Lecture Notes for MtSE 688 "Mathematical and statistical methods..."

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Abstract

These lecture notes will contain some theoretical material related to Kreyszig, 9th ed. (*abbreviated* KR) , which is the main textbook. Notes for all lectures will be kept in a single file and the table of contents will be automatically updated so that each time you can print out only the updated part.

The *Mathematica* appendix is included for reference; you do not have to print it out since there will be other files which illustrate how this program works.

Please report any typos to vitaly@oak.njit.edu

Contents

I. INTRODUCTION

This course contains more topics than a rigorous 1-semester mathematical course. As a result, we will spend less time on rigorous proofs and definitions and more time on qualitative discussions, examples and problem solving (by hand, and using *Mathematica*). However, not to loose contact with math, you are expected to complete reading assignments - indicated as *READING: ...* below. Do not expect to understand everything, but it is always useful to have a idea of the more general picture, even if a bit faint. Occasional sections which do require an in-depth analysis will be indicated as **work-through: ...** .

Homeworks are important part of the course; if done by hand they must be clearly written in pen (black or blue), if done using *Mathematica* they must be printed out as a clear hard copy (adding neat hand-written corrections on this hard copy is ok). No electronic submissions of *Mathematica* notebooks will be accepted.

II. THE *MATHEMATICA* PROGRAM AND REVIEW OF INTRODUCTORY MATH

Introduction to *Mathematica* is described in a separate file "IntroToMathematica.doc" (see also Appendix A). The examples refer to numbers and elemetary functions, which should not cause any difficulties. For complex numbers here is an (optional) reading assignment: *READING: KR, Ch. 13., Sects. 1-4 & 5-7.* You are not expected to be experts in analytical functions at this point, but rather should understand that the definition of the derivative

$$\frac{df}{dz} = \lim_{\Delta z \to 0} \frac{f(z + \Delta z) - f(z)}{\Delta z} \tag{1}$$

which looks very similar to what you used for real numbers, is a very strong requirement on $f(z)$ since *any* Δz, including complex ones can be used and the limit is expected to remain the same (!).

HW: *reproduce the Mathematica output described in the file "IntroToMathematica.doc" , slightly changing the input functions compared to what we discussed in class. Print out your notebook.*

HW: *KR, p. 707, 16.1: 15, 18, 20. Find the 1st 3 terms in each case. Do not worry about region of convergence (although evaluating the distance to the nearest singularity can be instructive). Laurent is like Taylor, but includes singular terms (negative powers) - is given by the same* **Series** *command in Mathematica. Plot any of the functions together with its 3-term approximation*

Introduction (cont.)

- Solving linear systems of equations; the **Solve** command
- Lists in *Mathematica*
- pure functions

see 688_intro2.doc for Solve and 688_intro2.nb for lists and pure functions.

A. Solving linear equations: The Wheatstone bridge

A general idea how to write Kirchoff's equations is given in Example 2, p. 290 in KR (you will not need Gauss elimination since we will using *Mathematica* where it is already implemented). Specifically, we consider Kirchoff's equations for a Wheatstone bridge (details will be discussed in class). Resistors r_1 and r_3 make the upper branch and r_2 and r_4 the lower; the midpoints of the two branches are connected by r_5. The system is connected to a $1-V$ battery; the goal is to find the equivqlent resistance r_{eq} . Steps:

- assign currents $i_1, \ldots, i_5$
- select loops, enough to cover every element in the circuit
- write the loop equations
- write the junction equation
- solve the equations to find currents
- voltage of the battery over total current will be equivalent resistance
- check the limits

For example, let all three loops contain the battery, the 1st one includes also the upper branch, the 2d the lower branch and the 3d loops includes resistors r_1, r_5 and r_4. Currents $i_1, \ldots, i_5$ will have the same indexes as the resistors. Then one has the loop equations:

$$
\begin{aligned}
i_1 r_1 + i_3 r_3 &= 1 \qquad (2)\\
i_2 r_2 + i_4 r_4 &= 1\\
i_1 r_1 + i_5 r_5 + i_4 r_4 &= 1
\end{aligned}
$$

The two junctions on both ends of r_5 will give

$$i_5 = i_1 - i_3 \tag{3}$$

$$i_5 = i_4 - i_2$$

(see 688_intro2.doc with full *Mathematica* realisation)

Note: the matrix of coefficients which appears in the equations must be non-singular.

READING: KR: Ch. 7.3

HW: *KR: p. 295, Nos. 1,9,14,15,17,18*

III. LINEAR ALGEBRA, VECTORS AND MATRICES

READING: KR: Ch. 7, Ch.8.1,8.3

work-through: all examples discussed in 688_vec.nb and 688_matrix.nb; Ch. 8.1

Note on notation and terminology:
following traditional confusion in engineering literature, KR uses "scalar multiplication" to indicate the product of a vector (matrix) by a scalar. This is hard to justify since such multiplication is trivial and hardly deserves a separate name. We will use the convention in mathematical (and physics) books where "scalar product" is equivalent to dot (or inner product) of two vectors and *results* in a scalar.

Next, KR defines "vector" as a "matrix with only one row and column" (p.274), while in fact "vector" is an object which obeys certain transformation rules (see below). More precise are his further clarifications for row (column) vectors, and whenever he is talking about a "vector" in connection with matrices it should be understood as a "row vector" or a "column vectors" depending on the context.

A. Vectors

A *vector* is characterized by the following *three* properties:

- has a magnitude
- has direction (Equivalently, has several components in a selected system of coordinates).
- obeys certain addition rules ("rule of parallelogram"). (Equivalently, components of a vector are transformed according to certain rules if the system of coordinates is rotated).

This is in contrast to a *scalar*, which has only magnitude and which is *not* changed when a system of coordinates is rotated.

How do we know which physical quantity is a vector, which is a scalar and which is neither? From experiment (of course). More general objects are *tensors* of higher rank, which transform in more compicated way. Vector is tensor of a first rank and scalr - tensor of zero rank. Just as vector is represented by a row (column) of numbers, tensor of 2d rank is represented by a matrix. (although matrices also appear indifferent contexes, e.g. for systems of linear equations).

1. *Single vector*

Consider a vector $\vec{a}$ with components a_x and a_y (let's talk 2D for a while). There is an associated scalar, namely the magnitude (or length) given by the Pythagoras theorem

$$a \equiv |\vec{a}| = \sqrt{a_x^2 + a_y^2} \tag{4}$$

Note that for a different system of coordinates with axes x', y' the components $a_{x'}$ and $a_{y'}$ can be very different, but the length in eq. (4) , obviously, will not change, which just means that it is a scalar.

Another operation allowed on a single vector is multiplication by a scalar. Note that the physical dimension ("units") of the resulting vector can be different from the original, as in $\vec{F} = m\vec{a}$.

2. *Two vectors: addition*

For two vectors, $\vec{a}$ and $\vec{b}$ one can define their sum $\vec{c} = \vec{a} + \vec{b}$ with components

$$c_x = a_x + b_x \ , \quad c_y = a_y + b_y \tag{5}$$

The magnitude of $\vec{c}$ then follows from eq. (4). Note that physical dimensions of $\vec{a}$ and $\vec{b}$ must be identical.

3. *Two vectors: scalar product*

If $\vec{a}$ and $\vec{b}$ make an angle ϕ with each other, their scalar (dotted) product is defined as $\vec{a} \cdot \vec{b} = ab\cos(\phi)$, or in components

$$\vec{a} \cdot \vec{b} = a_x b_x + a_y b_y \tag{6}$$

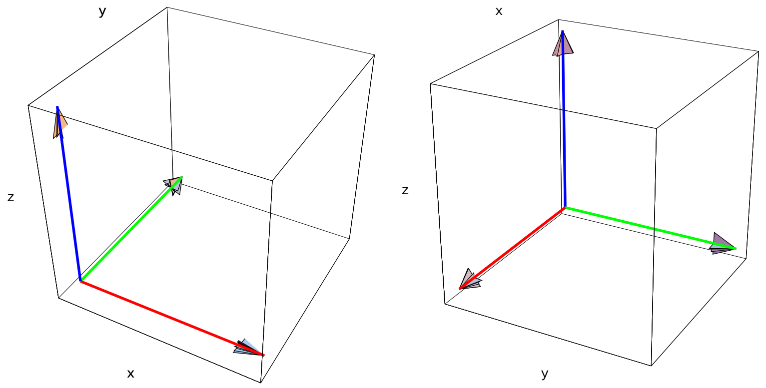

FIG. 1: The correct, "right-hand" systems of coordinates. Checkpoint - curl fingers of the RIGHT hand from x (red) to y (green), then the thumb should point into the z direction (blue). (Note that axes labeling of the figures is outside of the boxes, not necessarily near the corresponding axes.

