MTH 420/520 Spring 2019 Class notes

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In this class ...

- We describe certain common discrete and continuous models and discuss the corresponding methods

  1. Equilibrium models: SPD systems, minimization of convex functions, basics of the calculus of variations
  2. Regression, and classification: Least Squares, and dimension reduction (SVD, PCA)
  3. Saddle point systems: Lagrange multipliers, constrained optimization
  4. Oscillatory systems and analyses: Fourier analysis and applications

- For each model, students learn the challenges, and derive the methods of analysis and solution

- Students use theory and MATLAB to solve the problem

This class is ...

- NOT a class on (abstract) linear algebra

  but you will use the concepts all the time.

  If needed, please review material from MTH 341. You can also take MTH 342 or MTH 443 to prove some of the facts we use in this class.

- NOT a class on differential equations (ODEs or PDEs)

  but many models will be formulated as ODEs or PDEs

  If needed, please review material from MTH 256. Other classes of interest include MTH 4/582, MTH 621-2-3.

- NOT a physics or chemistry or CS or ... class

  but many models will require intuition from college level classes

- NOT a numerical analysis or programming class ...

  but we will use MATLAB in examples and HW.

  If needed, please consult resources such as

- NOT a machine learning (data science) class

  but you will see some examples and their mathematical models

- NOT a WIC

  but you will be expected to write at the MTH 4XX level. Typing is encouraged!

References and math you will need

- [GS] G. Strang, Introduction to Applied Math, Wellesley-Cambridge, 1986

- [LO] J.D. Logan, "Applied Mathematics", Wiley 1987

- [HA] P.S. Hansen, "Discrete Inverse Problems. Insight and Algorithms", SIAM 2010

- [DL] D.P. O'Leary, "Scientific Computing with Case Studies", SIAM 2009

- [CM] Cleve Moler's books and materials; http://www.mathworks.com/moler/

- [GE] A. Geron, Hands-on Machne Learning with Scikit-Learn & TensorFlow, O'Reilly, 2017

If needing a refresher on MTH 341, please consult https://tinyurl.com/yc8lxz2u. For those interested in the theory behind the concepts, please consult https://www.math.brown.edu/~treil/papers/LADW/LADW_2017-09-04.pdf or https://www.math.ucdavis.edu/~anne/linear_algebra/mat67_course_notes.pdf (some of the material is covered in MTH 342).

You will be expected to work through the examples in these course notes. Please contact the instructor immediately if you are struggling: identify what "math" or "computational skills" you are missing.

Linear algebra notation and MATLAB

We will work primarily in $\mathbb{R}^n$ (as opposed to C^n).

- Column vectors can be written as $u = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$ or $u = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \in \mathbb{R}^3$. In these class
  notes we will blend the latter notation with the shorthand MATLAB
  notation for column vectors `u=[1;2;3]=[1,2,3]'` so we will write
  $u = [1; 2; 3]$ or $u = [1, 2, 3]^T$.
  In turn, $v = [0, -1, 5]$ will denote a row vector so that $v^T = [0; -1; 5]$.
- Dot product (inner product) of $a, b \in \mathbb{R}^3$ is $a^T b = \sum_j a_j b_j$; in MATLAB
  `a'*b`. We will also write $(u, v) = v^T u$. Dot product is symmetric
- Norm of a vector $\|x\|_2$ is the usual Euclidean norm. We will also consider
  alternative norms.
- For matrices, we write $A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}$ as $A = [1, 2, 3; 4, 5, 6]$. In MATLAB
  you can also write the same matrix as `A=[1,2 3;4,5 6]`.

<u>Pbm.</u> I.1 MATLAB expertise. Work through
http://math.oregonstate.edu/~mpesz/teaching/420-520_S19/matlab_intro.html

LA concepts to be fluent in

1 **Vectors:** linearly independent, orthogonal ($u^T v = 0$), orthonormal (if $\|u\| = 1$, basis. Angle between vectors.

> <u>Pbm.</u> I.2 Consider $u = [1,2,0]^T$, $v = [-1,0,5]^T$. Check if (u,v) are linearly independent, orthogonal, orthonormal; check their angle. Find a third vector w if possible so that (u,v,w) is a basis for $\mathbb{R}^3$. Write $a = [2,0,-5]^T$ in this basis. Find a vector $\tilde{v}$ so that $(u,\tilde{v})$ is an orthogonal (orthonormal) set (an orthogonal set spanning $Col(u,\tilde{v})$) ? Repeat for $(u,\tilde{v},\tilde{w})$ for some $\tilde{w}$ that you would determine. Is it possible to do this for $(u,\tilde{v},a,\tilde{w})$? Check how to use MATLAB to check your answers.

2 **Square matrices:** singular, invertible; determinants; inverse matrix. Eigenvalues and eigenvectors. Diagonalizable matrices. *Algebraic multiplicity and geometric multiplicity of an eigenvalue.*

3 **Rectangular matrix** A. Consider $Col(A), Range(A), Ker(A), Null(A)$, A^T. Linear solvable systems, underdetermined and overdetermined systems. (For systems, use some unit vector on the right hand side).

<u>Pbm.</u> I.3 Work with matrices below to practice concepts in (2-3). Use hand calculations and MATLAB.
$A = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}$, $A = \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}$, $A = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$, $A = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$, $A = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$,
$A = \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$. $A = \begin{bmatrix} 3 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$, $A = \begin{bmatrix} 2 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$.

Equilibrium model: spring-mass system

Example I.1 (Spring-mass system)

Variables and coefficients (data and unknowns)

n masses: $m_i, i = 1 \ldots n$, external forces f_i, displacements x_i,
$n + 1$ springs: elasticity constant $c_j; j = 1, \ldots n + 1$; elongations e_j,
internal forces y_j.

Draw a picture.

Model connects data and unknowns with physics laws:

Define $e_j = x_j - x_{j-1}$, use convention $x_0 = 0, x_{n+1} = 0$. ($e = Ax$)
Hooke's law $y_j = c_j e_j$. ($y = Ce$)
Newton's law $f_i + y_{i+1} - y_i = 0$ ($f = A^T y$)

Check.

