du}{dx}}_{Au} w(x)\, dx.$$

  2. From the boundary condition $u(0) = 0$ and $w(1) = c\frac{d}{dx}u(1) = 0$,

$$\underbrace{\int_0^1 \frac{du}{dx} w(x)\, dx}_{(Au,w)} = \underbrace{-\int_0^1 u\frac{dw}{dx}\, dx}_{(u,A^T w)} + \underbrace{[uw]_{x=0}^{x=1}}_{=0}$$

  Hence, $A^T w = -\frac{dw}{dx}$ with $w(1) = 0$!! Great!

- $e = Au,\ w = Ce,\ f = A^T w \Rightarrow A^T CAu = f$

- The differential equation $A^T CAu = f$ can be solved directly.

  1. Recall $A^T CAu = -\frac{d}{dx}\left(c\frac{du}{dx}\right) = f$.
  2. $w(x) = \int_x^1 f dx = (A^T)^{-1} f$. Here, we use $w(1) = 0$
  3. $u(x) = \int_0^x \frac{w}{c} dx = A^{-1}C^{-1}w$ with $u(0) = 0$. We can say that $A = \frac{du}{dx}$ with $u(0) = 0$ is invertible.

Example: $-\frac{d^2u}{dx^2} = 1$ with $u(0) = 0$ and $u(1) = b$.

1. The solution $u(x) = bx + \frac{1}{2}(x - x^2)$ is the sum of two terms: a uniform stretching bx by fixing the end $x = 1$ at $u = b$, and a multiple of $(x - x^2)$ that vanishes at both ends.
2. The stress in the bar is $w = b + (\frac{1}{2} - x)$. One part comes from the boundary condition and the other part from the force.
3. We should make small change in the inner product (Au, w) and $(u, A^T w)$:

$$
\begin{aligned}
(Au, w) &= \int_0^1 \frac{du}{dx}\, w\, dx \quad + u(0)w(0) \\
(u, A^T w) &= \int_0^1 u \left(-\frac{dw}{dx}\right) dx \quad + u(1)w(1)
\end{aligned}
$$

♣ Boundary Conditions on A^T ♣

- If A has BC $u(0) = 0$, A^T must have $w(0) = 0$. (Why?)
- If A has BC $u(0) = 0 = u(1)$, A^T has no conditions. (Why?)
- If A has no conditions, A^T has BC $w(0) = 0 = w(1)$. (Why?)

♣ The equation $-(cu')' = f$ has other applications ♣

If u is the temperature u, then f is a heat source and c is the diffusivity. The condition $u(0) = T$ fixes the temperature at on end, and $w(1) = 0$ insulates the other end.

Example : Strum-Liouville Problem $-\frac{d}{dx}\left(c\frac{du}{dx}\right) + qu = f$ with boundary condition $[uw]_0^1 = 0$.

- Fortunately, the extra term qu does not spoil the symmetry, and fit completely into the same framework.

$$\underbrace{\begin{bmatrix} -\frac{d}{dx} & I \end{bmatrix}}_{A^T} \underbrace{\begin{bmatrix} c(x) & 0 \\ 0 & q(x) \end{bmatrix}}_{C} \underbrace{\begin{bmatrix} \frac{d}{dx} \\ I \end{bmatrix}}_{A} = -\frac{d}{dx}\left(c\frac{d}{dx}\right) + q$$

  Applied to u, it gives f.

Example : For small c, compare the solution of $-\frac{d}{dx}\left(c\frac{du}{dx}\right) + u = 1$ with the limit $U = 1$. Here, BC is $u(0) = 0 = u(1)$.

There are two approaches:

- (Exact solution) Fit the general solution

$$u = \underbrace{d_1 e^{x/\sqrt{c}} + d_2 e^{-x/\sqrt{c}}}_{-c\Box'' + \Box = 0} + \underbrace{1}_{particular\ sol.}$$

  to BC(boundary conditions) $u(0) = 0 = u(1)$.

- (Singular Perturbation) Near each end find a solution that connects $u(0) = 0 = u(1)$ to the interior value $U = 1$. There is a boundary layer at each end in which all action occurs. The special solution $u = 1 - e^{-x/\sqrt{c}}$ climbs from $u(0) = 1$ to $u = 1 - e^{-8} \approx 1$ at $x = 8\sqrt{c}$. At $x = 8\sqrt{c}$, it has virtually met the interior solution $U = 1$. Do a similar exponential to connect $U = 1$ with $u(1) = 0$. The perturbation is singular because the unperturbed solution $U = 1$ completely misses BC. The leading term $-cu''$ is disappearing as $c \to 0$, but it remains powerful insider the layer.

Example : For small q, compare the solution of $-\frac{d}{dx}\left(\frac{du}{dx}\right)+qu=1$ with that of $-\frac{d^2U}{dx^2}=1$. Here, BC is $u(0)=0=u(1)$.

- For the exact u, fit the general solution

$$u=\underbrace{d_1e^{\sqrt{q}x}+d_2e^{\sqrt{-q}x}}_{-\Box''+q\Box=0}+\underbrace{1/q}_{particular\ sol.}$$

  to $u(0)=0=u(1)$.

- (Regular Perturbation) $U=\frac{1}{2}(x-x^2)$ almost solve $-u''+qu=1$ with zero BC provided the error term qU is small compared with 1.
  1. Starting with U at $q=0$, look for a solution of the form (Taylor's expansion w.r.t. q)

  $$u=U+qV+q^2W+O(q^3)$$

  2. The first correction term qV is determined by substituting into $-u''+qu=1$ and we get $V=\frac{x^3}{12}-\frac{x^4}{24}-\frac{x}{24}$.

- Both methods gives the same solution. The first is exact but its behavior is not so clear for small q. The second form $u=U+qV+q^2W+O(q^3)$ clarifies that behavior but is not satisfactory for large q.

In the previous examples, we identify $A = \frac{d}{dx}$ and $A^T = -\frac{d}{dx}$ with BC and $A^TCAu = f \;\Leftrightarrow\; -\frac{d}{dx}\left(c\frac{du}{dx}\right) = f$. Now, let us study minimum principle for u and w.