A different system of coordinates can be used, with different individual components but with the same result. For two orthogonal vectors $\vec{a} \cdot \vec{b} = 0$. The main application of the scalar product is the concept of work $\Delta W = \vec{F} \cdot \Delta\vec{r}$, with $\Delta\vec{r}$ being the displacement. Force which is perpendicular to displacement does not work!

4. Two vectors: vector product

At this point we must proceed to the 3D space. Important here is the correct system of coordinates, as in Fig. 1. You can rotate the system of coordinates any way you like, but you cannot reflect it in a mirror (which would switch right and left hands). If $\vec{a}$ and $\vec{b}$ make an angle $\phi \leq 180^o$ with each other, their vector (cross) product $\vec{c} = \vec{a} \times \vec{b}$ has a magnitude $c = ab\sin(\phi)$. The direction is defined as perpendicular to both $\vec{a}$ and $\vec{b}$ using the following rule: curl the fingers of the right hand from $\vec{a}$ to $\vec{b}$ in the shortest direction (i.e., the angle must be smaller than 180^o). Then the thumb points in the $\vec{c}$ direction. Check with Fig. 2.

Changing the order changes the sign, $\vec{b} \times \vec{a} = -\vec{a} \times \vec{b}$. In particular, $\vec{a} \times \vec{a} = \vec{0}$. More generally, the cross product is zero for any two parallel vectors.

Suppose now a system of coordinates is introduced with unit vectors $\hat{\imath}$, $\hat{\jmath}$ and $\hat{k}$ pointing in the x, y and z directions, respectively. First of all, if $\hat{\imath}$, $\hat{\jmath}, \hat{k}$ are written "in a ring", the cross product of any two of them equals the third one in clockwise direction, i.e. $\hat{\imath} \times \hat{\jmath} = \hat{k}$,

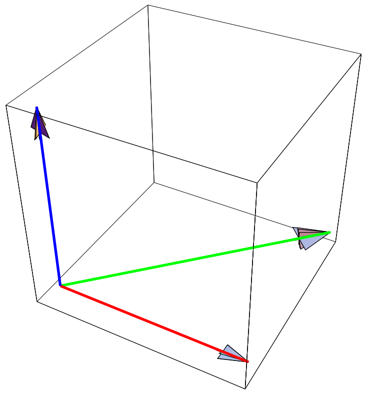

FIG. 2: Example of a cross product $\vec{c}$ (blue) = $\vec{a}$ (red) $\times$ $\vec{b}$ (green). (If you have no colors, $\vec{c}$ is vertical in the example, $\vec{a}$ is along the front edge to lower right, $\vec{b}$ is diagonal).

$\hat{j} \times \hat{k} = \hat{\imath}$, etc. (check this for Fig. 1 !). More generally, the cross product is now expressed as a 3-by-3 determinant

$$\vec{a} \times \vec{b} = \begin{vmatrix} \hat{\imath} & \hat{j} & \hat{k} \\ a_x & a_y & a_z \\ b_x & b_y & b_z \end{vmatrix} = \hat{\imath} \begin{vmatrix} a_y & a_z \\ b_y & b_z \end{vmatrix} - \hat{j} \begin{vmatrix} a_x & a_z \\ b_x & b_z \end{vmatrix} + \hat{k} \begin{vmatrix} a_x & a_y \\ b_x & b_y \end{vmatrix} \tag{7}$$

The two-by-two determinants can be easily expanded. In practice, there will be many zeroes, so calculations are not too hard.

B. Rotational matrix

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix} \cdot \begin{pmatrix} x \\ y \end{pmatrix} \tag{8}$$

HW: *Show that det* $[A_{rot}] = 1$

HW: *Show that rows are orthogonal to each other* **HW:** *For selected* ϕ *(or in a general form) find the eigenvalues - they will be complex. Show that their absolute values are* 1 *and that they are conjugate.* **HW:** *write a "reflection matrix" which reflects with respect to the y-axes. Make a plot similar to rotation - see 688_vec.nb*

C. Matrices

1. Rectangular matrices, product

Examples of matrices, vector-rows and vector columns. Index-free notations. Innner and outer product. Transposition. Special matrices (identity, diagonal, symmetric, skew-symmetric, triangular, stochastic). **HW:** *KR: p. 277, 7,8; p. 286, 1,11,14*

2. Rank of a matrix

Definition. Equivalence of row and column rank.
Vector space: *if* $\vec{a}$ *and* $\vec{b}$ *part of v.s., then* $\alpha\vec{a}+\beta\vec{b}$ *also....* Dimension, basis.

HW: *KR: p. 301. 1-6, 14,21*

3. Linear systems of equations

Submatrix and augmented matrix.
$dim(A) = m \times n$, $dim\,(\vec{x}) = n$

$$\hat{A} \cdot \vec{x} = \vec{b} \tag{9}$$

a) existence: if $rank(A) = rank\left(\tilde{A}\right)$, $\tilde{A} \equiv \left(A|\vec{b}\right)$
b) uniqueness: if $rank(A) = rank\left(\tilde{A}\right) = n$
c) if $rank(A) = rank\left(\tilde{A}\right) = r < n$ - infinitely many solutions. Values of $n-r$ variables can be chosen arbitrary.

Homogeneous system:

$$\hat{A} \cdot \vec{x} = \vec{0} \tag{10}$$

a) alvays has a trivial solution $\vec{x} = \vec{0}$
b) if $rank(A) = n$ this solution is unique
c) if $rank(A) = r < n$ non-trivial solutions exist which form a vector space -*null* space- (together with $\vec{x} = \vec{0}$) with $dim = n - r$.

For $m < n$ (fewer equations than unknowns) - always non-trivial solution.

4. *Determinants*

Explicit calculations. Operations with columns. Minor.

Square $n \times n$ matrix:

$$rank(A) < n \iff det(A) = 0 \tag{11}$$

Applications to linear equations. Cramer's rule: $x_1 = D_1/D, \ldots$.

Other properties:

$$det(A.B) = det(B.A) = det(A)det(B) \tag{12}$$

HW: *KR. p. 314. 5,6,7,18 (use Cramer's rule - check with Mathematica).*

5. *Inverse of a matrix*

$$\det(A) \neq 0$$

$$\left(A^{-1}\right)_{jk} = \frac{1}{det(A)}(-1)^{j+k}M_{kj} \tag{13}$$

(note different order!) **HW:** *find inverse of a 2×2 matrix with elements a, b, c, d. KR: p. 322, 2,3, 7*

D. The eigenvalue problem

$$\hat{A} \cdot \vec{x} = \lambda\vec{x} \tag{14}$$

$$\left(\hat{A} - \lambda\hat{I}\right) \cdot \vec{x} = \vec{0} \tag{15}$$

Thus,

$$det\left(\hat{A} - \lambda\hat{I}\right) = 0 \tag{16}$$

HW: *p. 338, 1 -6*

1. *Spectrum*

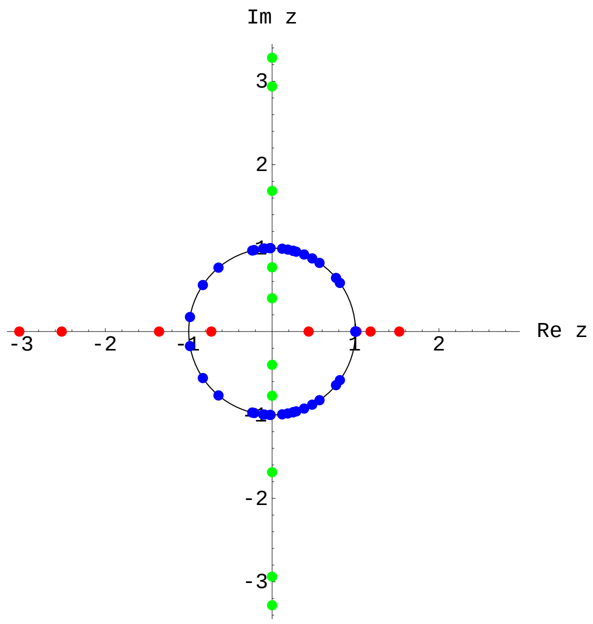

FIG. 3: Typical spectra of an orthogonal (blue), symmetric (red) and skew-symmetric (green) matrices. See 688_matrix.nb.

Dr. Vitaly A. Shneidman, Phys/MtSE 688, 4th Lecture

E. Eigenvectors

READING: KR., sect. 8.4 + 688_matrix2.nb

Eigenvectrors corresponding to distinct eigenvectors are orthogonal. This is true for both symmetric and orthogonal matrices. However, for orthogonal matrices the eigenvalues, and hence the eigenvectors will be complex. The definiton of the inner (dot) product then needs to be generalised:

$$\vec{a} \cdot \vec{b} = \sum_{i}^{N} \bar{a}_i b_i \tag{17}$$

where bar determines complex conjugation.

