1. MATH547 HOMEWORK 4

Topic: Math@UNC environment

Post date: May 25, 2020 Due date: May 28, 2020

1.1. Background: modeling binary interaction in science and engineering

Many systems consist of point interactions. The iconic Eiffel Tower can be modeled through the trusses linking two points with coordinates $x_i, x_j \in \mathbb{R}^3$. The unit vector along direction from point i to point j is

$$\boldsymbol{l}_{ij} = \frac{\boldsymbol{x}_j - \boldsymbol{x}_i}{\|\boldsymbol{x}_j - \boldsymbol{x}_i\|}.$$

Suppose that structure deformation changes the coordinates to $x_i + u_i$, $x_j + u_j$. The most important structural response is that on point i a force f_{ij} is exerted that can be approximated as

$$f_{ij} = \mathbf{l}_{ij} \mathbf{l}_{ij}^T (\mathbf{u}_i - \mathbf{u}_j),$$

in appropriate physical units. An opposite force $f_{ji} = -f_{ij}$ acts on point j. Note the projector along the truss direction $l_{ij}l_{ij}^T$. Adding forces on a point from all trusses leads to the linear relation

$$f = Ku \tag{1}$$

with $f, u \in \mathbb{R}^m, K \in \mathbb{R}^{m \times m}, d = 3$ the number of dimensions, N the number of points, and m = dN, the number of degrees of freedom of the structure. Point interactions arise in molecular or social interactions, cellular motility, and economic exchange much in the same form (1). The techniques in this homework are equally applicable to physical chemistry, sociology, biology or business management.

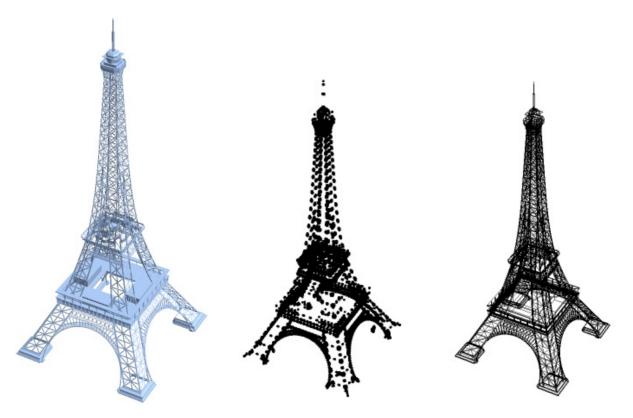


Figure 1. Eiffel Tower models

Load the Eiffel Tower data.

```
octave] cd /home/student/courses/MATH547ML/data/EiffelTower;
load EiffelPoints; X=Expression1; [NX,ndims]=size(X);
load EiffelLines; L=Expression1; [NL,nseg]=size(L);
octave] m=3*NX; disp([NX NX^2 NL m])

26464 700343296 31463 79392
octave]
```

Of the possible $N^2 \cong 7 \times 10^8$ linkages between points in the structure, only $N_l = 31462$ are present. It is wasteful, and often impossible, to store the entire matrix of couplings between points $K \in \mathbb{R}^{m \times m}$ ($m^2 \cong 6 \times 10^9$), but storing only the nonzero elements corresponding to the interacting can be carried out through a *sparse matrix*. After allocating space with spalloc, the matrix is initialized with zeros along the truss directions.

```
octave] K=spalloc(m,m,3*NL);
    for k=1:NL
        i = L(k,1); j = L(k,2);
        p = 3*(i-1)+1; q = 3*(j-1)+1;
        for id=1:3
            for jd=1:3
                K(i+id,j+jd) = 0;
        end;
        end;
        end
octave]
```

The matrix *K* can be formed by loops over the trusses. The following computation takes a few minutes. The matrix *K* has been pre-computed, and can be loaded from a disk file when answering the questions below, rather than executing the following loops.

```
octave] for k=1:NL
    i = L(k,1); j = L(k,2);
    lij = (X(j,:)-X(i,:))'; Pij = lij*lij';
    p = 3*(i-1)+1; q = 3*(j-1)+1;
    for id=1:3
        for jd=1:3
            K(i+id,j+jd) = K(i+id,j+jd) + Pij(id,jd);
        end;
    end;
    end
octave] save "K.mat" K
```

1.2. Theoretical questions

Provide a proof or counter-example for these true or false questions.