Minimization Problem

- *In finite dimensions,*

$$u = \arg\min_{u\in\mathbb{R}^n} P(u) \quad\Rightarrow\quad A^TCAu = f$$

where

$$P(u) = \frac{1}{2}(Au)^TC(Au) - f^Tu.$$

- *In the continuous case, if* $u \in H_0^1(0,1)$ *minimizes the potential energy*

$$u = \arg\min_{u\in H_0^1} P(u) \quad\Rightarrow\quad -\frac{d}{dx}\left(c\frac{du}{dx}\right) = f$$

where $H_0^1(0,1) = \{\phi \;:\; \int_0^1 |\phi|^2 + |\phi'(x)|^2 dx < \infty,\; \phi(0) = 0 = \phi(1)\}$ *and*

$$P(u) = \int_0^1 \left[\frac{c}{2}\left(\frac{du}{dx}\right)^2 - f(x)u(x)\right]dx$$

- *Moreover, the minimizer* u *satisfies*

$$\int_0^1 \left[c\,\frac{du}{dx}\,\frac{d\phi}{dx}\right]dx = \int_0^1 f(x)\phi(x)dx \qquad \forall\phi \in H^1(0,1)$$

Finite elements are based on the "weak form" with the test function ψ.

Proof. Use generalized derivative $\partial P(u)$ with respect to test function ϕ. That is all.

§0.2 Poisson equation and Potential flow in 2D

The equation $div(c\nabla u) = f$ is built from two operations, the gradient of u and the divergence of ∇u. One beautiful observation by Gauss-Green formula is $(gradient)^T = -divergence$. In fact, the Laplace equation fits exactly into the framework of $A^T CAu = f$:

$$-\nabla \cdot (c\nabla u) = \begin{bmatrix} -\frac{\partial}{\partial x} & -\frac{\partial}{\partial y} \end{bmatrix} cI \begin{bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{bmatrix} u = A^T CAu = f$$

(Why?)

- $(v = Au)$ The velocity v is $v = \nabla u$ (the gradient of the potential).
- $(w = Cv)$ The flow rate w is $w = cv$ (mass× velocity)
- $(f = A^T w)$ Conservation of mass is $-div(w) = f$ if there are sink $(f > 0)$ or sources $(f < 0)$.
- From Gauss-Green formula,

$$\underbrace{\int\int \nabla u \cdot w}_{(Au,w)} = \underbrace{\int\int u\ (-div(w))}_{(u,A^T w)} + \text{boundary terms}$$

§1 Applied Linear Algebra

§1.1 Four Special Matrices

Often we see the matrix as an operator.

$\boldsymbol{A}$ acts on vectors $\boldsymbol{x}$ to produce $\boldsymbol{Ax}$.

- The components of $\boldsymbol{x}$ have a meaning-displacements or pressures or voltages or prices or concentrations.
- The operator $\boldsymbol{A}$ also have meaning. In this chapter, $\boldsymbol{A}$ takes difference. Then $\boldsymbol{Ax}$ represents pressure differences or voltage drops or price differentials.
- $\boldsymbol{K} = \boldsymbol{A}^T\boldsymbol{A}$ may take *Laplacian with a boundary condition (Neumann, Dirichlet, periodic, Robin).*

We look first at the properties of the following four special families of matrices-*simple and useful, absolutely basic.*

Four sparse symmetric $n \times n$ matrix K_n, C_n, T_n, B_n

$$K_4 = \underbrace{\begin{pmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{pmatrix}}_{Toeplitz\ matrix} \quad C_4 = \underbrace{\begin{pmatrix} 2 & -1 & 0 & -1 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ -1 & 0 & -1 & 2 \end{pmatrix}}_{Circulant\ matrix}$$

and

$$T_4 = \begin{pmatrix} 1 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{pmatrix} \quad B_4 = \begin{pmatrix} 1 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 1 \end{pmatrix}$$

- K_n and T_n are invertible and positive definite.
- C_n and B_n are singular and positive semidefinite.
- The nullspaces of C_n and B_n contain all the constant vectors $u = (c, c, \ldots, c)$.

※ MATLAB Command:

- K_4=toeplitz([2 -1 zeros(1,2)])
- K_3=[2 -1 0; -1 2 -1; 0 -1 2]
- We can build K_8 from " eye" and "ones":

  E=-diag(ones(7,1),1) K_8=2 eye(8) + E+E'

  where $eye(8) = 8 \times 8$ identity matrix.

Homework (due to Oct 31): Solve the following

- **Sec 1.1 : 2,3,5,13,17,19,20,25,27**
- **Sec 1.2 : 1,3,4,8,9,10,12,14-21**
- **Sec 1.4 : 1–15**
- **Sec 1.5 : 23–31**

§1.2 Differences, Derivatives, Boundary Conditions

The matrices K_n and C_n and T_n and B_n are all involved in approximating the following Poisson equation

$$-\frac{d^2u}{dx^2} = f(x) \quad \text{with boundary conditions at} \quad x = 0 \quad \text{and} \quad x = 1$$

Finite Differences

How can we approximate $\frac{du}{dx}$ *and* $\frac{d^2u}{dx^2}$ *? We use Taylor series approximation of* $u(x+h)$ *and* $u(x-h)$*:*

$$u(x \pm h) = u(x) \pm hu'(x) + \frac{1}{2}h^2u''(x) + O(|h^3)$$

- *Forward difference*

$$\frac{\Delta_+ u}{h} = \frac{u(x+h) - u(x)}{h} = u'(x) + \underbrace{\frac{1}{2}hu''(x) + O(h^2)}_{error\ is\ O(h)}$$

- *Backward difference*

$$\frac{\Delta_- u}{h} = \frac{u(x) - u(x-h)}{h} = u'(x) - \underbrace{\frac{1}{2}hu''(x) + O(h^2)}_{error\ is\ O(h)}$$

- *Centered difference*

$$\frac{\Delta_0 u}{h} = \frac{u(x+h) - u(x-h)}{2h} = u'(x) + \underbrace{O(h^2)}_{error}$$

The matrix for centered differences is antisymmetric (like the first derivative):

Centered difference matrix $\triangle_0^T = -\triangle_0$

$$\begin{pmatrix} \ddots & & & \\ -1 & 0 & 1 & \\ & -1 & 0 & 1 \\ & & & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ u_i \\ u_{i+1} \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ u_{i+1} - u_{i-1} \\ u_{i+2} - u_i \\ \vdots \end{pmatrix}$$