HW: *KR., p. 355, 1-3 (eigenvectors only)*

F. Similarity transformation

$$\tilde{A} = P^{-1} \cdot A \cdot P \tag{18}$$

with non-singular P.

Theorem 3 $\tilde{A}$ has the same eigenvalues as A and eigenvectors $P^{-1}\vec{x}$ where $\vec{x}$ is an eigenvector of A.

work-through: KR., example 3 on p. 351; reproduce it with Mathematica + examples in 688_matrix2.nb

G. Diagonalization by similarity transformation

Let $\vec{x}_1\,,\vec{x}_2\,,\ldots\,\vec{x}_n$ be eigenvectors of an $n \times n$ matrix A with eigenvalues $\lambda_1\,,\ldots\,,\lambda_n$. Construct a matrix X with $\vec{x}_1\,,\vec{x}_2\,,\ldots\,\vec{x}_n$ as its columns. Then

$$D = X^{-1} \cdot A \cdot X = \mathrm{diag}\,[\lambda_1\,,\ldots\,,\lambda_n] \tag{19}$$

HW: *KR., p. 355, 1-3 (complete diagonalization); 4-6*

1. *Specifics of symmetric matrices*

If matrix A is symmetric, matrix X is orthonormal (or can be made such if normalised eigenvectors

$$\vec{e}_i = \frac{\vec{x}_i}{\sqrt{\vec{x}_i \cdot \vec{x}_i}}$$

are used). Then,

$$D = X^T \cdot A \cdot X \tag{20}$$

(orthogonal transformation) gives a diagonal matrix.

Major application: Quadratic forms

$$Q = \vec{x} \cdot A \cdot \vec{x} = \sum_{ij}^{n} x_i A_{ij} x_j \tag{21}$$

(a scalar!). With

$$y = X^T \cdot x \tag{22}$$

one gets

$$Q = \vec{y} \cdot D \cdot y = \lambda_1 y_1^2 + \ldots + \lambda_n y_n^2 \tag{23}$$

H. Applications of matrix techniques to molecules

1. Rotation

We will treat a molecule as a solid body with continuos distribution of mass described by density ρ. In terms of notations this is more convenient than summation over discrete atoms. Transition is given by a standard

$$\int \rho\left(\vec{r}\right) dV \left(\ldots\right) \;\rightarrow\; \sum_n m_n \left(\ldots\right) \tag{24}$$

with m_n being the mass of the n-th atom

For a solid body

$$\vec{v} = \vec{\Omega} \times \vec{r}$$

The kinetic energy is then

$$K = \frac{1}{2} \int \rho\left(\vec{r}\right) v^2 \left(\vec{r}\right) dV \tag{25}$$

With

$$\left(\vec{\Omega} \times \vec{r}\right)^2 = \Omega^2 r^2 - \left(\vec{\Omega} \cdot \vec{r}\right)^2$$

(**HW:** *prove the above vector identity; you can use Mathematica*)

one gets

$$K = \frac{1}{2} \vec{\Omega} \cdot \hat{I} \cdot \vec{\Omega} \tag{26}$$

Here

$$I_{ik} = \int \rho \left(r^2 \delta_{ik} - r_i r_k\right) dV \tag{27}$$

is the rotational inertia tensor.

If the molecule is symmetric and axes are well chosen from the start, tensor I will be diagonal. Otherwise, one can make it diagonal by finding principal axes of rotation:

$$\hat{I} = \mathrm{diag}\left\{I_1 \;,\; I_2 \;,\; I_3\right\} \tag{28}$$

see 688_rot.nb for examples.

HW. Show that for a diatomic molecule with r being the separation between atoms

$$I = \mu r^2 \;,\;\; 1/\mu = 1/m_1 + 1/m_2 \tag{29}$$

with μ being the reduced mass.

HW: *Consider HCl with $r \sim 1\AA$ (a) find I; (b) estimating the rotational energy as $1/2k_BT$, find Ω at room temperature.*

2. Vibrations of molecules

We will need some information on mechanics.

Lagrange equation

$$\mathcal{L}\left(\vec{q},\ \dot{\vec{q}},\ t\right) = K - U \tag{30}$$

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}_i} = \frac{\partial \mathcal{L}}{\partial q_i} \tag{31}$$

HW: *show that for a single particle with* $K = 1/2m\dot{x}^2$ *and* $U = U(x)$ *one gets the standard Newton's equation.*

Molecules

Let a set of 3D vectors $\vec{r}_n(t)$ $(n = 1, \ldots, N)$ determine the positions of atoms in a molecule, with r_n^0 being the equilibrium positions. We define a multidimensional vector

$$\vec{u}(t) = \left(\vec{r}_1 - \vec{r}_1^{\,0}\,,\ \ldots\ , \vec{r}_N - \vec{r}_N^{\,0}\right) \tag{32}$$

With small deviations from equilibrium, both kinetic and potential energies are expected to be quadratic forms of $\dot{\vec{u}}$ and $\vec{u}$:

$$K = \frac{1}{2}\dot{\vec{u}} \cdot \hat{M} \cdot \dot{\vec{u}} > 0 \tag{33}$$

$$U = \frac{1}{2}\vec{u} \cdot \hat{k} \cdot \vec{u} \geq 0 \tag{34}$$

Introduce "inertial matrix"

$$\hat{M} = \frac{\partial}{\partial \dot{\vec{u}}}\,\frac{\partial}{\partial \dot{\vec{u}}}\mathcal{L} \tag{35}$$

and "elastic matrix"

$$\hat{k} = -\frac{\partial}{\partial \vec{u}}\,\frac{\partial}{\partial \vec{u}}\mathcal{L} \tag{36}$$

Then the Lagrange equations take the form:

$$\hat{M} \cdot \ddot{\vec{u}} = -\hat{k} \cdot \vec{u} \tag{37}$$

We look for a solution

$$\vec{u}(t) = \vec{u}_0 \exp\left(i\omega t\right) \tag{38}$$

$$-\omega^2 \hat{M} \cdot \vec{u}_0 + \hat{k} \cdot \vec{u}_0 = 0 \tag{39}$$

$$\hat{M}^{-1} \cdot \hat{k} \cdot \vec{u}_0 = \omega^2 \vec{u}_0 \tag{40}$$

ω^2 - eigenvalues of a matrix $\hat{M}^{-1} \cdot \hat{k}$ ("secular matrix").

Normal coordinates

Once the secular equation is solved, one can find $3N$ generalized coordinates Q_α which are linear combinations of all $3N$ initial coordinates, so that

$$\mathcal{L} = \frac{1}{2} \sum_\alpha \left(\dot{Q}_\alpha^2 - \omega_\alpha^2 Q^2\right) \tag{41}$$

Q_α determine shapes of characteristic vibrations

Example: diatomic molecule

$$\mathcal{L} = \frac{1}{2}\left(m_1 \dot{x}_1^2 + m_2 \dot{x}_2^2\right) - \frac{1}{2} k_1 \left(x_2 - x_1\right)^2$$

$$x_2 = -\frac{m_1 x_1}{m_2} \ , \ \ X = x_2 - x_1$$

Now

$$\mathcal{L} = \frac{1}{2} \mu \dot{X}^2 - \frac{1}{2} k_1 X^2$$

with

$$\mu = \frac{m_1 m_2}{m_1 + m_2} \tag{42}$$

and

$$\omega = \sqrt{\frac{k_1}{\mu}}$$

Above is a human way to solve the problem - we eliminated the motion of center of mass from the start and then found the frequency. A more formal, matrix way is given in 688_vibrations.nb.

HW: consider a hypothetical molecule with one atom of mass 1 amu (hydrogen) and the other 20 amu. The spring constant is $1000N/m$ *and the equilibrium distance is* $1\AA$
a) find the frequency b) (optional) estimating the vibrational energy as $k_B T$*, with* T *being the room temperature, find the amplitude of vibrations. Compare this to equilibrium distance - must be small in order to treat vibrations as harmonic.*

Linear triatomic molecule

Consider a linear ABA molecule with spring constants k_1 and additional energy dependence on the angle between bonds. Solution as well as pictures of normal shapes are given in 688_vibrations.nb.