Count the unknowns and equations. Check dimensions.

Solve the EQ problem

Summarize and solve.

Decide on the unknowns. Choose $x = (x_i)_i$; define $K = A^T C A$.

$$Kx = f. \tag{1}$$

Example I.2 (Equilibrium as minimization)

Equation (1) is related to finding the minimizer of the potential energy function

$$x = \operatorname{argmin} \phi(r), \quad \phi(r) = \tfrac{1}{2} r^T K r - r^T f \tag{2}$$

(Elastic energy $\sum_j \tfrac{1}{2} c_j e_j^2$: each $c_j e_j^2$ arises from the work of internal force ce done on the stretch de; integrate $\int cede$; balanced by the external work on the masses $\sum_i x_i f_i$).

Analyze: are (1) and (2) solvable? Are they equivalent?

Yes and yes.
We show this later via the spd property of the matrix K.

Other equilibrium (stationary) models with structure as in (1)

Example I.3 (Models in 1d)

Heat conduction. Diffusion equation. (Linear) elasticity. Electric circuits. Flow in porous media.

Pbm. I.4 Connect the laws below to the applications. What are the unknowns? Are they constitutive or balance laws?

Energy conservation. Darcy's law. Fourier's law. Fick's law.
Kirchoff's law. Hooke's law. Ohm's law. Mass conservation.

Example I.4 (Discrete (network) models)

Primary variables: scalar, defined at the nodes of a network, connected by an incidence matrix A (representing a directed graph or a network)
Secondary variables: fluxes. defined on the edges.

Connect them by constitutive and balance laws.
Summarize. Analyze. Solve.

Does the order ("direction" in network) matter?

Example I.5 (Spring-mass system, revisited)

Rewrite constitutive equations for spring-mass system changing the signs in some of the definitions of e_j. (or the interpretation of x_i or of f_i). For example, write $e_2 = x_1 - x_2$ instead of $e_2 = x_2 - x_1$.

Check properties of matrix K. Better yet: check the entries!

Solve the problem, apply the new interpretation of x_i, y_j, f_i.

Convince yourself that the physical solution does not depend on the signs you prescribed in your definitions.

<u>Pbm.</u> I.5 What if there are no walls? One wall only?

Example I.6 (Network)

Draw a triangle with vertices $1, 2, 3$; assign to these some "potential" values x_1, x_2, x_3, and some sources f_1, f_2, f_3. Assign some direction to the edges e_1, e_2, e_3. Write the model, with appropriate definitions of e_j given by the direction of the edges (e.g., if edge e_1 is from node 1 to 2, write $e_1 = -x_1 + x_2$). Also, write $y_j = c_j e_j$ for every edge. Close with balance laws $f_i = \dots$ (total flow in minus total flow out).

Check properties of the matrix K. Is the problem $Kx = f$ solvable?

Redo the problem by changing the direction of the edges. The matrix K should not change.

The problem is not solvable unless we fix (ground) one of x_i. Apply and redo.

Symmetric positive definite matrices

Definition I.7

$A \in \mathbb{R}^{n \times n}$ is symmetric if

$$A = A^T \tag{3}$$

Let $A \in \mathbb{R}^{n \times n}$ be symmetric. It is positive definite (spd) if

$$x^T A x > 0, \forall x \in \mathbb{R}^n, x \neq 0. \tag{4}$$

One can also define semidefinite (nonnegative definite) matrices.
These satisfy $x^T A x \geq 0$.

Pbm. I.6 Work out conditions that guarantee that $A \in \mathbb{R}^{2 \times 2}$ is spd,
using the definition (4).

Hint: start by assuming $A = \begin{bmatrix} a & b \\ b & c \end{bmatrix}$ *with some* $a, b, c \in \mathbb{R}$.

Write out what $x^T A x$ *is. Now, how do you guarantee the inequality (4) holds for
any* x? *Find the conditions on* a, b, c.

Answer: We must have $a > 0$, and $ac - b^2 > 0$.

Characterization of spd matrices

Assume $A = A^T$.

Theorem I.8 (Characterization of spd matrices (a-b))

(a) *A is spd iff its leading principal minors are all positive
(this connects to the pivots found during LU decomposition)*

The kth leading principal minor of a matrix is the determinant of its upper-left $k \times k$ submatrix.

(b) *A is spd iff its eigenvalues are all positive
(this connects to diagonalization of A and an equivalent inner product on $\mathbb{R}^n$).*

Recall the connection between the eigenvalues, the trace, and the determinant of the matrix, i.e., $\lambda_1 + \lambda_2 = \ldots$ and $\lambda_1 \lambda_2 = \ldots$.

<u>Pbm.</u> I.7 Determine the conditions that guarantee that $A \in \mathbb{R}^{2 \times 2}$ is spd using the characterization (a) and (b). Compare to the conditions you found in Pbm I.6.

Spd matrix and convexity

Recall the concept of functions on $\mathbb{R}$ that are "convex up" from calculus. Generalize this concept to $\mathbb{R}^n$.
(It can be also generalized to functionals = functions of functions).

Definition I.9

$\phi : V \to \mathbb{R}$ is strictly convex if its graph lies always strictly below its secants, or

$$\phi(tx + (1-t)y) < t\phi(x) + (1-t)\phi(y), \quad \forall t \in (0,1), \ \forall x, y \in \mathbb{R}^n. \quad (5)$$

The vector $tx + (1-t)y$ is called a convex combination of x, y.

Pbm. I.8 Start with $n = 1$. Convince yourself that $\phi(x) = ax^2$ is convex using (5), as long as $a > 0$. What happens if $a = 0$? What about $ax^2 + dx + f$?

Pbm. I.9 Consider $A = [a, 0; 0, c]$ and $\phi(x) = ax_1^2 + cx_2^2$. What conditions on a, c guarantee that $\phi(\cdot)$ is convex?