Second difference $\frac{d^2u}{dx^2} \approx \frac{u_{i+1}-2u_i+u_{i-1}}{h^2}$

Watch how the second difference $\Delta_-\Delta_+ u$ *is centered around point* i:

$$\frac{d^2u}{dx^2} \approx \frac{1}{h}\Delta_-\left[\frac{\Delta_+ u(i)}{h}\right] = \frac{1}{h}\left(\underbrace{\left[\frac{u_{i+1}-u_i}{h}\right]}_{\Delta_+ u(i)/h} - \underbrace{\left[\frac{u_i-u_{i-1}}{h}\right]}_{\Delta_+ u(i-1)/h}\right)$$

$$= \frac{u_{i+1}-2u_i+u_{i-1}}{h^2}$$

Here are second differences of special column vectors.

$$\checkmark \underbrace{\begin{pmatrix} \ddots & & & & \\ & 1 & -2 & 1 & \\ & & 1 & -2 & 1 \\ & & & & \ddots \end{pmatrix}}_{\frac{d^2}{dx^2}} \underbrace{\begin{pmatrix} 1 \\ 4 \\ 9 \\ 16 \end{pmatrix}}_{x^2} = \underbrace{\begin{pmatrix} \vdots \\ 2 \\ 2 \\ \vdots \end{pmatrix}}_{2}$$

$$\checkmark \underbrace{\begin{pmatrix} \ddots & & & & \\ & 1 & -2 & 1 & \\ & & 1 & -2 & 1 \\ & & & & \ddots \end{pmatrix}}_{\frac{d^2}{dx^2}} \underbrace{\begin{pmatrix} 0 \\ 0 \\ 1 \\ 2 \end{pmatrix}}_{Ramp} = \underbrace{\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}}_{\text{delta}}$$

$$\checkmark \underbrace{\begin{pmatrix} \ddots & & & & \\ & 1 & -2 & 1 & \\ & & 1 & -2 & 1 \\ & & & & \ddots \end{pmatrix}}_{\frac{d^2}{dx^2}} \underbrace{\begin{pmatrix} \sin t \\ \sin 2t \\ \sin 3t \\ \sin 4t \end{pmatrix}}_{\sin tx} = \underbrace{(2\cos t - 2)\begin{pmatrix} \sin t \\ \sin 2t \\ \sin 3t \\ \sin 4t \end{pmatrix}}_{\lambda \cdot (\text{Sines})}$$

Finite Difference Equation

We can create a discrete form of

$$-d^2u/dx^2 = f(x) \quad \textit{with fixed ends} \quad u(0) = 0 = u(1)$$

- *Divide the interval* $[0, 1]$ *into equal piece of meshlength* $h = \frac{1}{n+1}$.
- *The goal is to compute approximations* $u_1, \ldots, u_n$ *to the true values* $u(h), \ldots, u(nh)$ *at those* n *meshpoints inside the* $[0, 1]$
- *Finite element equation is*

$$\frac{-u_{i+1} + 2u_i - u_{i-1}}{h^2} = f_i \quad \textit{with fixed ends } u_0 = 0 = u_{n+1}$$

Example: Compare solutions of the differential and difference equations:

$$-\frac{d^2u}{dx^2} = 1 \quad \text{with} \quad u(0) = 0 = u(1)$$
$$\frac{-u_{i+1} + 2u_i - u_{i-1}}{h^2} = 1 \quad \text{with} \quad u_0 = 0 = u_{n+1}$$

[Error Estimate]

- The complete solution has two parts

$$u_{\text{complete}} = \underbrace{u_{\text{particular}}}_{-x^2/2} + \underbrace{u_{\text{nullspace}}}_{Cx+D}$$

- The boundary condition $u(0) = 0 = u(1)$ will determine C and D in the null space part. The exact solution is $u = \frac{1}{2}x - \frac{1}{2}x^2$.
- Finite difference solution is $u_i = \frac{1}{2}(ih - i^2h^2)$.
- Hence, $u_i = u(ih)$: perfect agreement which is unusual!

Example :Compare the differential and difference equations

Compute the error of the difference equations starting from zero slope.

$$(1) \qquad -\frac{d^2u}{dx^2} = 1 \quad with \quad \frac{du}{dx}(0) = 0 \ \& \ u(1) = 0$$

$$(2) \qquad \frac{-u_{i+1}+2u_i-u_{i-1}}{h^2} = 1 with \quad \frac{u_1-u_0}{h} = 0 \ \& \ u_{n+1} = 0$$

[Error Estimate]

- The free-fixed solution of (1) is $u(x) = \frac{1}{2}(1-x^2)$.
- The discrete solution of (2) can be obtained by computing $u = h^2 T_n^{-1} ones$ where

$$T_n = \underbrace{\begin{pmatrix} 1 & 0 & & \\ -1 & 1 & 0 & \\ & \ddots & \ddots & 0 \\ & & -1 & 1 \end{pmatrix}}_{\textbf{backward}} \underbrace{\begin{pmatrix} 1 & -1 & & \\ 0 & 1 & -1 & \\ & \ddots & \ddots & -1 \\ & & 0 & 1 \end{pmatrix}}_{\textbf{-forward}}$$

- Direct computation yields

$$u_i = \frac{1}{2}h^2(n+i)(n+1-i) \qquad \text{where} \quad h = \frac{1}{n+1}$$

Hence,

$$u_i = \frac{1}{2}(1+ih-h)(1-ih) = u(ih) - \underbrace{\frac{h(1-ih)}{2}}_{error}$$

- The first-order error $u_0 - u(0) = -\frac{1}{2}h$ is caused by replacing the zero slope at $x = 0$ by the one-sided condition $u_1 = u_0$.

Example: Is there a way to avoid this $O(h)$ error from the one-side BC $u_1 = u_0$?

Yes. The natural idea is a **centered difference** *by extending the difference equation to $x = 0$:*

$$(u_1 - u_{-1})/2h = 0 \qquad [u'(0) = (u(h) - u(-h))/2h + O(h^2)]$$

For example, consider the function $u(x) = cos(\pi x/2)$ satisfying

$$-u'' = f = (\pi/2)^2 cos(\pi x/2) \quad \text{with} \quad u'(0) = 0, u(1) = 0$$

How close to u are the solutions U and V of the finite difference equations $T_n U = f$ and $T_{n+1} V = g$?