HW: *Consider a symmetric triangular molecule; find the frequencies and normal shapes of vibrations. Note: it is convenient to express elongations in terms of vectors locating the atoms, similarly to the example of a linear triatomic molecule. Also, if you have trouble finding the eigenvector due to degeneracy of eigenvalues, try breaking the symmetry by modifying e.g., one of the masses by a small* ϵ *and taking the limit* $\epsilon \to 0$ *in the answer.*

HW: *Consider a molecular group of 3 identical masses which can move in a ring of constant radius* r*. Masses are connected by different springs:* k_1 *(1 & 2) ,* k_2 *(2 & 3) and* k_3 *(3 & 1) (and imagine that they are elongated/contracted along the ring). Find and classify frequencies and vibrational shapes*

HW: *(optional). Consider vibrations of a tetrahedron described in the lecture on molecular rotations. All spring constants* (k_1) *are identical.*

IV. FOURIER

READING: KR., Ch. 11

work-through: KR., Ch. 11, pp. 478-490, 496-498, 506-519, 531 + 688_fourier.nb .

A. Orthogonality

$$\int_{-\pi}^{\pi} dx\, 1 \cdot \cos(nx) = 2\pi\delta_{n\,0} \tag{43}$$
$$\int_{-\pi}^{\pi} dx\, 1 \cdot \sin(nx) = 0$$

For $m,\, n \neq 0$:

$$\int_{-\pi}^{\pi} dx\, \cos(nx)\cos(mx) = \pi\,\delta_{mn} \tag{44}$$
$$\int_{-\pi}^{\pi} dx\, \cos(nx)\sin(mx) = 0$$
$$\int_{-\pi}^{\pi} dx\, \sin(nx)\sin(mx) = \pi\,\delta_{mn}$$

HW: *show/check that*

B. Fourier series and formulas for coefficients

$$f(x) = a_0 + \sum_{n=1}^{\infty} \left(a_n \cos(nx) + b_n \sin(nx)\right) \tag{45}$$

Coefficients:

$$a_0 = \frac{1}{2\pi}\int_{-\pi}^{\pi} dx\, f(x) \tag{46}$$
$$a_n = \frac{1}{\pi}\int_{-\pi}^{\pi} dx\, f(x)\cos(nx) \tag{47}$$
$$b_n = \frac{1}{\pi}\int_{-\pi}^{\pi} dx\, f(x)\sin(nx) \tag{48}$$

Note: even function: $b_n = 0$; odd function: $a_n = 0$.

HW: *p. 485, 2,3,7-12, 13-15 (show combined plots of a function and its approximations), 21. Example 3 on p. 489 - reproduce with Mathrmatica and plot for a selected $\omega \neq 1$; p. 496, 3-6.*

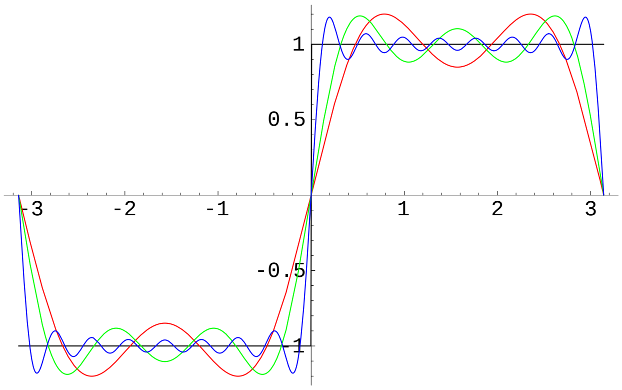

FIG. 4:

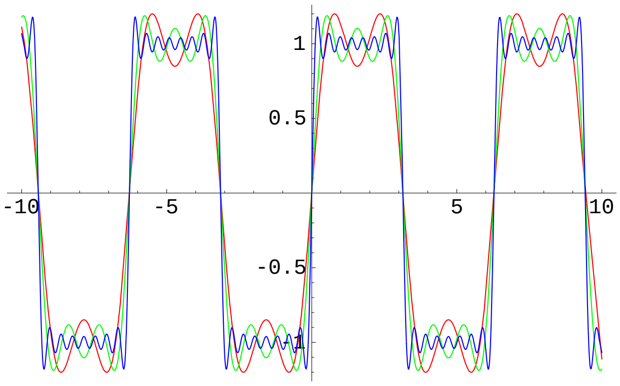

FIG. 5:

C. Complex series

1. *Orthogonality*

"Scalar product" of two functions $f(x)$ and $g(x)$ on an interval $[-\pi, \pi]$:

$$\langle f|g\rangle = \int_{-\pi}^{\pi} dx\, f(x)^* g(x) \tag{49}$$

Introduce:

$$e_n(x) = e^{inx} \tag{50}$$

Then:

$$\langle e_n|\, e_m\rangle \equiv \int_{-\pi}^{\pi} dx\, e^{i(m-n)x} = 2\pi\delta_{mn} \tag{51}$$

(note: more compact than real sin/cos). **HW:** *Show/check that*

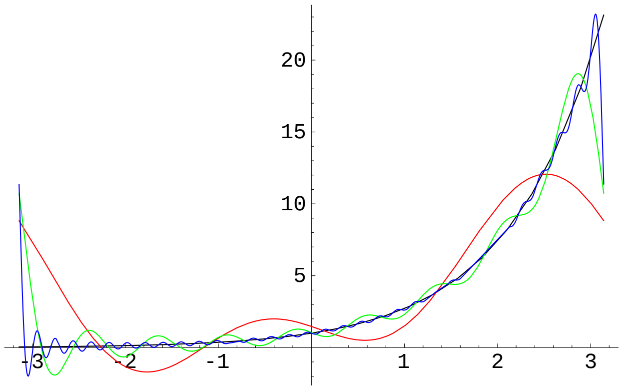

FIG. 6: Approximations of e^x by trigonometric polynomials (based on complex Fourier expansion). Red - 2-term, green - 8-term and blue - the 32 term approximations.

2. Series and coefficients

$$f(x) = \sum_{n=-\infty}^{n=\infty} c_n e^{inx} \tag{52}$$

or

$$|f\rangle = \sum_{n=-\infty}^{n=\infty} c_n \, |e_n\rangle \tag{53}$$

From orthogonality:

$$c_n = \frac{1}{2\pi} \langle e_n | \, f \rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} dx \, e^{-inx} f(x) \tag{54}$$

Again, note much more compact than sin/cos.

HW: *p. 499, Nos. 2, 9-12*

D. Dirac delta

(mostly, not in KR. - use notes below).

1. Basic definitons

$$\delta(x) = 0 \, , \quad x \neq 0 \tag{55}$$

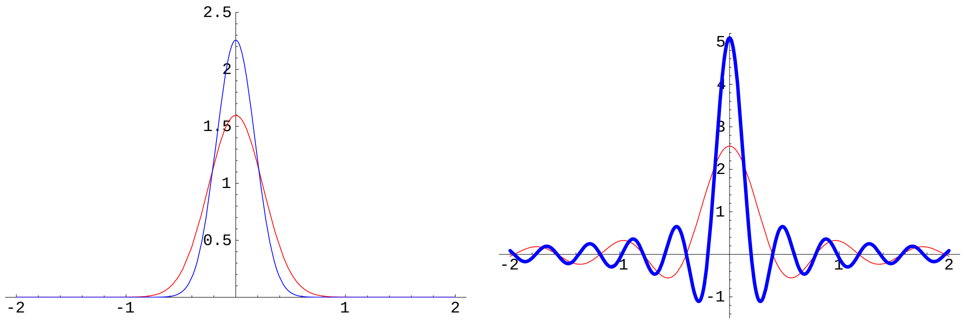

FIG. 7: Two represenations of δ_n which lead to Dirac delta-function for $n \to \infty$.

$$\delta(x) = \infty \;, \quad x = 0$$
$$\int_{-\epsilon}^{\epsilon} \delta(x)\, dx = 1 \;, \quad \text{for any } \epsilon > 0$$

Then,

$$\int_{-\epsilon}^{\epsilon} \delta(x) f(x)\, dx = f(0) \;, \quad \text{for any } \epsilon > 0 \tag{56}$$

Note: the real meaning should be given only to integrals. E.g., $\delta(x)$ can oscillate infinitely fast, which does not contradict $\delta(x) = 0$ once an integral is taken.