Convexity and spd condition, cd

Consider again a general $A \in \mathbb{R}^{n \times n}$ with $A = A^T$.

Theorem I.10 (Another characterization of spd $A = A^T$ is spd.)

(c) *A is spd iff the function $\phi(x) = x^T A x$ is strictly convex.*

<u>Pbm.</u> I. 10   Determine the conditions that guarantee that $A \in \mathbb{R}^{2 \times 2}$ is spd using the characterization (c).

Hint: there is a lot of algebra involved. Write out $\phi(x)$ and check the convexity condition (5).

<u>Pbm.</u> I. 11   Recall multivariable calculus problem: checking for the extreme values of $\phi(x) = ax_1^2 + 2bx_1x_2 + cx_2^2 + dx_1 + ex_2 + f$.
Write the equations to find the critical point.

The second derivative of ϕ is the Hessian $D^2\phi = \begin{bmatrix} a & b \\ b & c \end{bmatrix}$. What conditions guarantee that you have a minimum of ϕ at the critical point?

Compare with Pbm.I 6.

We will not be proving the general case $\mathbb{R}^{n \times n}$.

Back to the equilibrium model (1) and (2)

Now we want to know if the problem (1) is well-posed, i.e. that it has a solution, and that the solution is unique. We also want to known the connection between (1) and (2).

First, check that $K = A^T CA$ is spd, as long as C and A are full rank.

Pbm. I.12 Show that for any nonsingular diagonal matrix C, $A^T CA$ is symmetric.

Next show it is nonnegative definite.

Now assume that C and A in the equilibrium problem are full rank.

Conclude K is of full rank. Show directly that K is spd.

Calculations on previous slides suggest now that $\phi(x)$ defined by (2) is convex.

Thus we must find its critical point, the same as its minimizer.

Pbm. I.13 Follow the calculations to convince yourself that the critical point of $\phi(\cdot)$ is $x : Kx = f$ ((1) holds).

In the end, since K is spd, it is nonsingular, and (1) has a unique solution. We also find that (1) is equivalent to (2).

Discrete vs continuum models for our example

Let $n \to \infty$ (springs $\to$ rod)

Displacements x_i, $i = 1, \ldots n$.
Fix $x_0 = 0, x_{n+1} = 0$
Elongation e_j
Difference $e_i = x_i - x_{i-1}$
Hooke's law $y_j = c_j e_j$
...
Model ((1))
$Kx = f$

Displacements $u(x)$, $x \in (0, l)$.
Boundary conditions $u(0) = 0, u(l) = 0$.
Strain e
Derivative $e = \frac{d}{dx}u$
Stress-strain $\sigma = ce$
...
Model (limit of (1)) we get

$$-\frac{d}{dx}\left(c(x)\frac{d}{dx}u(x)\right) = f \qquad (6)$$

Example I.11 (Beyond 1 spatial dimension)

In more than one spatial dimension the model becomes

$$-\nabla \cdot (c\nabla u) = f, \ x \in \Omega \qquad (7)$$

and requires boundary conditions on $\partial\Omega$.

Continuous problem cast as a minimization

In the discrete spring-mass model (or other such stationary model) recall that (1) defines the minimizer for (2).
What about the continuous model (6)?

Define $J(u) = \int_0^l \frac{1}{2}c(u')^2 - fu$. It is known that (6) defines the minimizer of $J(\cdot)$ over the set of sufficiently smooth functions satisfying $u(0) = u(l) = 0$. The equation (6) is the so-called Euler-Lagrange equation for the functional $J(\cdot)$.

To derive the Euler-Lagrange equations for some $J(\cdot)$, we proceed as follows. Calculate the first variation of $J(\cdot)$ $\frac{1}{t}(J(u + tv) - J(u))$, and take a limit (if possible) as $t \to 0$. Interpret this quantity $J'(u)(v)$ as the directional (Gateau) derivative of J at u in the direction of v.

Set $J'(u)(v) = 0$ for any v. Work (by integration by parts) to identify the equation that the minimizer u must satisfy.

Details in variational calculus: spaces and boundary conditions

Define space of functions $V = C_0^2 = C^2[0,1] \cap \{v : v(0) = 0 = v(1)\}$.

Example I.12 (Minimize $J(u) = \int_0^1 (u')^2 - fu$ over V)

Following the strategy outlined above, (recall $v \in V$)

$$J'(u)(v) = \int_0^1 u'v' - fv = 0.$$

Integrating by parts and using boundary conditions we obtain

$$\int_0^1 (-u'' - f)v = 0$$

Use FLCV (below) to conclude $-u'' = f$. Apply BC to solve for u.

Lemma I.13 (FLCV (Fundamental Lemma of Calculus of Variations))

If $\phi(\cdot) \in C^0[a,b]$ and $\int_a^b \phi(x)\psi(x)dx = 0$ for every $\psi \in C_0^2[a,b]$, then $\phi(x) = 0$, $\forall x \in [a,b]$.

Different BC

Example I.14 (Same functional, different V)

Consider $\int_0^1 (u')^2 - fu$ over $V = C^2[0,1] \cap \{v : v(0) = 0\}$.
Following calculations as above we derive ...

$$\int_0^1 (-u'' - f)v + u'(1)v(1) = 0 \tag{8}$$

Now test this equation with v which happens to satisfy $v(1) = 0$. We conclude $-u'' = f$. From this it follows from (8) that $u'(1)v(1) = 0$ regardless what the value of $v(1)$ is, i.e., $u'(1) = 0$ (this is the natural or Neumann condition).

Pbm. I. 14 Follow the Euler-Lagrange strategy for ϕ defined in (2). You should get (1).

Pbm. I. 15 Follow the Euler-Lagrange strategy for $J(u) = \int_0^1 \frac{1}{2}u^2 - u$ for $u \in C^2[0,1]$. What is the extremal?

Try also $J(u) = \int_0^1 \frac{1}{2}e^x(u')^2 - sin(x)u$.