1. If **R** is an upper-triangular matrix, its singular values are the same as the diagonal values r_{ii} .

SOLUTION. Counterexample

```
octave] R=[1 1;0 1]
```

R =

- 1 1
- 0 1

```
octave] svd(R)
```

ans =

- 1.61803
- 0.61803

octave]

2. If $A = A^T$, the singular values of A are the same as its eigenvalues.

SOLUTION. Not quite, singular values are positive, while eigenvalues can be negative. Counterexample

A =

- 1 (
- 0 -1

ans =

- 1 -1
- 1 1

octave]

3. If **T** is of full rank, **A** and $\mathbf{B} = \mathbf{T}^{-1}\mathbf{A}\mathbf{T}$ have the same singular values.

SOLUTION. No, counterexample

```
octave] A=[1 2;0 1]; T=[0 2; 1 0]; T1=inv(T); B=T1*A*T; disp([A B])
```

- 1 2 1 0
- 0 1 1 1

```
octave] [svd(A) svd(B)]
```

ans =

- 2.41421 1.61803
- 0.41421 0.61803

octave]

4. For $A, B \in \mathbb{R}^{m \times m}$, the matrices AB and BA have the same eigenvalues.

SOLUTION. Yes. Consider $ABx = \lambda x$, with $x \neq 0$. Compute

$$\lambda \mathbf{B} \mathbf{x} = \mathbf{B} (\lambda \mathbf{x}) = \mathbf{B} (\mathbf{A} \mathbf{B} \mathbf{x}) = (\mathbf{B} \mathbf{A}) (\mathbf{B} \mathbf{x}).$$

Set y = Bx, and obtain

$$(\boldsymbol{B}\boldsymbol{A})\,\mathbf{v}=\lambda\,\mathbf{v},$$

the same eigenvalue as for AB.

1.3. Reduced order modeling

Load data, and define functions to draw the deformed structure.

```
octave] cd /home/student/courses/MATH547ML/data/EiffelTower;
        load EiffelPoints; X=Expression1; [NX,ndims]=size(X);
        load EiffelLines; L=Expression1; [NL,nseg]=size(L);
        m=3*NX; load K;
octave] function drawXu(X,u,L,is)
          clf; view(-30,45); [NX,nd]=size(X);
          [nL,nseg]=size(L); x=[]; y=[]; z=[];
          U=reshape(u,3,NX)';
          for k=1:is:nL
            x=[x X(L(k,1),1)+U(L(k,1),1) X(L(k,2),1)+U(L(k,2),1)];
            y=[y X(L(k,1),2)+U(L(k,1),2) X(L(k,2),2)+U(L(k,2),2)];
            z=[z X(L(k,1),3)+U(L(k,1),3) X(L(k,2),3)+U(L(k,2),3)];
          end;
          plot3(x,y,z);
        end
octave] drawXu(X,zeros(m,1),L,20)
octave] function drawXU(X,U,L,is)
          clf; view(-30,45); [NX,nd]=size(X);
          [nL,nseg]=size(L); x=[]; y=[]; z=[];
          for k=1:is:nL
            x=[x X(L(k,1),1)+U(L(k,1),1) X(L(k,2),1)+U(L(k,2),1)];
            y=[y X(L(k,1),2)+U(L(k,1),2) X(L(k,2),2)+U(L(k,2),2)];
            z=[z X(L(k,1),3)+U(L(k,1),3) X(L(k,2),3)+U(L(k,2),3)];
          end;
          plot3(x,y,z);
octave] drawXU(X,zeros(NX,3),L,20)
octave]
```

The following questions only require a few Octave lines to solve correctly. Be careful to not request output of the large vectors and matrices that arise. Use visualization with the draw function to represent results, and concentrate

on the mathematical formulation. For example, imposing displacement u = (z, 0, 0) at each node, i.e., a horizontal displacement along the x direction proportional to the z coordinate is accomplished by:

```
octave] U=zeros(NX,3); U(1:NX,1)=X(1:NX,3);
octave] drawXU(X,U,L,20)
octave]
```

1.3.1. Least squares solution on singular modes

Find the linear combination s of the first 10 singular modes that best approximates a force $f = (z \cos \theta, z \sin \theta, 0)$ on the structure. Randomly choose θ . Show the first 3 singular modes and the linear combination you find.