1. h=1/(n+1);u=cos(pi∗(1:n)'∗h/2); c=(pi/2)^ 2; f=c ∗ u;
2. U=h∗h∗T\ f; % **There is a typo. Find it.**
3. e=1-U(1) % First-order error at $x = 0$
4. g=[c/2;f]; T=...; % Create T_{n+1}. Note $g_1 = f(0)/2$. Why?
5. V=h∗h∗T\ g; % Solution $u_0, \ldots, u_n$ with centered condition $u_{-1} = u_1$
6. E=1-V(1) % Second-order error

The term $g = [c/2; f]$ comes from

$$\underbrace{-u_{-1} + 2u_0 - u_1}_{u_{-1}=u_1} = h^2 f_0 \quad \Rightarrow \quad u_0 - u_1 = \frac{1}{2} h^2 f_0$$

Homework: Find typo in 2 & 5.

§1.3 Elimination Leads to $K = LDL^T$

Goal: Solve $Ku = f$

- *Solving a system* $Ku = f$ *is exactly the same as finding* **a combination of the columns of K that produces the vector f.**
- *Our method of computing* $u = K \setminus f$ *(MATLAB) is Gaussian elimination (not Cramer's rule and not determinant!)*
- *The* **symmetric factorization** $\mathrm{K} = \mathrm{LDL^T}$ *takes two steps. First, elimination factors* K *into* LU. *Second, the symmetry of* K *leads to* $U = DL^T$. *The steps from* K *to* U *and back to* K *are by* **lower triangular matrices**-*rows operation on lower rows.*

For example, consider

$$\underbrace{\begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix}\begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \begin{pmatrix} 4 \\ 0 \\ 0 \end{pmatrix}}_{Ku=f} \quad \text{is} \quad \begin{matrix} 2u_1 & -u_2 & & = 4 \\ -u_1 & +2u_2 & -u_3 & = 0 \\ & -u_2 & +2u_3 & = 0 \end{matrix}$$

The solution vector is $u = (3, 2, 1)$. It means

$$\begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix}\begin{pmatrix} 3 \\ 2 \\ 1 \end{pmatrix} = 3\begin{pmatrix} 2 \\ -1 \\ 0 \end{pmatrix} + 2\begin{pmatrix} -1 \\ 2 \\ -1 \end{pmatrix} + 1\begin{pmatrix} 0 \\ -1 \\ 2 \end{pmatrix}$$

When we divide $Ku = (4, 0, 0)^T$ by 4, the right side becomes (1,0,0) which is the first column of I.

$$\text{Column 1 of inverse} \quad \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix}\begin{pmatrix} \frac{3}{4} & * & * \\ \frac{2}{4} & * & * \\ \frac{1}{4} & * & * \end{pmatrix} = \begin{pmatrix} 1 & * & * \\ 0 & * & * \\ 0 & * & * \end{pmatrix} = I$$

If we really want K^{-1}, its columns come from Ku = columns of I. So $K^{-1} = K/I$.

Elimination Produces $K = LU$

Suppose forward elimination use the multipliers in L to change the rows of K into the rows of U (upper triangular). **Then K is factored into L times U.**

$$\underbrace{\begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix}}_{K} = \underbrace{\begin{pmatrix} 1 & 0 & 0 \\ -\frac{1}{2} & 1 & 0 \\ 0 & -\frac{2}{3} & 1 \end{pmatrix}}_{L} \underbrace{\begin{pmatrix} 2 & -1 & 0 \\ 0 & \frac{3}{2} & -1 \\ 0 & 0 & \frac{4}{3} \end{pmatrix}}_{U}$$

The solution step compute $\boldsymbol{c}$ (forward substitution) and then $\boldsymbol{u}$ (back substitution).

$$\begin{aligned} \boldsymbol{Lc} &= \boldsymbol{f} \quad \rightarrow \quad \boldsymbol{c} = \boldsymbol{L}^{-1}\boldsymbol{f} \\ \boldsymbol{Uu} &= \boldsymbol{c} \quad \rightarrow \quad \boldsymbol{u} = \boldsymbol{U}^{-1}\boldsymbol{c} \\ \Rightarrow & \quad \boldsymbol{u} = \boldsymbol{U}^{-1}\boldsymbol{L}^{-1}\boldsymbol{f} = \boldsymbol{K}^{-1}\boldsymbol{f} \end{aligned}$$

Singular Systems When the column has all zeros in the pivot position and below, this is our signal that the matrix is **singular**. It has no inverse.

Example 1

$$C = \begin{pmatrix} \underline{2} & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix} \longrightarrow \begin{pmatrix} \underline{2} & -1 & -1 \\ 0 & \underline{\frac{3}{2}} & -\frac{3}{2} \\ 0 & 0 & 0 \end{pmatrix} = U.$$

In linear algebra, the rows of C are **linearly dependent**. With only two pivots, C is **singular**.

No row exchanges to get n pivots : A is invertible and A=LU.
Row exchanges by P to get n pivots : A is invertible and PA=LU.
No way to find n pivots : A is singular. There is no inverse matrix A^{-1}.

Symmetry Converts $K = LU$ to $K = LDL^T$

Symmetry is lost

$$\underbrace{\begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix}}_{K} = \underbrace{\begin{pmatrix} 1 & & \\ -\frac{1}{2} & 1 & \\ 0 & -\frac{2}{3} & 1 \end{pmatrix}}_{L} \underbrace{\begin{pmatrix} 2 & -1 & 0 \\ & \frac{3}{2} & -1 \\ & & \frac{4}{3} \end{pmatrix}}_{U}$$

The lower factor L has ones on the diagonal. The upper factor U has the pivots. This is unsymmetric, but the symmetry is easy to recover.

Symmetry is recovered

$$K = \begin{pmatrix} 1 & & \\ -\frac{1}{2} & 1 & \\ 0 & -\frac{2}{3} & 1 \end{pmatrix} \begin{pmatrix} 2 & & \\ & \frac{3}{2} & \\ & & \frac{4}{3} \end{pmatrix} \begin{pmatrix} 1 & -\frac{1}{2} & 0 \\ & 1 & \frac{2}{3} \\ & & 1 \end{pmatrix} = LDL^T$$

The product LDL^T is automatically a symmetric matrix, if D is diagonal. More than that, A^TCA is automatically symmetric if C is symmetric. The factor A is not necessarily square and C is not necessarily diagonal.