Generalizations of Euler-Lagrange equations

The general form of Euler-Lagrange equations for the functional
$J(u) = \int_a^b L(x, u(x), u'(x))dx$ over $u \in C^2[a, b], u(a) = A, u(b) = B$ is

$$L_u - \frac{d}{dx}L_{u'} = 0. \qquad (9)$$

Its solution, the critical point of $J(\cdot)$ is called the stationary solution, since the equation provides the necessary but not always the sufficient condition for the minimum.
The difficulty most of the time is not deriving the EL equations, but rather solving them.

These equations can be generalized to $\mathbb{R}^d$, $d > 1$, to higher order derivatives, and multiple functions.

Pbm. I.16 Classical examples include the brachistochrone problem, minimal surface problem, Fermat problem in geometrical optics, the Plateau problem, and systems of reaction-diffusion equations. Look these up and discuss (for extra credit).

Convexity of functionals

Above you have gained some working experience with $J(u)$, for $u \in V = C^2[a, b]$.

We call $J(\cdot)$ a functional (i.e., a function of functions with values in $\mathbb{R}$).

Recall the definition of convexity (5) which we now restate for functionals and say that $J : V \to \mathbb{R}$ is convex if

$$J(tu + (1 - t)v) < tJ(u) + (1 - t)J(v), \quad \forall t \in (0, 1), \ \forall u, v \in V. \quad (10)$$

<u>Pbm.</u> I. 17 Show that $J(u) = \int_0^1 u^2$ is convex. What about the Dirichlet functional $J(u) = \int_0^1 \frac{1}{2}(u')^2? - uf$?

One can prove that if a functional is convex (and if some additional conditions hold), then its extremal found by Euler-Lagrange equations is the minimizer of the functional.

Norms and inner products

Recall $x \cdot y = y^T x = \sum_i x_i y_i$ is the "dot product" or scalar product of two vectors $x, y \in \mathbb{R}^n$. This notion is extended to any vector space V, and denoted by (x, y), for $x, y \in V$.

An inner product on any space V (with scalars in $\mathbb{R}$) should be symmetric, bilinear, and positive definite. (A more general notion is defined on $\mathbb{C}^n$ and with scalars in $\mathbb{C}$.)

Euclidean norm of a vector $\|x\|_2 = \sqrt{x^T x} = \sqrt{(x,x)} = \sqrt{\sum x_i^2}$. (Sometimes we skip the subscript "2").

Pbm. II.1 Check if $(x,y)_{my} = \sum 2x_i y_i$ is an inner product. Also, for what $A \in \mathbb{R}^{2 \times 2}$, is $(x,y)_{yours} = y^T A x$ an inner product?
(Answer to the second: A must be spd).

Example II.1 (Inner product space of functions)

For $f, g \in V = C[0,1]$, define $(f,g) = \int_0^1 f(x)g(x)dx$.

Pbm. II.2 Check that the inner product for functions satisfies the desired properties.

Least squares (LSQ) and normal equations

Consider some data $(x_i, y_i)_{i=1}^n$, with $n \geq 2$. Assume that there is a linear trend $y_i \approx \theta x_i + b$. We try to identify this trend i.e., to find θ, b.

This is known as a "linear regression" problem, or "linear least squares". In machine learning, b is called a "bias" and θ is called a feature weight, and (x_i, y_i) are known as training data.

To find θ, b, we see that the system of equations $y_i = \theta x_i + b$ is overdetermined, thus there is no solution. We can, however, try to minimize $\| y - (\theta x + b) \|$.
If the norm is Euclidean, this is the LSQ problem, where we minimize $\| y - (\theta x + b) \|_2^2$, or try to find

$$\text{argmin} \quad \phi([\theta, b]) = \sum_i (y_i - \theta x_i - b)^2. \tag{11}$$

<u>Pbm.</u> II.3 Use calculus to find the minimizer of $\phi([\theta, b])$.

Definition II.2 (The LSQ solution to an overdetermined pbm $Au \approx f$)

is the solution $\hat{u}$ to the normal equations (well-posed if A is full rank)

$$A^T A \hat{u} = A^T f \tag{12}$$

<u>Pbm.</u> II.4 Set $u = [\theta, b]^T$ and find A for (11) to be framed as $Au \approx f$.
<u>Pbm.</u> II.5 Set $u = [\theta; b]$, write $\phi(u)$ as $u^T K u + \dots$ for some K, and work out by hand its minimizer. Is $\phi(u)$ convex ?

Examples of LSQ

Example II.3 (LSQ in MATLAB)

Given the following data `t=[0.5, 1.5, 2, 5]; b = [3.1 6.8 10.3 25];`, solve
the least squares problem for $x = [a; c]$ fitting the data (t, b) to the linear model
$b = at + c$.

  (i) Setup the matrix A and right hand side f.
 (ii) Solve for x: `x=A\ f;` Compare with the use of normal equations.
(iii) Plot the curve and mark the points.
        `plot(t,b,'*',t,a*t+c,'-');legend('data','linear fit');`

MATLAB function `polyfit` can be used to achieve the same as what you did in A.
Learn how, and compare to A. Try the quadratic model $b = at^2 + dt + c$ next.

Example II.4 (Nonlinear data fitting)

Use data from Ex. II.3 for the model $b = ce^{at}$ describing the concentration of
microbes that are growing with rate a in time t, with initial condition c. Can you
use linear LSQ ? What if you knew a and wanted c ? What if you knew c and
wanted a ? How can you combine these two ?
`Pbm.` II. 6 Provide details why this exponential model might be a good
model. Can you think of an appropriate differential equation describing
microbe growth ?
`Pbm.` II. 7 Learn how to use lsqnonlin (MATLAB) and apply to this example.

Examples. Beyond normal equations

Instead of the linear (strictly speaking, affine) model $y = \theta x + b$, one can have a multi-linear model $y = \sum_{k=1}^{K} \theta_k X_k + b$, where X_k are different variables (features), and θ_k are feature weights. (Typically b is set as θ_0, with $X_0 = 1$.)