2. Sequences leading to a δ-function for $n \to \infty$

$$\delta_n(x) = n \text{ for } |x| < 1/2n \;, \quad 0 \;\; \text{otherwise} \tag{57}$$

$$\delta_n(x) = \frac{n}{\sqrt{\pi}} \exp\left(-n^2 x^2\right) \tag{58}$$
$$\delta_n(x) = \frac{\sin(nx)}{\pi x} \tag{59}$$

HW: *check normalization and reproduce plots*

3. Derivative

$$\int \delta'(x) f(x) = -f'(0) \tag{60}$$

HW: *Show that integrating by parts*

E. Fourier integral

in class

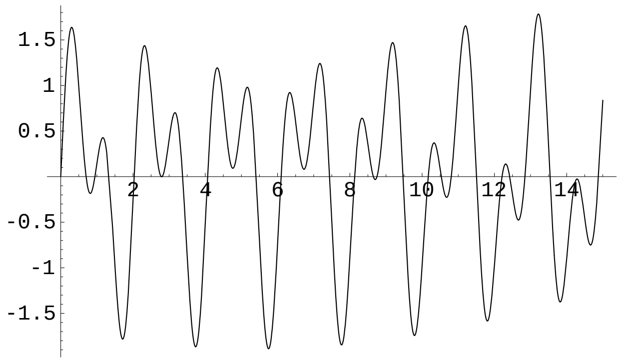

FIG. 8: An "almost periodic" function $e^{-0.001x}\left(\sin\left(3x\right)+0.9\sin(2\pi x)\right)$

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HW: *Check any 6 formulas from Table III, p. 531 in KR.*

F. Power spectra for near-periodic functions

(not in KR., will be discussed in class). Note

$$\mathcal{F}\left[1\right]=\sqrt{2\pi}\delta\left(k\right) \tag{61}$$

Similarly,

$$\mathcal{F}\left[e^{-ik_0x}\right]=\sqrt{2\pi}\delta\left(k-k_0\right) \tag{62}$$

i.e. an ideally periodic signal gives an infinite peak in the power spectrum.

A real signal can lead to a finite peak for 2 major reasons:

- signal is not completely periodic
- the observation time is *finite*

This is illustrated in Fig. 9.

G. Convolution theorem

work-through: KR. p.523 + 688_convol.nb

$$\mathcal{F}\left[\int_{-\infty}^{\infty}f(y)g(x-y)\,dy\right]=\sqrt{2\pi}\mathcal{F}\left[f\right]\mathcal{F}\left[g\right] \tag{63}$$

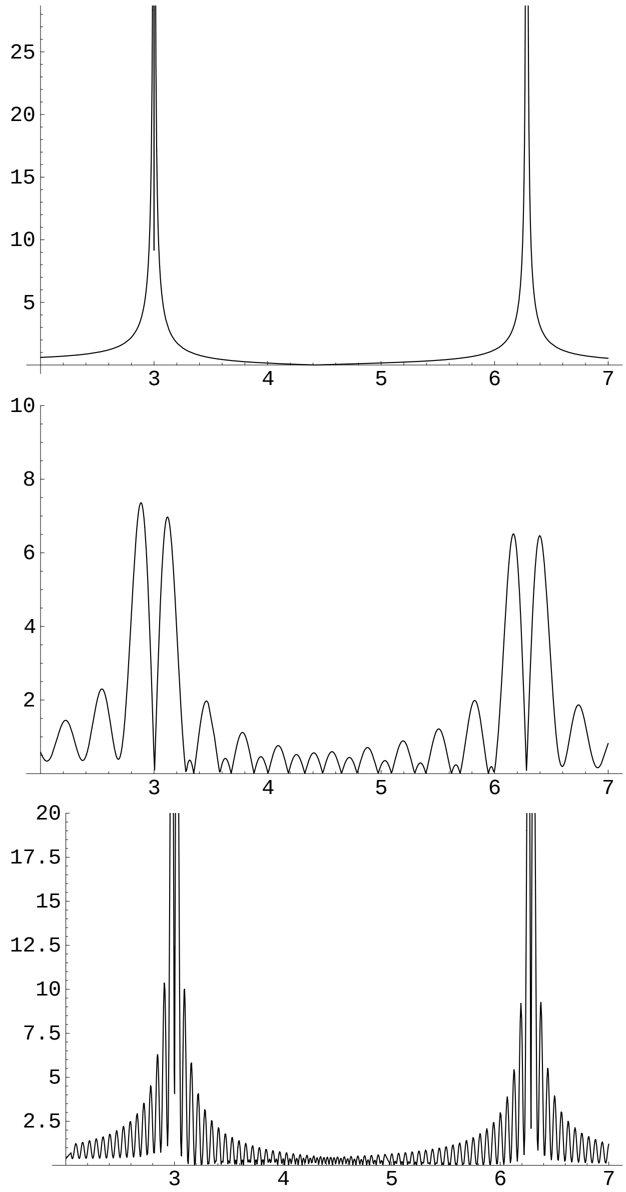

FIG. 9: Power spectrum of the previous function obtained using a cos Forier transformation (infinite interval) and finite intervals $L = 10$ and $L = 100$.

H. Discrete Fourier

work-through: KR. pp. 524,25 + 688_discFour.nb

Consider various lists of N (complex) numbers. They can be treated as vectors, and any vector $\vec{f}$ can be expanded with respect to a basis:

$$\vec{f} = \sum_{n=1}^{N} f_n \vec{e}_n \tag{64}$$

with

$$\vec{e}_1 = (1,0,0,\ldots)\ ,\ \vec{e}_2 = (0,1,0,\ldots)\ ,\ \ \ldots \tag{65}$$

Scalar (inner) product is defined as

$$\vec{f}\cdot\vec{g} = \sum_{n=1}^{N} f_n^* g_n \tag{66}$$

(note complex conjugation).

Alternatively, one can use another basis with

$$\vec{e}_n{}' = \Big(1,\ e^{2\pi i\,(2-1)\,(n-1)/N},\ \ldots\ ,\ e^{2\pi i\,(m-1)\,(n-1)/N},\ \ldots\ ,\ e^{2\pi i\,(N-1)\,(n-1)/N}\Big) \tag{67}$$

Note: KR. uses m instead of our $(m-1)$ but his sum is from 0 to $N-1$, so it is the same thing.

1. Orthogonality

$$\vec{e}_n{}'\cdot\vec{e}_k{}' = N\delta_{nk} \tag{68}$$

Indeed,

$$\vec{e}_n{}'\cdot\vec{e}_k{}' = \sum_{m=1}^{N} r^{(k-n)(m-1)}\ ,\quad r\equiv e^{2\pi i/N} \tag{69}$$

Summation gives

$$\vec{e}_n{}'\cdot\vec{e}_k{}' = \frac{1-r^{(k-n)N}}{1-r^{(k-n)}} \tag{70}$$

Note that for k,n integer the numerator is always zero. The denominator is non-zero for any $k-n\neq 0$, which leads to a zero result. For $k=n$ one needs to take a limit $k\to n$

HW: *do that*

Now we can construct a matrix ("Fourier matrix" $\hat{F}$) of $\vec{e}_n{}'$ for all $n\leq N$ and use it to get components in a new basis

$$\hat{F}\cdot\vec{f} \tag{71}$$

This will be Fourier transform. Applications will be discussed in class.

HW: *construct $\hat{F}$ for $N=3$*

V. ORDINARY DIFFERENTIAL EQUATIONS

A. 1st order

HW: *KR. p. 18, 2-6, 10-12.*

1. *Separation of variables. Example :growth and decay of grains*

$$\frac{dR}{dt} = \frac{R_*}{\tau}\left(1 - \frac{R_*}{R}\right) \tag{72}$$

Here R_* is the critical size and τ is the time scale. Interface-limited kinetics is assumed.

First, switch to dimensionless variables t/τ (will use the same notation, t) and $r = R/R_*$. Now

$$\frac{dr}{dt} = 1 - \frac{1}{r} \tag{73}$$

Write it as

$$\frac{dr}{1 - 1/r} = dt$$

to obtain an implicit solution

$$r + \ln|r - 1| = t + C \tag{74}$$

The constant C follows from initial conditions, $r(0) = r_0$. Thus

$$t = r - r_0 + \ln\frac{r - 1}{r_0 - 1} \tag{75}$$

(Note: the absolute value under the ln is not required anymore.)

The family of solutions is plotted (parametrically since this is an implicit solution!) in Fig. 10.

HW: *Consider and explore the equation for diffusion-limited growth and decay:*

$$\frac{dR}{dt} = \frac{R_*^2}{\tau R}\left(1 - \frac{R_*}{R}\right) \tag{76}$$

Make the plots.

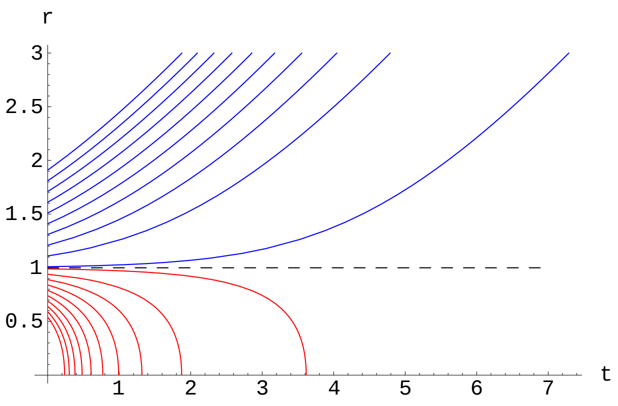

FIG. 10: The family of solutions for eq. (73). Note that supercritical nuclei ($r_0 > 1$ - blue) grow while subcritical nuclei ($r_0 < 1$ -red) decay with time. The singular solution $r(t) = 1$ (the "critical nucleus") is shown by a dashed line; it is unstable, however.