§1.4 Inverses and Delta function

We are comparing matrix equations with differential equations. One is $Ku = f$, the other is $-u'' = f(x)$. The solutions are vectors u and functions $u(x)$. We consider the case when $f(x) = \delta(x-a)$ which represents a "spike" or a "point load" or an "impulse" concentrated at $x = a$.

In $Ku = f$, take $f = \delta_j$ = j-th column of eye(n).

The solution $u(x, a)$ is the **Green's function**. When we know the Green's function for all point loads $\delta(x-a)$, we can solve $-u'' = f(x)$ for any load $f(x)$.

Example : Solve $-u'' =$ point load

$$-\frac{d^2u}{dx^2} = \delta(x-a) \quad with \quad \begin{cases} u(0) = 0 \ \& \ u(1) = 0 \\ u'(0) = 0 \ \& \ u(1) = 0 \end{cases}$$

[Solution]

The solution u can be decomposed into

$$u(x) = \underbrace{R(x-a)}_{particular\ sol.} + \underbrace{Cx + D}_{sol.\ to\ u''=0}$$

where $R(x-a) = \begin{cases} 0 & \text{for} \quad x \le a \\ x-a & \text{for} \quad x \ge a \end{cases}$ If $u(0) = 0$ & $u(1) = 0$ (fixed ends), the solution is

$$u(x) = -R(x-a) + (1-a)x = \begin{cases} (1-a)x & \text{for} \quad x \le a \\ (1-x)a & \text{for} \quad x \ge a \end{cases}$$

If $u'(0) = 0$ & $u(1) = 0$ (free-fixed), the solution is

$$u(x) = \begin{cases} 1-a & \text{for} \quad x \le a \\ 1-x & \text{for} \quad x \ge a \end{cases}$$

Please note the symmetry between x and a in the two parts. The response at x to a load at a equals the response at a to a load at x. It is the "Green function".

Discrete Vectors : Load and Step and Ramp

The **delta vector** $\boldsymbol{\delta}$: $\boldsymbol{\delta}_{(\cdot)-j} = (\dots, 0, 0, 1, 0, 0, \dots)$

(Its peak is at the position j.)

The **step vector** $\boldsymbol{S}$: $\boldsymbol{S}_{(\cdot)-j} = (\dots, 0, 0, 1, 1, 1, \dots)$

The **ramp vector** $\boldsymbol{R}$: $\boldsymbol{R}_{(\cdot)-j} = (\dots, 0, 0, 0, 1, 2, \dots)$

Example : The Discrete Equations $Ku = \delta_{(\cdot)-j}$ and $Tu = \delta_{(\cdot)-j}$

- *Notations: The $\boldsymbol{\delta}_{(\cdot)-j}$ has component $\boldsymbol{\delta}_{i-j}$, zero except when $i = j$. The shifted step and shifted ramp have components $\boldsymbol{S}_{(\cdot)-j}$ and $\boldsymbol{R}_{(\cdot)-j}$, also centered at j.*

- *If $\boldsymbol{u} = (u_1, \cdots, u_n)^T$ is the solution of the fixed-ends difference equation*

$$-u_{i+1} + 2u_i - u_{i-1} = \delta_{i-j} \quad \textit{with} \quad u_0 = 0 = u_{n+1}$$

then

$$u_i = -R_{i-j} + \left(1 - \frac{j}{n+1}\right) i = \begin{cases} \left(\frac{n+1-j}{n+1}\right) i & \textit{for } i \le j \\ \left(\frac{n+1-i}{n+1}\right) j & \textit{for } i \ge j \end{cases}$$

- *The solution of* **free-fixed** *discrete equation $Tu = \delta_j$ is*

$$u_i = -R_{i-j} + (n + 1 - j) = \begin{cases} \mathrm{n + 1 - j} & \textit{for } i \le j \\ \mathrm{n + 1 - i} & \textit{for } i \ge j \end{cases}$$

The above formulas for the vector $\boldsymbol{u}$ are exactly parallel to Green's functions for the continuous problems.

Green's function and the inverse matrix

If we can solve for point loads, we can solve for any loads.

Why? In the matrix case, this is immediate and worth seeing.

- Any vector $f = [f_1\ f_2\ \cdots\ f_n]^T$ is a combination of n-point loads:

$$f = f_1\delta_1 + \cdots + f_n\delta_n$$

The inverse matrix multiplies each column to combine n-point loads:

$$K^{-1}f = f_1 \underbrace{K^{-1}\delta_1}_{column\ 1} + \cdots + f_n \underbrace{K^{-1}\delta_n}_{column\ n}$$

- In continuous case, the combination gives an integral not a sum. The load $f(x)$ is an integral of point loads $f(a)\delta(x-a)$. Then the solution $u(x)$ is an integral over all a of responses $G(x,a)$ to those loads at each point a:

$$-u''(x) = f(x) = \int_0^1 f(a)\delta(x-a)da$$

is solved by

$$u(x) = \underbrace{\int_0^1 f(a)\ G(x,a)\ da}_{K^{-1}f}$$

where $G(x,a)$ is the Green's function which is the solution of

$$-G''(x-a) = \delta(x-a) \quad with \quad u(0) = 0\ \& u(1) = 0.$$

- The Green's function $G(x,a)$ corresponds to row x and column a to a continuous K^{-1}.

Woodbury-Sherman-Morrison formula will find K^{-1} from T^{-1}.

If $K = T - uv^T$ (rank-one change), then

$$K^{-1} = T^{-1} + \frac{T^{-1}uv^TT^{-1}}{1 - v^TT^{-1}u}$$

§2.1 Equilibrium and Stiffness matrix

$Ku = A^TCAu = f$ is the framework of linear equilibrium. The goal is to understand A and C and the product $K = A^TCA$. In mechanics, K is the stiffness matrix and forces f produce movements u. It will be extended in two directions. One is to escape from linearity. The other is to escape from equilibrium. Ohm's Law and Hooke's Law are close approximation to the truths, but not perfect. Nonlinearity starts to be important when voltages and forces are large. The other major extension is to time-dependent problems (or dynamic problem) such as

$$\frac{du}{dt} = Ku - f \qquad or \qquad M\frac{d^2u}{dt^2} = Ku - f$$

Our system can be changed to a PDE $Ku = \nabla \cdot (c\nabla u)$ with the primary unknown $u = u(x, y, z, t)$.

Example: Fig. 2.1 (a) fixed-fixed problem

Fig. 2.1 (a) shows three masses m_1, m_2, m_3 connected by a line of springs.