Example II.5 ("Quality of life" model)

One can predict "happiness" y depending on variable X_1 which is the GDP/capita in a country, and variable X_2 which is the mean annual temperature in that country.

See data in `http:/goo.gl/OEht9W` and `http:/goo.gl/j1MSKe`

If the number of variables K is really large, solving normal equations directly is not advantageous. One uses instead the QR algorithm, or an iterative algorithm such as a gradient based method.

Once the linear model is found, ... we can use this model to predict the output y for some new inputs x (or X). This is called "interpolation" or "extrapolation".

<u>Ex.</u> For example, we can predict the ``happiness'' for a country knowing its temperature and GDP/capita.

Orthogonal projections and LSQ

Recall how you calculate a projection $\hat{v}$ of a vector v on the direction of another vector q of unit length. The length of the projection is $\|\hat{v}\| = (q, v) = v^T q$, and the projection vector $\hat{v} = q(v, q) = qq^T v$.

If q is not of unit length, we replace q by $\frac{q}{\|q\|}$ in the calculations. We obtain

$$\hat{v} = \frac{q}{\|q\|} \frac{q^T}{\|q\|} v = \ldots = q(q^T q)^{-1} q^T v. \tag{13}$$

Pbm. II.8 Work out the formula for the projection of vector v on the space spanned by several orthogonal vectors $q_1, q_2, \ldots$ forming matrix Q.
Answer: $\hat{v} = QQ^T v = \sum_j q_j (v, q_j)$.
Repeat for the case when q_j form Q of full rank, but which is not orthogonal. Answer:

$$\hat{v} = Q(Q^T Q)^{-1} Q^T v = \sum_j q_j \frac{1}{(q_j, q_j)} (v, q_j). \tag{14}$$

The coefficients (q_j, v) of expansion of $\hat{v}$ in the basis of columns of Q are sometimes called Fourier coefficients.

Another way to find the LSQ solution to $Au \approx f$ is to realize that this problem has no solution unless f is the column space of A. So we calculate a projection $\hat{f}$ of f onto $Col(A)$, and then solve $A\hat{u} = \hat{f}$. This gives the LSQ solution (if A has full rank)

$$\hat{u} = (A^T A)^{-1} A^T f, \tag{15}$$

LSQ via pseudo-inverse A^+

Here we assume again that A is not square but has full rank.

Definition II.6 (Pseudo-inverse for a full rank matrix $A \in \mathbb{R}^{m \times n}$, with $m \geq n$ is)

$$A^+ = (A^T A)^{-1} A^T. \tag{16}$$

Notice this is the matrix appearing in (15) so that $\hat{u} = A^+ f$.

Pbm. II.9 Find pseudo-inverse for $A = [1,1]^T$, $A = [1,1]$.
If A is invertible, show that $A^+ = A^{-1}$.

In practice, we never form the pseudo-inverse when solving least-squares.
Pseudo-inverse is formed using SVD (Singular Value Decomposition), defined below.

Dimension reduction via SVD aka PCA

The SVD (singular value decomposition) can be found for every matrix. Assume $\mathbb{R}^{m \times n} \times A$ has rank r. Then one can find

$$A = U\Sigma V^T. \tag{17}$$

Here $U \in \mathbb{R}^{m \times m}, V \in \mathbb{R}^{n \times n}$ are orthogonal matrices, and $\Sigma \in \mathbb{R}^{m \times n}$ includes a diagonal $n \times n$ matrix of r nonzero singular values $\sigma_1 \geq \sigma_2 \geq \ldots \sigma_r \geq 0$. followed by zeros on the diagonal, and padded by zeros.

If $A = A^T$, then $V = U$. What about Σ if A is spd?

How to find SVD

(i) Calculate $K = A^T A$, find its eigenvalues $\sigma_1^2 \geq \sigma_2^2 \geq \ldots \sigma_n^2 \geq 0$, and the corresponding eigenvectors $v_1, v_2, \ldots$. Recall $Kv_j = \sigma_j^2 v_j$.

(ii) Find the columns $u_j = \frac{1}{\sigma_j} Av_j$ in U for each nonzero σ_j.

(iii) Check the dimensions of V and U. If not enough vectors u_j, augment by additional columns so U is orthogonal.

Once SVD (17) is known, we can calculate its pseudo-inverse $A^+ = V\Sigma^+ U^T$. Here Σ^+ contains the reciprocals of the nonzero singular values of A in Σ.

Pbm. II.10 Calculate SVD and A^+ for the matrices from Pbm.I 3. For A of full rank, check that A^+ via SVD is the same as in (16).

Using SVD for dimension reduction

With (17) we can write A as a sum of rank-1 matrices. In this context, SVD is also known as PCA (Principal Component Analysis)

$$A = \sum_{j=1}^{r} \sigma_j u_j v_j^T \approx \sum_{j=1}^{K} \sigma_j u_j v_j^T = \tilde{A}. \tag{18}$$

This approximation (Eckart-Young Theorem) is the best among all matrices of rank K, r: it minimizes the Frobenius norm of $A - \tilde{A}$.

<u>Pbm.</u> II. 11 Convince yourself that each uv^T is rank 1. Then use orthogonality of U and of V to show the first identity in (18).

In addition to full SVD (17), one also considers thin ($U_n, \Sigma_n \in \mathbb{R}^{n \times n}$), compact (thin without the zero singular values), and truncated versions (only $\sigma_1, \ldots \sigma_K$).

Example II.7 (Dimension reduction for images)

A now classical application of SVD is when $A \in \mathbb{R}^{n \times m}$ represent pixels of an image. A reduced version of the image in (18) can be transmitted **much** faster than A when $K << r$.

This is mathematically related to the Eckart-Young theorem.