SOLUTION. Construct the force at each node, first as an $N \times d$ table, and then as a vector with m = dN components. Check correct representation of the three components of the force as successive elements in a vector.

From the singular value decomposition $K = Y\Sigma Z^T \in \mathbb{R}^{m\times m}$, denote by $Y_k, Z_k \in \mathbb{R}^{m\times k}$ the matrices formed by the first k columns of Y, Z. The matrix Y is a basis for the codomain, and the matrix Z is a basis for the domain of the linear mapping represented by the matrix X. The matrices Y_k, Z_k are therefore bases for subspaces within the codomain, domain, respectively. From the full model f = Ku, obtain a reduced model

$$\mathbf{v} = \mathbf{R}\mathbf{x}, \ \mathbf{x}, \mathbf{v} \in \mathbb{R}^k, \ \mathbf{R} \in \mathbb{R}^{k \times k}$$

with the reduced system matrix defined by

$$\mathbf{R} = \mathbf{Y}_k^T \mathbf{K} \mathbf{Z}_k .$$

(Note: choosing the same reduced basis for approximation, e.g., $g = \mathbf{Z}_k \mathbf{y}$, of both forces and displacements is acceptable but not optimal)

Solution of the reduced model gives an approximation of the solution to the full model

$$f \cong g = Y_k y, u \cong s = Z_k x$$
.

If given a force on the full model, the approximation of the force on the reduced model is obtained as the solution of the least squares problem

$$\min_{\mathbf{y}} \|\mathbf{f} - \mathbf{Y}_k \mathbf{y}\|.$$

Since Y_k has normalized, orthogonal columns, the solution to the least squares problem is $y = Y_k^T f$. Carry out the above steps, through the following five Octave instructions.

```
octave] [Yk,Sigmak,Zk]=svds(K,10);
octave] y=Yk'*f; R=Yk'*K*Zk; x=R\y; s=Zk*x;
```

octavel

Display the requested singular vectors and the approximate solution obtained from the reduced model. The displacements can be scaled to obtain a more comprehensible visualization.

```
octave] cd /home/student/courses/MATH547ML/homework; mkdir hw04; cd hw04
octave] figure(1); drawXu(X,0*Zk(:,1),L,20); print -depsc Fig1a.eps; figure(2);
octave] drawXu(X,250*Zk(:,1),L,20); print -depsc Fig1b.eps
octave] drawXu(X,250*Zk(:,2),L,20); print -depsc Fig1c.eps
octave] drawXu(X,250*Zk(:,3),L,20); print -depsc Fig1d.eps
octave] drawXu(X,5000*s,L,20); print -depsc Fig1e.eps
octave]
```

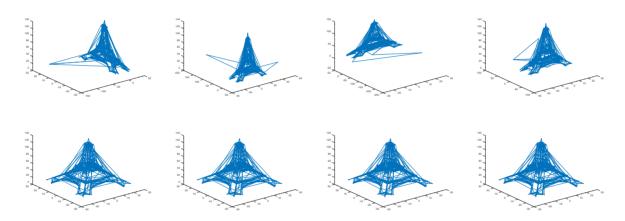


Figure 2. Representation of deformation of the Eiffel Tower. Top row contains first 3 singular vectors, showing "squeezing" of the structure along different spatial directions, and the approximation given by the reduced model solution for a force $f = (z\cos\theta, z\sin\theta, 0)$.