- $\mathbf{u} = (u_1, u_2, u_3)^T$=*displacement of the mass*
- $\mathbf{e} = (e_1, e_2, e_3, e_4)^T$=*elongations of springs*
- $\mathbf{w} = (w_1, w_2, w_3, w_4)^T$=*tension in the springs*
- $\mathbf{f} = (f_1, f_2, f_3)^T$=*external forces*

Question: Derive the stiffness matric K, connecting the primary unknown u to the force f.

Answer: Stretching $\mathbf{e} = A\mathbf{u}$, Hooke's Law $\mathbf{w} = C\mathbf{e}$, and balance of forces $A^T\mathbf{w} = \mathbf{f}$ lead to

$$K\mathbf{u} = A^TCA\mathbf{u} = \mathbf{f}\,, \quad A = \underbrace{\begin{pmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & -1 & 1 \\ 0 & 0 & -1 \end{pmatrix}}_{\text{derivative}}, \quad C = \underbrace{\begin{pmatrix} c_1 & & & \\ & c_2 & & \\ & & c_3 & \\ & & & c_4 \end{pmatrix}}_{\text{spring constants}}$$

Minimum Principles. There are two ways to describe the laws of mechanics, by equations and also by minimum principles.

Example: Connection between the equation and the minimum principle.

Question: Explain why $u = K^{-1}f$ minimize the following total potential energy

$$P(u) = \frac{1}{2}u^T Ku - u^T f$$

We can minimize $P(u)$ by solving $\nabla P(u) = 0$. At the minimum, $\nabla P(u) = Ku - f = 0$.
***
$P(u) = \frac{1}{2}u^T Ku - u^T f$ means that the masses lose potential energy by $f^T u$. Equilibrium comes when $\frac{\partial P}{\partial u} = 0$, a little more displacement Δu gives $\Delta P = 0$ (energy gain=energy loss). Note that $P_{min} = P(K^{-1}f) = -\frac{1}{2}f^T u$ is negative. The mass lost potential energy when they were displaced. It is quite interesting that exactly half of that loss is stored in springs as $\frac{1}{2}u^T Ku = \frac{1}{2}u^T f$.

§2.2 : Oscillation by Newton's Law

Compare $F = ma$ with the previous section about equilibrium. There, the mass didn't move since each mass was in balance between the force f and spring force Ku. That balance $F = f - Ku = 0$ is now gone and mass are in motion: $Mu_{tt} = f - Ku$ if we ignore damping or friction.

§2.2.1 : Special Case $u'' + u = 0$: One mass and one spring

Key word: Understanding stability and accuracy on Numerical Algorithm

The general solution is $u = a_1 \cos t + a_2 \sin t$. We can write equation

$$u'' + u = 0 \quad \Rightarrow \quad u' = v \;\; \& \;\; v' = -u$$

Then

$$u(t)^2 + v(t)^2 \quad = \quad \text{a constant}$$

because $\frac{d}{dt}(u(t)^2 + v(t)^2) = 2u'u + 2v'v = 2vu - 2uv = 0.$

Four Finite difference method :

$u'' + u = 0 \quad \Leftrightarrow \quad u' = v \; \& v' = -u$

Question: Compare four FDM **(Forward Euler, Backward Euler, Trapezoidal Method, Leapfrog)** *of*

$$\frac{d}{dt}\begin{pmatrix} u(t) \\ v(t) \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} u(t) \\ v(t) \end{pmatrix}, \qquad \begin{pmatrix} u(0) \\ v(0) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

With each time step $h = \Delta t$,

$$\frac{U_{n+1} - U_n}{h} = \begin{cases} V_n & (* \text{ Forward E.}) \\ V_{n+1} & (\natural \text{ Backward E.}) \\ (V_n + V_{n+1})/2 & (\dagger \text{ Trapezoidal}) \\ V_n & (\ddagger \text{ Leapfrog}) \end{cases}$$

$$\frac{V_{n+1} - V_n}{h} = \begin{cases} -U_n & (* \text{ Forward E.}) \\ -U_{n+1} & (\sharp \text{ Backward E.}) \\ -(U_n + U_{n+1})/2 & (\dagger \text{ Trapezoidal}) \\ -U_{n+1} & (\ddagger \text{ Leapfrog}) \end{cases}$$

- **Forward Euler Method.**

$$\begin{pmatrix} U_{n+1} \\ V_{n+1} \end{pmatrix} = \underbrace{\begin{pmatrix} 1 & h \\ -h & 1 \end{pmatrix}}_{G_F} \begin{pmatrix} U_n \\ V_n \end{pmatrix}, \quad \lambda = 1 \pm ih$$

The growth matrix $G_F = \begin{pmatrix} 1 & h \\ -h & 1 \end{pmatrix}$ at each time step $h = \Delta t$ is officially stable, but $O(h)$ errors are unacceptable. The eigenvalue λ of G_F produces growth since $|\lambda| = |1 \pm ih| > 1$.

- **Backward Euler Method.** The growth matrix is $G_B = \begin{pmatrix} 1 & -h \\ h & 1 \end{pmatrix}^{-1}$.
Hence, its eigenvalue λ produces decay since $|\lambda| = \frac{|1 \pm ih|}{1+h^2} < 1$. See Fig 2.5.

- **Trapezoidal Method.** The growth matrix is

$$G_T = \begin{pmatrix} 1 & -h/2 \\ h/2 & 1 \end{pmatrix}^{-1} \begin{pmatrix} 1 & h/2 \\ -h/2 & 1 \end{pmatrix}$$

Its eigenvalue satisfies $|\lambda| = 1$ and every (U_n, V_n) stays exactly on the circle. Energy is conserved because G_T is orthogonal. See Fig 2.6.

- **Leapfrog Method.** The growth matrix is $G_B = \begin{pmatrix} 1 & h \\ -h & 1 - h^2 \end{pmatrix}$.
Hence, it has also $|\lambda| = 1$, but G_L is an not orthogonal matrix and orbit follows an ellipse. The ellipse comes closer to the circle as $h \to 0$. See Fig 2.7. Leapfrog has a great advantage: **it is explicit.**

- Multiplication by G_T and G_L preserves areas in the phase plane. All triangle from $(0, 0)$ to (U_n, V_n) to (U_{n+1}, V_{n+1}) have the same area. This property is fundamental for sucess in long-time integration.