Karhunen-Loeve and statistical meaning of PCA

SVD = PCA(Principal Component Analysis)

If the rows of data matrix A are vectors of observations and have zero mean, then $A^T A \sim$ covariance matrix which measures the correlation between variables. (Recall $cov(A) = \frac{1}{n-1} \sum_{j=1}^{n} (a_i - \mu)(a_j - \mu)$).

```
A = [3 -4 7 1 -4 -3; 7 -6 8 -1 -1 -7], mean(A,2)
cov(A'), A*A'/5
```

Example II.8 (Independent stochastic realizations of data)

Another related application of SVD (PCA) is the Karhunen-Loeve decomposition (via Mercer's therem) which allows to create random realizations of images close to A but which maintain a structure *statistically* similar to A.

MATLAB illustration: rows of A hold observations of amount of rain per month
```
rain= [20 25 23 18 20 15 5 2 2 4 12 15];
% generate some random data with mean "rain"
randn('seed',0); for k=1:10 raindata(k,:)=rain+randn(1,12);end;
clf; hold on; for k=1:10 plot(raindata(k,:));end; hold off; % treat this as original data
% calculate sample mean and covariance
randave=sum(raindata,1)/10; clf; cc = cov(raindata); [u,s,v]=svd(cc); rmat = sqrt(s)*v';
% plot new random independent realizations of the same data
plot(randave'+rmat*randn(12,1))
```

Singular Value Expansion=SVD in continuous setting

Example II.9 (Seeking a burried treasure)

Assume that a treasure of mass density $f(t)$ is burried D feet below surface.
Horizontal position of the treasure is measured in t, and of the receiver in s; the
distance of f from g is $|s - t|$. The source f does not move, but we can move the
receiver as much as necessary. The vertical component of gravity g produced by f
is given by (best derived with a picture)

$dg = \frac{\sin(\theta)}{r^2} f(t) dt \implies g(s) = \int_0^1 \frac{D}{(D^2+(s-t)^2)^{3/2}} f(t) dt.$

This is a special case of Fredholm integral equation

$$\int_0^1 K(s,t) f(t) dt = g(s). \tag{19}$$

Its discrete form can be derived, e.g., as $Kg = f$, e.g., by numerical integration or
by *collocation*

$$\sum_j K(s_i, t_j) f(t_j) = g(s_i). \tag{20}$$

Pbm. II. 12 Describe what challenges you see in solving (20) or $Kg = f$.
Start with dimensions: the number of observations versus the resolution
at which you seek $f(t)$.

Sensitivity of inverse problems

The problem: given f, calculate g, is a "forward" problem.
The problem: given g, find f, is known as an "inverse problem". One can analyze its solvability using the SVE $K(s,t) = \sum_{m=1}^{\infty} \mu_m u_m(s) v_m(t)$. If many μ_m are zero or close to 0, the problem is ill-posed.

In general, you have to use some form of LSQ to solve (20). The main difficulty is that we may not have a full rank matrix K, thus $K^T K$ is singular, and we cannot form K^+ with (16). Instead, we form it via SVD $K^+ = U\Sigma^+ V^T$, where Σ^+ contains only the inverses of nonzero singular values.

Example II.10 (Bar-code reading)

Another example giving rise to (19) is barcode reading. The original signal $f(t)$ is piecewise constant (0 for white) and (1 for black). Due to imperfections of the barcode and of a scanner, we get a blurry signal $g(s)$ which is given by (19) with $K(s,t) = exp(-\frac{(t-s)^2}{\sigma^2})$, where σ is a constant which depends on the accuracy of a scanner.

Both examples Ex. II.10 and Ex. II.9 have the kernel $K(s,t)$ in the "convolution" form, so that $K(s,t)$ only depends on $s - t$. Solving the inverse problem with such a kernel is called "deconvolution".

Further inverse problem examples

<u>Pbm.</u> II. 13 Play with different values of σ in Ex. II.10 and of D in
Ex. II.9 to understand the sensitivity of solutions. Assume a piecewise
constant input $f(t)$, and study the shape of the output $g(s)$ depending on
D and σ. **Hint:** this should be done numerically.

The pseudo-inverse K^+ mentioned above is defined with SVD. One can show it is
a limit of regularizations of the rank-deficient LSQ problems where, instead of
solving argmin $\|Kx - f\|^2$, we seek

$$\text{argmin } \|Kx - f\|^2 + \alpha \|x\|^2. \tag{21}$$

Yet another example of an inverse problem which requires regularization is *image
deblurring*.

Example II.11 (Deblurring)

Given K, and f, find the solution x to argmin $\|Kx - f\|^2 + \alpha \|x\|^2$. Here x is the
unknown image (pixel by pixel value representing greyscale), and K is the blurring
or compression transformation. The regularization parameter α is chosen to
smooth out the process, since $K^T K$ might be close to singular.

Google Page Rank using eigenvectors

PageRank of web network

When using web search, you type a keyword and get a list of web urls in a certain order known as PageRank, a measure of popularity (# of links to that url).

Example II.12 (Class website)

Consider the following set of 3 web pages for a class.
Page 1 has a link to page 2 with HW, and page 3 with extra resources, and to page 4, class Canvas website. Page 2 has a link to page 4, Canvas website. Page 3 lists various extra resources, but has no links. Page 4 is the class CANVAS website which links back to Page 1.

We encode this network in adjacency network with $A_{ij} = 1$ if there is a link from page j to page i. We can also create a transition matrix G which tells us how likely we are to go from node j to i, i.e., we encode the probabilities that a random user will choose a particular outgoing link. This matrix has a property that its columns have sum 1, and therefore it is called a stochastic matrix. Finally we account for the fact that someone can just randomly land on any of the nodes, with probability α.

Page rank, cd

We obtain

$$
A = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{bmatrix} ;\ G = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0.5 & 0 & 0 & 0 \\ 0.3 & 0 & 0 & 0 \\ 0.2 & 1 & 0 & 0 \end{bmatrix} ;\ \mathrm{One} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix} \tag{22}
$$

From this we calculate matrix $M = (1-\alpha)G + \frac{\alpha}{4}\mathrm{One}$.