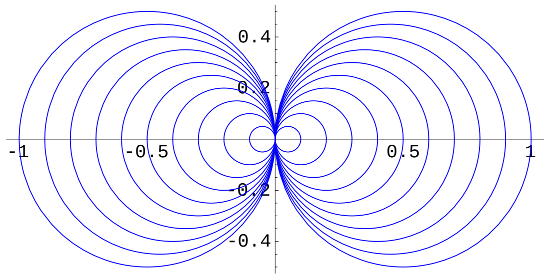

FIG. 11: A family of solutions of eqs.(77, 78).

2. The "homogeneous" equations. Example from KR., p.17

General:

$$y' = f\left(y/x\right) \tag{77}$$

Note that the solution will remain valid if the scales of x and of y are changed simultaneously.

Example:

$$f(y/x) = \frac{y^2 - x^2}{2xy} \tag{78}$$

using $u = y/x$ one separates variables (as will always happen in such equations!). The resulting plot (a family of cirles) is in figure 11.

work-through: Kr., p.17 and 688_ode.nb

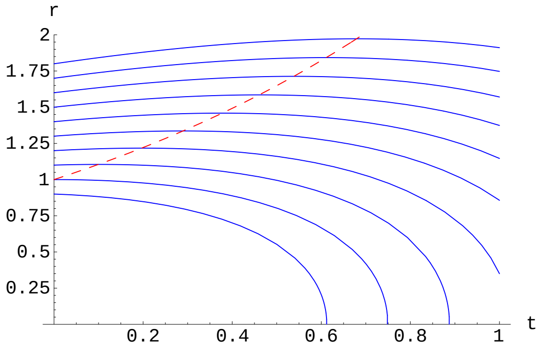

FIG. 12: Solutions of eq. (79) describing growth and decay of nuclei for a time-dependent critical size. The red dashed line indicates the "critical size" value; once it catches up with a certain nucleus the latter starts to decay.

3. Equations with no analytical solution

Consider the same problem of grain growth and decay, but for a rapid cahnge in time of R_*. Note that part of the dependence can be eliminated by switching to a new time

$$t_{new} = \int R_*(t)dt/\tau$$

However, for the reduced radius we need $r = R/R_*(0)$ (otherwise, dr/dt will involve extra terms). Specifying the strong time-dependence as exponential (we again further use t instead of t_{new}) one gets

$$\frac{dr}{dt} = 1 - \frac{e^t}{r} \tag{79}$$

Equation looks simple but cannot be solved exactly *in principle* since variables cannot be separated. (Such equations are known as Ricatti equations). Numerical integration is possible - see the 688_ode.nb and Fig. 12 below - but one needs to be careful due to singularity at $r = 0$. (Alternatively, one can use t as dependent variable and r as independent. That would simplify numerics. **HW:** *(optional) do that*).

B. Linear 2d order equations

1. *free oscillations with one degree of freedom*

Generic equation:

$$\ddot{x} + \omega_0^2 x = 0 \tag{80}$$

Physical meaning:

Mechanical:

$$\omega_0 = \sqrt{\frac{k}{m}} \tag{81}$$

k - spring constant, m -mass, x - displacement.

E& M (simple LC contour, $x \to q$, the charge, $\dot{x} \to I$, the current, $m \to L$, $1/k \to C$):

$$\omega_0 = \sqrt{\frac{1}{LC}} \tag{82}$$

2. *General solution*

$$x(t) = Ae^{i\omega_0 t} + B^{-i\omega_0 t} \tag{83}$$

A and B can be complex and follow from initial conditions and x is real. Alternatively, one can use

$$x = Re\left[Ae^{i\omega_0 t}\right]$$

where again $Re[A]$, $Im[A]$ follow from intial conditios. Finaly,

$$x = A\cos(\omega_0 t) + B\sin(\omega_0 t)$$

with real A, B gives the same thing.

3. *Damping*

If there is viscous friction $-fv$ then the generic equation is:

$$\ddot{x} + 2\gamma\dot{x} + \omega_0^2 x = 0 \tag{84}$$

with

$$\gamma = f/2m$$

Alternatively, in E& M

$$\gamma = R/2L$$

R-resistance.

Note: you always must cast the equation in the above standard form if you have to solve it; otherwise things get too messy

Solution is looked for as

$$x \propto e^{i\omega t}$$

which leads to two complex conjugated

$$\omega_{1,2} = \pm\Omega + i\gamma\ , \quad \Omega \equiv \sqrt{\omega_0^2 - \gamma^2} \tag{85}$$

The full solution will be

$$x(t) = Ae^{i\omega_1 t} + B^{i\omega_2 t} = \tag{86}$$

$$e^{-\gamma t}\left(Ae^{i\Omega t} + B^{-i\Omega t}\right) \tag{87}$$

Note that for small damping $\Omega \approx \omega_0$ i.e. γ affects only the imaginary part.

See Fig. 13 for $x(t)$ and Fig. 14 for the phase portrait $\dot{x}$ vs x (will be discussed in class, see also the 688_ode.nb).

HW: *Find A, B and write the final trigonometric expression for (a) $x(0) = x_0$, $v(0) = 0$ and (b) $x(0) = 0, v(0) = v_0$*

4. Driving and resonance

the generic equation is:

$$\ddot{x} + 2\gamma\dot{x} + \omega_0^2 x = De^{-i\omega_d t}\ ,\ D = \frac{F}{m}$$

F is the amplitude of the driving force (or, $D = V_0/L$ in LRC circuit, V_0 the amplitude of driving voltage).

Look for

$$x = Ae^{-i\omega_d t}$$

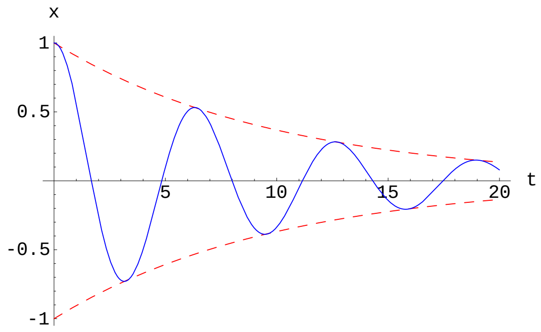

FIG. 13: Decay with time of free oscillations.

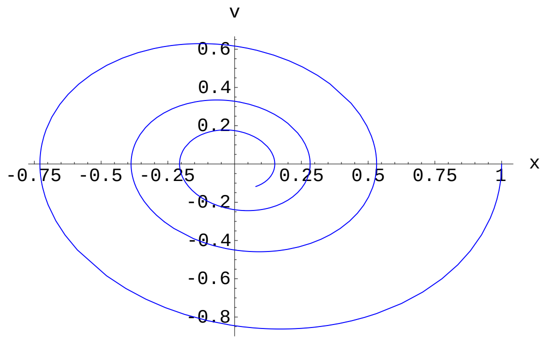

FIG. 14: Phase portrait of a damped system.

and solve for A:

$$A = \frac{D}{\omega_d^2 - 1 + 2\gamma\omega_d}$$

(note - $\omega_0 = 1$ here, to comply with 688_ode.nb)

Resonance - rapid increase in $|A|$ when $\omega_d = \omega_0$ (note: not Ω!) see Fig. 15.

The homogeneous solution can be added to comply with initial conditions, but due to $e^{-\gamma t}$ it quickly decays (i.e. a driven system "forgets" initial conditions). Exception is $\gamma = 0$ when initial conditions always play a role - see Fig. 16.

HW: *find an explicit solution for* $\omega_d = \omega_0 + \delta$, $\gamma = 0$, $x(0) = 0$, $\dot{x}(0) = 0$ *for a small* δ*. Consider the limit* $\delta \to 0$.

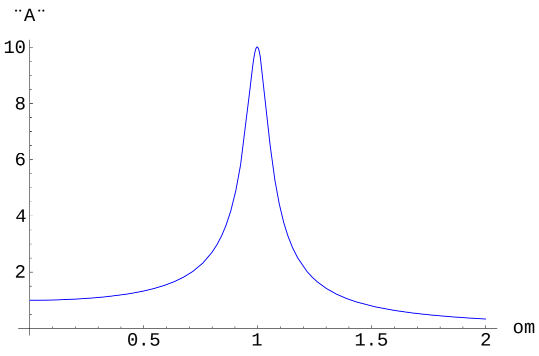

FIG. 15: Amplitude (absolute value) as a function of driving frequency for $\gamma = 0.05$.