1.3.2. Least squares solution on eigenmodes

Find the linear combination t of the first 10 eigenmodes that best approximates a force $f = (z \cos \theta, z \sin \theta, 0)$ on the structure. Show the first 3 eigenmodes and the linear combination you find.

SOLUTION. The procedure is similar to the previous case, but with a different choice of bases. The eigenvectors are no longer guaranteed to be be orthogonal, so a QR procedure is applied to obtain the reduced model bases. In this case the basis for the domain and codomain are the same.

```
octave] [Vk,Lambdak] = eigs(K,10); [Rk,Tk] = qr(Vk,0);
octave] y = Rk'*f; R = Rk'*K*Rk; x = R\y; t = Rk*x;
octave]
```

Display the requested eigenvectors and the approximate solution obtained from the reduced model. Again, the displacements are scaled to obtain a more comprehensible visualization.

```
octave] cd /home/student/courses/MATH547ML/homework; mkdir hw04; cd hw04
octave] figure(1); drawXu(X,0*Rk(:,1),L,20); print -depsc Fig2a.eps; figure(2);
octave] drawXu(X,250*Rk(:,1),L,20); print -depsc Fig2b.eps
```

```
octave] drawXu(X,250*Rk(:,2),L,20); print -depsc Fig2c.eps
octave] drawXu(X,250*Rk(:,3),L,20); print -depsc Fig2d.eps
octave] drawXu(X,5000*t,L,20); print -depsc Fig2e.eps
octave]
```

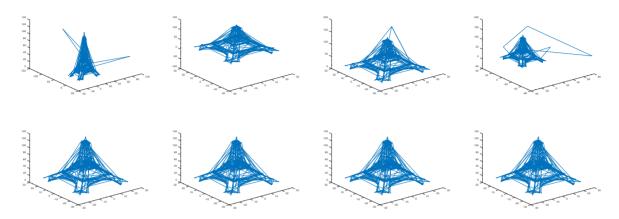


Figure 3. Representation of deformation of the Eiffel Tower. Top row contains first 3 eigenvectors, again showing "squeezing" of the structure along different spatial directions, and the approximation given by the reduced model solution for a force $f = (z\cos\theta, z\sin\theta, 0)$. Note that the eigenmode reduced solution is very different from that obtained from the singular vector model reduction.

1.3.3. Least squares solution on Krylov modes

Replace singular modes or eigenmodes by orthogonal Q, with $QR = [f K f K^2 f ... K^9 f]$ (known as Krylov modes). Find the linear combination w of the first 10 Krylov modes that best approximates a force $f = (z \cos \theta, z \sin \theta, 0)$ on the structure. Show the first 3 Krylov modes and the linear combination you find.

SOLUTION. Again, the procedure is similar, but with a different choice of bases. The Krylov modes must be computed and then orthogonalized. In this case also the basis for the domain and codomain are the same.

```
octave] k=10; Kk = [f];
    for i=2:k
        Kk = [Kk K*Kk(:,i-1)];
    end;
    [Wk,Tk]=qr(Kk,0);

octave] y=Wk'*f; R=Wk'*K*Wk; x=R\y; w=Wk*x;

octave]
```

Display the requested eigenvectors and the approximate solution obtained from the reduced model. Again, the displacements are scaled to obtain a more comprehensible visualization.

```
octave] cd /home/student/courses/MATH547ML/homework; mkdir hw04; cd hw04
octave] figure(1); drawXu(X,0*Wk(:,1),L,20); print -depsc Fig3a.eps; figure(2);
octave] drawXu(X,250*Wk(:,1),L,20); print -depsc Fig3b.eps
octave] drawXu(X,250*Wk(:,2),L,20); print -depsc Fig3c.eps
octave] drawXu(X,250*Wk(:,3),L,20); print -depsc Fig3d.eps
```

octave] drawXu(X,250*w,L,20); print -depsc Fig3e.eps

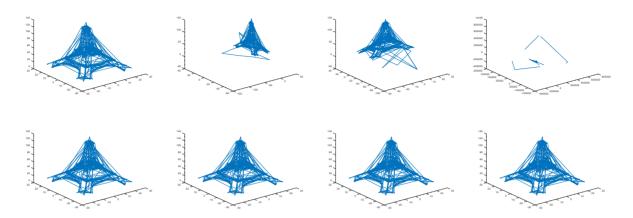


Figure 4. Representation of deformation of the Eiffel Tower. Top row contains first 3 Krylov modes, and the approximation given by the reduced model solution for a force $f = (z \cos \theta, z \sin \theta, 0)$. Note that the Krylov reduced solution does not seem realistic.