Pbm. II.14 Show that M a stochastic matrix.

Example II.13 (Finding PageRank)

One can prove that M has the leading eigenvalue 1. The corresponding eigenvector (normalized) is called the PageRank. How to find it?
Consider a random vector r^0 whose entries are positive and have sum 1. (In Matlab you can generate one using `r0=rand(4,1);r0=r0/sum(r0);`). Calculate Mr^0, M^2r^0,...$M^{131}r^0$,.... After each step you can normalize the result so it has sum 1. (Your result is the PageRank vector.).

Pbm. II.15 Why does the algorithm in Ex. II.13 work? Explain.

Pbm. II.16 What happens if $\alpha = 0$?, i.e., when $M = G$. Can you find an initial vector r^0 for which the PageRank is the zero vector? What does this mean algebraically?

The theory behind this example is the Perron-Frobenius theorem. The computation of PageRank is essentially the so-called *power method* *for finding the dominant eigenvalue of a matrix.*

Use SVD for classification in data science

Example II.14 (Projections: eigenfaces)

Approximation in inner product spaces

Recall that when given a subspace $V_N = span(Q_N)$, with $Q_N = span\{q_1, \ldots q_N\}$ of dimension N of some inner product space V, the best approximation $\tilde{u}_N = \sum_j u_j q_j$ to $u \in V$ is found as the orthogonal projection which satisfies

$$(u - \tilde{u}_N, q_j) = 0, \quad \forall j = 1, \ldots N. \tag{23}$$

<u>Pbm.</u> III. 1   Show $\tilde{u}_N = \text{argmin}_{v \in V_N} \phi(v)$ with $\phi(v) = \|u - v\|^2$.

If u is known, we can find $\tilde{U}_N$ using projections; see Pbm.II. 8.
The ideal situation is when the basis Q_N is orthogonal, and when the following is satisfied that $Q_1 \subset Q_2 \subset \ldots Q_N \subset \ldots$ basis for V. (This approach is known as the Galerkin method).

What if we do not "know" u?
For example, of interest is the case when u is a solution to $Au = f$, some high dimensional problem. We want to approximate u without knowing it.
One convenient way to solve this problem is when q_j are eigenvectors of A (with the corresponding λ_j). If they are orthogonal, then we can calculate $u_j = \frac{f_j}{\lambda_j}$, and we have

$$u = \sum_j u_j q_j \approx \sum_{j=1}^N u_j q_j = \tilde{u}_N \tag{24}$$

Eigenfunctions and approximating BVP

Recall the boundary value problems which describe equilibria (stationary heat conduction, mechanical equilibria, potential flow). In particular, recall Ex. I.12. We have to solve

$$- u'' = f, x \in (0,1), \ u(0) = 0 = u(1). \tag{25}$$

The goal is to approximate u by some $\tilde{u}_N$. We pursue the ideas expressed above.

First we identify A as "the operator $-\frac{d^2}{dx^2}$ with the homogeneous Dirichlet boundary conditions".
Next we find its eigenvalues λ and eigenfunctions $q(x)$ so that
$Aq = \lambda q$. We find $\lambda_j = (j\pi)^2$ and $q_j(x) = sin(j\pi x)$ for $j = 1, 2, \ldots$.
Next we check if $\{q_j\}_j$ is an orthogonal basis. (Some trig tricks are useful here.) It might also be useful to normalize q_j.
Finally we calculate $f_j = \frac{1}{(q_j, q_j)}(f, q_j)$, and apply (24) to get $\tilde{u}_N$.

There is a lot of deep math hidden above. In particular, we have not addressed the space spanned by all q_j (this is the so called space $L^2(0,1)$). In addition, we did not address the question how to prove that $\lim_{N \to \infty} \tilde{u}_N = u$.

Other examples

Next we want to consider the general case, of Fourier series expansions of any square-integrable function $u \in L^2(-\pi, \pi)$. We find that the general basis we need are the functions used in the following Fourier series expansion

$$
u(x) \approx \tilde{u}_N(x) \quad = \quad \frac{a_0}{2} + \sum_{j=1}^{N} a_j \cos(jx) + b_j \sin(jx), \tag{26a}
$$

$$
a_j \quad = \quad \frac{1}{\pi} \int_{-\pi}^{\pi} u(x) \cos(jx) dx, \quad j \geq 0, \tag{26b}
$$

$$
b_j \quad = \quad \frac{1}{\pi} \int_{-\pi}^{\pi} u(x) \sin(jx) dx, \quad j \geq 1. \tag{26c}
$$

<u>Pbm.</u> III. 2 This example is easily extended to $u \in L^2(-L, L)$, with $L > 0$. Complete the expansion and formulas.

<u>Pbm.</u> III. 3 Calculate the expansions of $u(x) = 1$, $u(x) = x$, $u(x) = x^2$, $u(x) = \sin(5\pi x) - \frac{1}{2}\cos(3\pi x)$, all on $(-1, 1)$. Separately consider the expansions of $u(x) = \text{sgn}(x)$, and $u(x) = |x|$.

<u>Pbm.</u> III. 4 Complete the matching of f1, f2, ...f6 to F1, F2, ...F6 as given in class worksheet.

Application of Fourier analysis

First we extend (25) and use Fourier series to solve a boundary value problem for the differential equation of heat conduction, with constant heat conductivity k, given as

$$-\frac{d}{dx}(k\frac{du}{dx}) = f, \ \ x \in (0, \pi); \ \ u(0) = 0, u(\pi) = 0. \tag{27}$$

for the temperature $u(x)$. We seek u_j so that

$$u(x) = \sum_{j=1}^{\infty} u_j \sin(jx) \tag{28}$$

Let f be given on $(0, \pi)$, and assume we know its Fourier series $f = \sum_j f_j \sin(nx)$.
Pbm. III.5 Write the formula for f_j. Find u_j so that $u(x)$ given by (28) solves (27). Now find $G(x, y)$ so that $u(x) = \int_0^\pi G(x, y) f(y) dy$.
The function $G(\cdot, \cdot)$ is known as the Green's function for (27); it plays a similar role to A^{-1} in $Au = f$.
Pbm. III.6 Calculate $-k\frac{d^2 G}{dx^2}$ to get an expression for Fourier series resembling the Dirac δ. Solve $-kG'' = \delta$ directly to get a different formula for G.