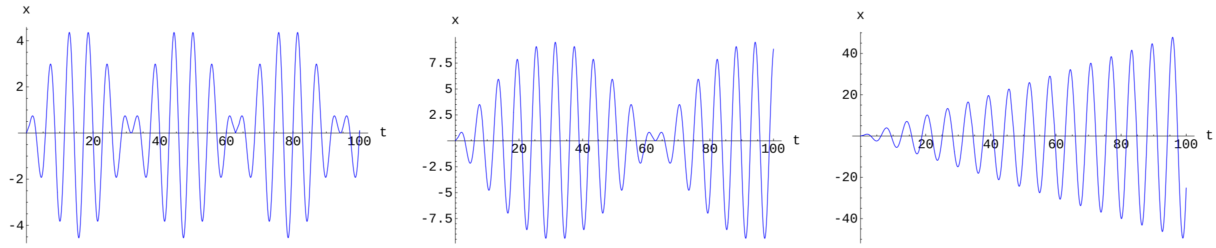

FIG. 16: Driven oscillations for different miss-match between the driving frequency ω and natural frequency $\omega_0 = 1$. 1st figure - $\omega = 1.2$, 2d- $\omega = 1.1$ (note increase of amplitude) and 3d - $\omega = 1$ (pure resonance).

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VI. GENERAL LINEAR 2D-ORDER ODE'S

Example: equation with non-constant coefficients (Airy)

$$y'' - xy = 0 \tag{88}$$

(This is the *normal* form, without y'). Two solutions are given in Fig. 17. Note:

- one solution, "first kind", remains finite near the singular point $x \to \infty$, the other solution, "second kind" tends to infinity.
- both solutions either oscillate ($x < 0$) or behave exponentially ($x > 0$)
- when oscillating, zeroes of the two solutions intermingle ("oscillation theorem")

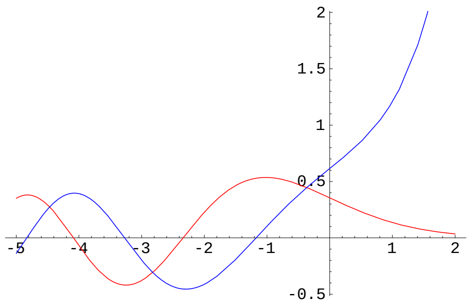

FIG. 17: The two Airy functions

A. Wronskian and method of variation of parameters

READING: Sect. 2.6 in KR.

work-through: Sect. 2.10 in Kr.

HW: *p. 101, Nos. 1-5. For all problems a) find the the 2 solutions of homogeneous equations; b) find their wronskian; c) construct a particular solution of the inhomogeneous equation; d) plot the result - see the example in 688_ode2.nb*

$$W\left(y_1\,,y_2\right)=y_1y_2'-y_2y_1' \tag{89}$$

HW: *Find wronskian for the following pairs:* $\sin x$, $\cos x$, $\exp(x)$, $\exp(-x)$ *and the two Airy functions - see 688_ode2.nb*

Particular solution:

$$y_p(x)=-y_1(x)\int^x\frac{y_2(z)r(z)}{W(z)}\,dz+y_2(x)\int^x\frac{y_1(z)r(z)}{W(z)}\,dz \tag{90}$$

Example (KR., p.99)

$$y''+y=1/\cos x \tag{91}$$

See Fig. 18 and 688_ode2.nb

VII. SYSTEMS OF ODE'S WITH CONSTANT COEFFICIENTS

$$\frac{d}{dt}\vec{y}=\hat{A}\cdot\vec{y} \tag{92}$$

Will be discussed in class.

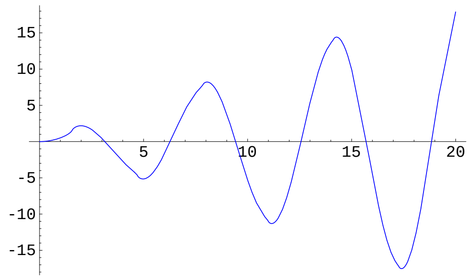

FIG. 18: Particular solution for eq.(91)

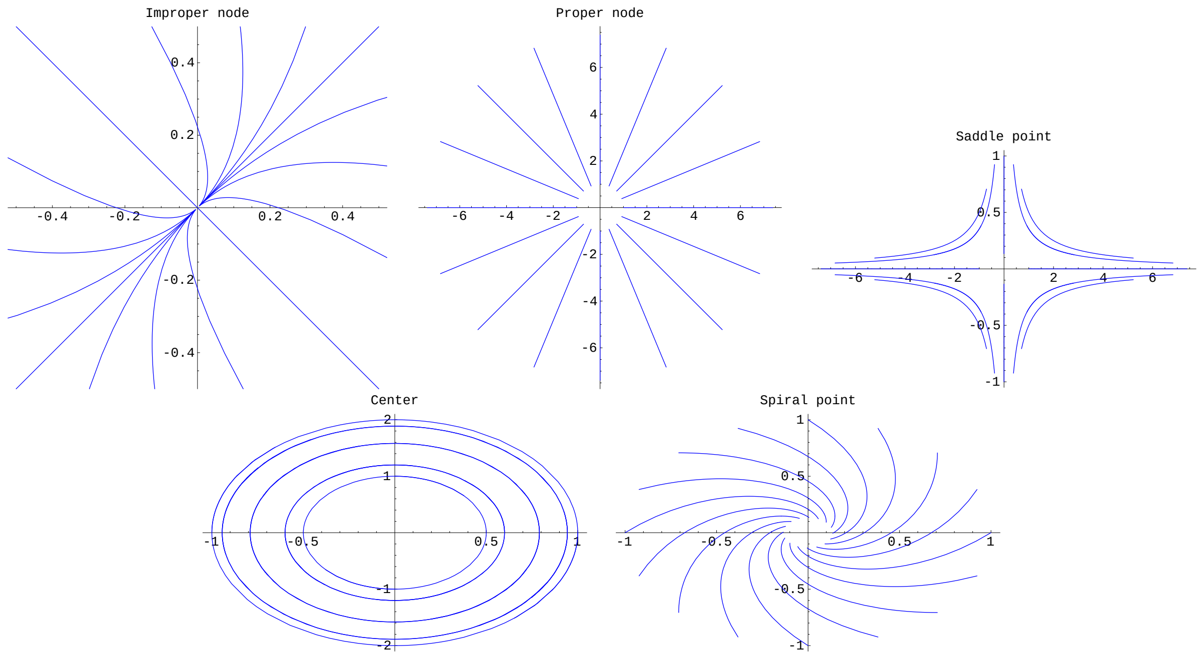

FIG. 19: Typical nodes for eq.(92).

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VIII. LAPLACE TRANSFORM

READING: KR., Ch.6.1-6.3

$$F(s) = \mathcal{L}\left[f\right] = \int_0^\infty e^{-st} f(t)\, dt \tag{93}$$

work-through: Examples 1,2, pp.321,22 in KR.

HW: *Reproduce Table 6.1, Mathematica is ok.*

A. s- and t-shifting

$$\mathcal{L}\left[f(t)e^{at}\right] = F(s-a) \tag{94}$$

$$\mathcal{L}\left[f(t-a)\theta(t-a)\right] = e^{-as}F(s) \tag{95}$$

where $\theta(x)$ is a unit-step theta-function ($u(x)$ in KR.) **HW:** *KR. p. 227, Nos. 43-48. p.240, Nos. 14-17.*

B. Derivatives and Integrals

work-through: KR., Ch. 6.2

$$\mathcal{L}\left[f'(t)\right] = sF(s) - f(0) \tag{96}$$

$$\mathcal{L}\left[\int_0^t f(\tau)\,d\tau\right] = \frac{1}{s}F(s) \tag{97}$$

HW: *KR. p. 232, eq.(10)*

IX. DIFFUSION EQUATION

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \tag{98}$$

The solution for $c(x,0) = \delta(x)$ ("Greens function") is given by

$$G(x,t) = \frac{1}{2\sqrt{\pi D t}}\exp\left\{-\frac{x^2}{4Dt}\right\} \tag{99}$$

General solution (1d):

$$c(x,t) = \int_{-\infty}^{\infty} dy G[x-y,t]c_0(y)$$

the above is general for initial distribution c_0; below is an example of a localized intial distribution between $x=0$ and $-\infty$:

$$c_1[x,t] = \frac{1}{2}\mathrm{erfc}\left[\frac{x}{2\sqrt{Dt}}\right] \tag{100}$$