Key word: Understanding the problem $M\mathbf{u}'' + K\mathbf{u} = \mathbf{f}(t)$

The framework $u \to e \to w \to f$ does not change much when $u(t)$ is measured from equilibrium. But force balance is different. That includes Newton's inertia term along with any applied force $f(t)$:

$$\begin{array}{llcll} \text{oscillations} & \mathbf{u}(t) = (u_1(t), \cdot, u_n(t)) & & \text{force balence} & M\mathbf{u}'' + K\mathbf{u} = \mathbf{f}(t) \\ & A \downarrow & & & \uparrow A^T \\ \text{elongations} & \mathbf{e}(t) = (e_1(t), \cdot, e_n(t)) & \xrightarrow{C} & \text{spring forces} & \mathbf{w}(t) = (w_1(t), \cdot, w_n(t)) \end{array}$$

The all important matrix K is still $A^T C A$.

Special case: $(*)$ $\quad Mu'' + Ku = 0$

Let $M = \begin{pmatrix} m_1 & & \\ & \ddots & \\ & & m_n \end{pmatrix}$ *where* $m_i > 0$. *Assume* K *is a positive definite matrix.*

1. *Show that* $\mathbf{u} = e^{i\omega t}\mathbf{x}$ *is the solution of* $M\mathbf{u}'' + K\mathbf{u} = 0$ *if and only if*
$$M^{-1}K\mathbf{x} = \lambda\mathbf{x}, \qquad \lambda = \omega^2$$
2. *There exist eigenvalues* $\lambda_1, \cdots, \lambda_n > 0$ *and eigenvectors* $\mathbf{x}_1, \cdots, \mathbf{x}_n$ *such that*
$$\mathbf{x}_i^T M \mathbf{x}_j = \delta_{ij} \qquad \& \qquad M^{-1}K\mathbf{x}_j = \lambda_j \mathbf{x}_j$$
3. *Explain why* $(*)$ $M\mathbf{u}'' + K\mathbf{u} = 0$ *has* $2n$ *linearly independent solutions. Find the general solution.*

Answer. (1) Substituting $\mathbf{u} = e^{i\omega t}\mathbf{x}$ into the equation leads to

$$0 = M\mathbf{u}'' + K\mathbf{u} = e^{i\omega t}(-\omega^2 M + K)\mathbf{x} \quad \Rightarrow \quad K\mathbf{x} = \omega^2 M\mathbf{x}$$

Hence, ($\lambda = \omega^2$ is eigenvalue and $\mathbf{x}$ is eigenvector of $M^{-1}K$.)

(2) Since $M^{-1/2}KM^{1/2}$ is symmetric and positive definite, there exist λ_j, y_j such that

$$y_i^T y_j = \delta_{ij}, \qquad M^{-1/2}KM^{1/2}y_j = \lambda_j y_j \qquad (i, j = 1, \cdots, n)$$

Setting $x_j = M^{-1/2}y_j$, we have

$$MKx_j = \lambda x_j, \qquad x_i^T M x_j = y_i^T y_j = \delta_{ij}$$

(3) We know that there exist a unique solution of $\mathbf{u} = (u_1, \cdots, u_n)$ satisfying

$$M\mathrm{u}'' + K\mathrm{u} = 0, \quad \mathrm{u}(0) = \mathrm{a}, \quad \mathrm{u}'(0) = \mathrm{b}.$$

Since we have $2n$ linearly independent choices of $\mathrm{a}, \mathrm{b} \in \mathbb{R}^n$, the problem has $2n$ linearly independent solutions. The general solution is

$$\mathrm{u}(t) = \sum_{i=1}^{n} \left(a_i \cos\sqrt{\lambda_i} t + b_i \sin\sqrt{\lambda_i} t \right) \mathrm{x}_i$$

Example 2: $(*)$ $Mu'' + Ku = 0$: See Figure 2.8 (b)

When $m_1 = 9, m_2 = 1, c_1 = 75, c_2 = 6$ *with fixed-free model(lower end free),*

$$M^{-1}K = \begin{pmatrix} 9 & 0 \\ 0 & 1 \end{pmatrix}^{-1} \begin{pmatrix} 75+6 & -6 \\ -6 & 6 \end{pmatrix} = \begin{pmatrix} 81/9 & -6/9 \\ -6 & 6 \end{pmatrix}$$

The general solution of $M\mathrm{u}'' + K\mathrm{u} = 0$ *is*

$$\mathrm{u}(t) = \left(a_1 \cos\sqrt{5}t + b_1 \sin\sqrt{5}t\right) \begin{pmatrix} 1 \\ 6 \end{pmatrix} + \left(a_2 \cos\sqrt{10}t + b_2 \sin\sqrt{10}t\right) \begin{pmatrix} 2 \\ -3 \end{pmatrix}$$

Question: Explain how the masses move.

Answer. The masses move together in the direction of eigenvector $(1, 6)^T$ with the speed related to the eigenvalue of $\lambda_1 = 5$. The eigenvector $(2, -3)^T$ moves the masses in opposite direction, faster because $\lambda_2 = 10 > \lambda_1 = 5$.

♣ Note that eigenvectors are not orthogonal, but they are $M-$orthogonal:

$$\begin{pmatrix} 1 \\ 6 \end{pmatrix}^T \begin{pmatrix} 2 \\ -3 \end{pmatrix} \neq 0 \quad but \quad \begin{pmatrix} 1 \\ 6 \end{pmatrix}^T M \begin{pmatrix} 2 \\ -3 \end{pmatrix} = 0$$

Standing Waves and Traveling Waves

The point is that a sum of standing waves (up and down, staying in place) produces a traveling waves. A violin string is the limiting case of more masses ($h \to 0$ or $n \to \infty$). The discrete jh becomes a continuous variable x. The discrete $M\mathrm{u}'' + K\mathrm{u} = 0$ becomes the wave equation $mu_{tt} - cu_{xx} = 0$. The normal modes become $\sin(k\pi\sqrt{c/m}t)\sin(k\pi x)$ for any $k = 1, 2, \cdots$

Total Energy is conserved. $Mu''(t) + Ku(t) = 0$

Prove that $Mu''(t) + Ku(t) = 0$ *leads to*

$$\frac{d}{dt}(\text{Kinetic Energy}(KE) + \text{Potenial Energy}(PE)) = 0$$

where

$$KE = \frac{1}{2}(u')^T M u' \quad \& \quad PE = \frac{1}{2}u^T K u$$

Proof.