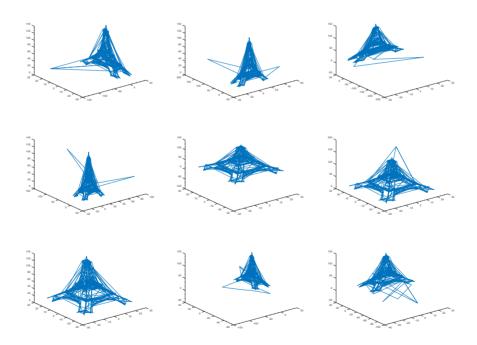


Figure 5. Comparison of the first 3 singular modes (top row), eigenmodes (middle row), Krylov modes (bottom row).

1.3.4. Reduced-rank singular mode approximation

From the SVD $K = Y \Sigma Z^T$ construct an approximate matrix

$$\tilde{\mathbf{K}} = \sum_{k=1}^{n} \sigma_k \mathbf{y}_k \mathbf{z}_k^T$$

and compare the force f with $\tilde{f} = \tilde{K}s$, s from question 1.3.1.

SOLUTION. The previous problem showed the approximate displacement obtained from the reduced model. Here the error in force is estimated

$$\tilde{f} = \tilde{K} s = \left(\sum_{k=1}^{n} \sigma_k y_k z_k^T\right) s = \sum_{k=1}^{n} \sigma_k y_k z_k^T s = \sum_{k=1}^{n} c_k y_k = Y_k c,$$

with $c_k = \sigma_k \mathbf{z}_k^T \mathbf{s}$.

```
octave] c=diag(Sigmak).*Zk'*s;
octave] ftilde=Yk*c;
octave] norm(f-ftilde)/norm(f)
```

ans = 0.99999

octave]

1.3.5. Reduced-rank eigenmode approximation

From the eigendecomposition $KR = R\Lambda$ construct an approximate matrix

$$\tilde{K} = \sum_{k=1}^{n} \lambda_k r_k r_k^T$$

and compare the force f with $\tilde{f} = \tilde{K}t$, t from question 1.3.2.

SOLUTION. Repeat the above procedure, now using eigenmodes,

$$\tilde{f} = \tilde{K} s = \left(\sum_{k=1}^{n} \lambda_k r_k r_k^T\right) t = \sum_{k=1}^{n} \lambda_k r_k r_k^T t = \sum_{k=1}^{n} d_k r_k = R_k d,$$

with $c_k = \sigma_k \mathbf{z}_k^T \mathbf{s}$.

```
octave] d=diag(Lambdak).*Rk'*t;
octave] ftilde=Rk*d;
octave] norm(f-ftilde)/norm(f)
```

ans = 0.99997

octave]

1.3.6. Reduced model convergence

Choose one of the reduced models from 1.3.1 to 1.3.4. Repeat the calculations for 15,20,25 modes, and comment on whether the solutions converge.

SOLUTION. Construct a function to return the error in the force estimation for k modes.

0.99999 0.99997 0.99996 0.99995

octave]

Notice that the relative error

$$\varepsilon_k = \frac{\|\tilde{f}_k - f\|}{\|f\|},$$

is decreasing, albeit slowly. Computation of a larger number of singular values (takes a few minutes to complete) leads to a plot from that indicates

octave] sig=svds(K,100);
octave] plot(log10(sig), 'o'); print -depsc Fig6a.eps
octave] SVDreduced(K,f,40)

ans = 0.99992

octave]