Transient heat conduction

If the heat conduction problem is transient, but we have f as above, we extend (27) to

$$cu_t - \frac{\partial}{\partial x}(k\frac{\partial u}{\partial x}) = f, \ \ x \in (0,\pi), u(0,t) = u(\pi,t) = 0 \tag{29}$$

supplemented by the initial condition $u(x,0) = u_{init}(x)$. Now it is natural to expect that

$$u(x,t) = \sum_{j=1}^{\infty} u_j(t)\sin(jx) \tag{30}$$

Pbm. III.7 Find $u_j(t)$ so that $u(x,t)$ given by (30) solves (29). You can assume first that $f_j = 0$ but $u_j(0) \neq 0$. Next assume $f_j \neq 0$ but $u_j(0) = 0$. Finally combine these two steps and exploit linearity of the equation. Or solve all at once.

More general context of solving this problem is known as the "method of separation of variables".

Wave equation, vibrations, and sound

Finally, we consider the wave equation

$$u_{tt} - c^2 u_{xx} = 0, \ \ x \in (0, \pi), u(0, t) = u(\pi, t) = 0 \tag{31}$$

supplemented by the initial conditions
$u(x, 0) = u_{init}(x), u_t(x, 0) = v_{init}(x).$

<u>Pbm.</u> III.8 Find equations which define $u_j(t)$ so that $u(x, t)$ given by (30)
solves (31).

The wave equation (31) models longitudinal vibrations of an elastic
rod discussed in Module I. It is also a linearized model for vibrations
of a string.
These vibrations have a certain amplitude (which is time-dependent),
and frequency (reciprocal of the period $T = \pi/j$ of vibrations) (which
is not time dependent).
Human ear can hear these vibrations if they have frequency between
20Hz and 20kHz.

MATLAB sounds

The frequency 220 in the example below corresponds to the note "A" in music (in the same octave as the "middle C"). The frequency 330 is "E". Doubling the frequency produces a sound one octave higher. The octave is divided 12 semitones, and is called an octave because it is made os seven intervals (of not equal length).

```
t=linspace(0,2*pi,2000);s=sin(220*t);sound(s)
%%
for f=[262 294 330 349 392 440 466 524],
   s=sin(f*t);
   plot(t,s);sound(s);pause;
end
```

Pbm. III.9 Does everything sound all right to your ear? Experiment trying to fix what is not right.
Now do the math. Report on the ratios of frequencies that you observe in this C major scale.
The major triad in C scale has frequency ratio 1, $3/2$, and $5/4$.
Identify these frequencies.
Pbm. III.10 Transcribe your favorite tune to a vector similar to f.

Provide the code in MATLAB to share with class.

Use Fourier transform for images and such

Above we discussed Fourier series. The coefficients of projection of the function $f(x)$ on the basis functions of Fourier basis are the f_j (or a_j, b_j, with $j = 1, \dots \infty$). Alternative formulation of (26) is with complex coefficients

$$f(x) = \sum_{j=-\infty}^{\infty} c_j e^{ijx} \qquad (32)$$

Here the basis functions are the complex valued functions $(e^{ijx}), j = 1, \dots \infty$.

Different Fourier series, integrals, and transforms

Fourier series for periodic $f(x), x \in (-\pi, \pi) \to c_j$ with $j = 1, \infty$

Fourier integral (transform) $f(x), x \in (-\infty, \infty) \to \hat{F}(\xi), \xi \in (-\infty, \infty)$

Discrete Fourier transform, $f_k = f(x_k), x_k = k\frac{2\pi}{n}, k = 0, 1, \dots n - 1 \to c_j$ with $j = 0, 1, \dots n - 1$

Example III.1 (How to find DFT)

Consider $n = 4$, and try to find the Fourier coefficients c_0, c_1, c_2, c_3 to match $c_0 + c_1 e^{ix} + c_2 e^{2ix} + c_3 e^{3ix}$ with the values f_0, f_1, f_2, f_3 given as some $f_n = f(x_n)$, and $x_0 = 0, x_1 = \frac{\pi}{2}, x_2 = \pi, x_3 = 3\frac{\pi}{2}$. Set it up as $Ac = f$.

Pbm. III.11 Practice with complex matrices in MATLAB and confirm the property $A^{-1} = \frac{1}{4}\overline{A}$ by hand calculation and in MATLAB.

FFT = Fast Fourier Transform

In Example III.1 we consider a linear algebra problem seeking c so that $Ac = f$. The trick is to notice the amazing property that

$$A^{-1} = \frac{1}{4}\overline{A}. \tag{33}$$

This property extends to any symmetric matrix F whose entries are (powers of) the roots of unity. Specifically, we have that for a given $n \geq 1$, if $w^n = 1$, then $w = e^{2\pi/n}$ and $1 + w + w^2 + \ldots w^{n-1} = 0$.

The (j, k) entry of the matrix F has entries w^{jk}. ($j = 0, 1, \ldots n - 1$, $k = 0, 1, \ldots n - 1$.)

Solving for c can be done extremely fast because of the (hierarchical) structure of this matrix. In addition to (33), the multiplication by F can be done in fewer than $n \log_2 n$ operations with an algorithm known as FFT.

(Fast Fourier Transform)

These properties helps, e.g., to solve very quickly problems such as the Poisson's equation $-\Delta u = f$ on simple regions, since the problem can be converted to FFT and the use of matrix F.

Pbm. III.12 For a demonstration and activity on Fourier image analysis, see http://math.oregonstate.edu/~mpesz/teaching/420-520_S19/fft.html

Optimization