$$\begin{aligned}
\frac{d}{dt}(KE) &= \frac{1}{2}(u'')^T M u' + \frac{1}{2}(u')^T M u'' \\
&= \frac{1}{2}(-M^{-1}Ku)^T M u' + \frac{1}{2}(u')^T M(-M^{-1}Ku) \\
&= -\frac{d}{dt}(PE)
\end{aligned}$$

√ This is an excellent check on our codes. Any solution $u(t)$ must satisfy

$$\begin{aligned}
&\frac{1}{2}(u'(t))^T M u'(t) + \frac{1}{2}u(t)^T K u(t) \\
&\qquad = \frac{1}{2}(u'(0))^T M u'(0) + \frac{1}{2}u(0)^T K u(0)
\end{aligned}$$

Explicit Finite difference: $Mu''(t) + Ku(t) = f(t)$

We begin with equal time steps Δt, and a centered difference to replace $U''(t)$:

$$U''(t) \approx \frac{U(t+\Delta t) - 2U(t) + U(t-\Delta t)}{(\Delta t)^2}$$

Explicit Finite Difference: Leapfrog method

- $Mu''(t) + Ku(t) = f(t)$ *can be expressed as*

$$M\frac{(U(t+\Delta t) - 2U(t) + U(t-\Delta t))}{(\Delta t)^2} + KU(t) = f(t)$$

- *Writing* $U_n = U(n\Delta t)$,

$$MU_{n+1} = [2M - (\Delta t)^2 K]U_n - MU_{n-1} + (\Delta t)^2 f$$

- *Introducing* $v = u'$, $Mu''(t) + Ku(t) = f(t)$ *becomes*

$$Mv' + Ku = f \qquad \& \qquad u' = v$$

- *Writing* $U_{n+1} - U_n = \Delta t V_{n+\frac{1}{2}}$, *we have first order leapfrog*

$$M\left(V_{n+\frac{1}{2}} - V_{n-\frac{1}{2}}\right) + \Delta t K U_n = \Delta t f$$
$$U_{n+1} - U_n = \Delta t V_{n+\frac{1}{2}}$$

Stability analysis: $Mu''(t) + Ku(t) = 0$

Key word: Stability places on essential limitation on the size of the step Δt.

$u''(t) + M^{-1}Ku(t) = 0$ produce leapfrog

$$(*) \qquad U_{n+1} - 2U_n + U_{n-1} = (\Delta t)^2 M^{-1} K U_n = 0$$

- Recall the example 2:

$$M^{-1}K = \begin{pmatrix} 9 & 0 \\ 0 & 1 \end{pmatrix}^{-1} \begin{pmatrix} 75+6 & -6 \\ -6 & 6 \end{pmatrix} = \begin{pmatrix} 81/9 & -6/9 \\ -6 & 6 \end{pmatrix}$$

  and eigenvalues are $\lambda = 5, 10$. This has the stability limit $\Delta t < 0.632$. $U_n \nearrow \infty$ if $\Delta t > 0.633 = \sqrt{\frac{4}{\lambda_{max}}}$. The slightly smaller step $\Delta t = 0.63$ has no explosion, but output is totally inaccurate. **Why?**

- Starting from $U_0 = x$ where x is an eigenvector $M^{-1}Kx = \lambda x$, look for leapfrog's growth factor in the discrete normal mode $U_n = G^n x$.

- Substituting $U_n = G^n x$ into (*) yields the equation for the growth factor:

$$(**) \qquad G^2 - (2 - \lambda(\Delta t)^2)G - 1 = 0$$

- If α, β are roots of (**), $\alpha + \beta = 2 - \lambda(\Delta t)^2 < 2 \quad \& \quad \alpha\beta = 1$.

- In order that $|\alpha|, |\beta| < 1$, the time step Δt must satisfies

$$\Delta t \le \sqrt{\frac{4}{\lambda}} \qquad \text{for all eigenvalues of } M^{-1}K$$

Implicit Trapezoidal : $u''(t) + M^{-1}Ku(t) = 0$

Aim: Large finite element codes need more stability that leapfrog offers. Discuss the way to remove limitations on Δt.

- Recall

$$Mu''(t)+Ku(t) = 0 \qquad \Leftrightarrow \qquad Mv'+Ku = 0 \quad \& \quad v = u'$$

- Trapezoidal rule for $u' = v$ is

$$U_{n+1} - U_n \approx \int_{n\Delta t}^{(n+1)\Delta t} u'dt \approx \frac{V_{n+1} - V_n}{2}$$

- Trapezoidal rule for $Mv' + Ku = 0 \quad \& \quad v = u'$ is

$$(*) \qquad V_{n+1} - V_n = -\Delta t M^{-1}K\frac{(U_{n+1} + U_n)}{2}$$

$$(**) \qquad U_{n+1} - U_n = \Delta t\frac{(V_{n+1} + V_n)}{2}$$

- Subtracting $(*) \times (V_{n+1} + V_n)^T M$ from $(**) \times (U_{n+1} - U_n)^T K$ gives energy indentity

$$V_{n+1}^T M V_{n+1} + U_{n+1}^T K U_{n+1} = V_n^T M V_n + U_n^T K U_n$$

Hence, energy is unchanged at time $n + 1$.

- The new V_{n+1}, U_{n+1} come from the old V_n, U_n by lock matrix

$$\begin{bmatrix} I & \frac{1}{2\Delta t}B \\ -\frac{\Delta t}{2}I & I \end{bmatrix} \begin{bmatrix} V_{n+1} \\ U_{n+1} \end{bmatrix} = \begin{bmatrix} I & -\frac{1}{2\Delta t}B \\ \frac{\Delta t}{2}I & I \end{bmatrix} \begin{bmatrix} V_n \\ U_n \end{bmatrix}$$

$$\Longrightarrow \begin{bmatrix} B & 0 \\ 0 & B \end{bmatrix} \begin{bmatrix} V_{n+1} \\ U_{n+1} \end{bmatrix} = \begin{bmatrix} I & -\frac{1}{2\Delta t}B \\ \frac{\Delta t}{2}I & I \end{bmatrix}^2 \begin{bmatrix} V_n \\ U_n \end{bmatrix}$$

where $B = \frac{\Delta t^2}{4}M^{-1}K$.