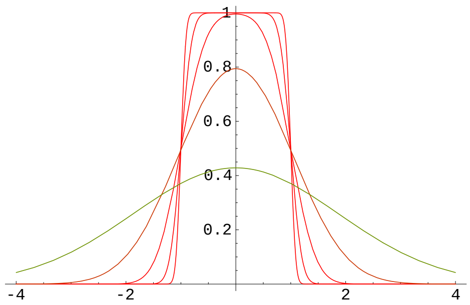

FIG. 20: Diffusion of an initially constant distribution in free space

Another example: $c_0 = 1$ for $-1 < x < 1$. From superposition principle:

$$c_{box}[x,t] = (c_1[x-1,t] - c_1[x+1,t])/2 \tag{101}$$

A. Problems with boundaries

1. *Semi-infinite: fixed concentration*

$$c(0,t) \equiv 1$$
$$c(x,t) = 2c_1[x,t] = \operatorname{erfc}\left[\frac{x}{2\sqrt{t}}\right]$$

guessed !! (yes, guessing is legal!); same figure as before, only now the region $x < 0$ is "unphysical"

2. *Semi-infinite: reflecting*

point source at $x = 1$ and reflecting boundary at $x = 0$. $j = 0$, thus $\partial c/\partial x = 0$ at the reflecting boundary.

$$c_{mir}[x,t] := G[x-1,t] + G[x+1,t]$$

3. *semi-infinite: absorbing*

Absorbing boundary at $x = 0$ and point source at $x = 1$.

$$c_{abs}[x,t] := G[x-1,t] - G[x+1,t]$$

Note : do not care about negative concentration at $x < 0$

B. Two absorbing boundaries: Fourier expansion

1. Formulation of the problem

A. Solve the equation

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \tag{102}$$

in the interval

$$0 \le x \le l$$

(assume $l = 1$) with boundary conditions (BC)

$$c(0,t) = c(l,t) = 0$$

The initial condition is

$$c(x,0) = f(x)$$

HW: *Select any simple function $f(x)$ (e.g., a linear function $f(x) = ax + b$ or a boxed function f(x)=1 for $l/2 - h/2 \le x \le l/2 + h/2$ - and make the calculation and graphick below explicitly*

Start: Dimensionalization: Switch to new time

$$t' = Dt/l^2$$

so that

$$\frac{\partial c}{\partial t'} = \frac{\partial^2 c}{\partial x^2} \tag{103}$$

(we not scale x since l is 1).

2. Analytical solution

Below the method of separation of variables is applied; other methods (Laplace transform, reflection etc.) also can be used. Primes will not be indicated further in eq.(103). Use separation of variables and look for

$$c(x,t) = \sum_{n=1}^{\infty} A_n T_n(t) X_n(x) \tag{104}$$

One obtains:

$$T_n(t) = \exp\left(-\lambda_n^2 t\right) \;,\;\; X_n(x) = \sin\left(\lambda_n x\right) \tag{105}$$

and fromt he 2d BC:

$$\lambda_n = n\pi \;,\;\; n = 1, 2, 3, \ldots \tag{106}$$

$$c(x,t) = \sum_{n=1}^{\infty} A_n \exp\left(-n^2 \pi t\right) \sin(n\pi x) \tag{107}$$

[Note: In each term of the sum the x- and t-dependences are separated. A simple exponential dependence on t is expected since there is only a first derivative in t and coefficients are t-independent. The function $\exp\left(-n^2\pi^2\right)\sin(n\pi x)$ satisfies the diffusion equation (103) for any n and for integer $n = 1, 2, 3...$ satisfies the BC.]

To obtain the expansion coefficients, A_n, we note that

$$\int_0^1 \sin(n\pi x)\sin(m\pi x)dx = 0$$

for $m \neq n$ and equals $1/2$ for $m = n$. Then, we consider eq.(107) at $t = 0$ with $c(x, 0) = f(x)$. Multiplying the expansion by $\sin(m\pi x)$ and integrating from 0 to one obtains

$$\int_0^1 dx f(x)\sin(n\pi x) = \frac{1}{2}A_n \tag{108}$$

For simple $f(x)$ the integral can be evaluated analytically (e.g, with *Mathematica*). After this, the expansion (107) gives the full analytical solution. If the time is not too small, the solution is accurately approximated the first few terms and can be plotted easily.

HW: *modify the formulas for* $l \neq 1$

C. Laplace Transform

After switching to the LT, the diffusion equation becomes an *ordinary* differential equation, and can be solved in elementary functions. Further, we expand the denominator assuming large s to emphasize the role of small t (and to simplify inversion). One obtains

$$W[x,s] = \frac{1 + e^{-\sqrt{s}} - e^{-\sqrt{s}x} - e^{-\sqrt{s}(1-x)}}{s}\sum_{m=0}^{\infty}(-1)^m e^{-m\sqrt{s}}$$

Inverse of

$$e^{-\sqrt{s}(x+m)}/s$$

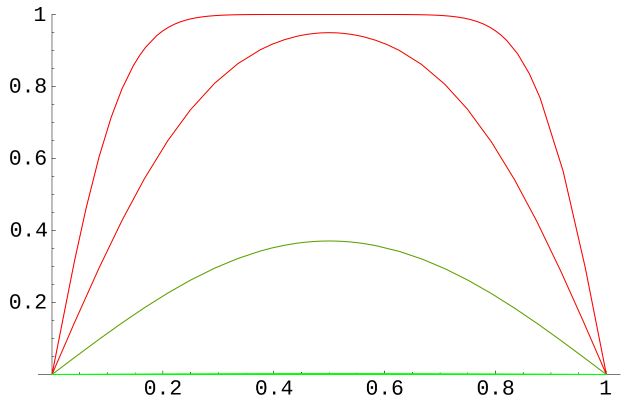

FIG. 21: Diffusion of an initially constant distribution between two absorbing boundaries. Note that at larger times the profile is practically sinusoidal, the first term in the Fourier expansion. At very small times Fourier expansion is not the best one, and the Laplace transform technique is more efficient.

is

$$i_m[x,t] \equiv \text{erfc}\left[\frac{m+x}{2\sqrt{t}}\right]$$

Thus,

$$c[x,t] = \sum_{m=0}^{\infty} \left(i_m[0,t] + i_m[1,t] - i_m[x,t] - i_m[1-x,t]\right)$$

For a given accuracy, $\epsilon \ll 1$ one has an estimation

$$m \sim 2\sqrt{t}\ln(1/\epsilon)$$

which is a modes number (for a computer) for not too large t. With such a cut-off on m evaluation of the sum (and plotting) are fast on any platform.

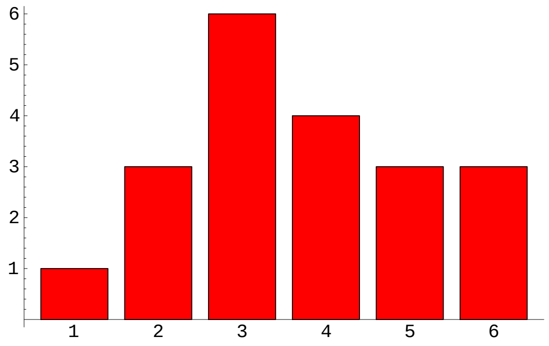

FIG. 22: A typical histogram after 20 rolls of a single die.

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X. ELEMENTS OF PROBABILITY AND STATISTICS

A. Representation of data. Histograms

READING: Kr. 24.1

1. *Mean and variance*

work-through: KR., p.996 + 688_probab.nb

see Fig. 22.

HW: *(a) Create a list of 100 random integer numbers between $a_0 = 0$ and $a_9 = 9$. (b) count frequencies for each a_i and plot a histogram. (c) calculate mean (d) calculate variance*

B. Sample space and events

work-through: KR. 24.2 Examples:

- flipping a coin $S = [head, \, tail]$ (or, $S = [0, 1]$, "binary")
- flipping n coins ("binomial") $S = [n \, heads, \ 0 tails \, , n-1 \, head, \ 1 tail \, , \ldots 0 heads, \ n \, tails]$ (or, $S = [0, \ldots, n]$, the number of "heads")
- rolling a die. $S = [1, \, \ldots, \, 6]$
- rolling 2 dice. $S = [2, \, \ldots, \, 12]$

1. *Sets. Unions, intersections, etc.*

see KR. and the *Mathematica* notebook.

HW: *Create your own examples of union and intersection of lists*

C. Probabilities and random variables

work-through: KR. 24.3 Intuitive "definition":

Relative frequency when the number of trials tends to ∞

Note: number of trials is unrelated to the sample space S, which can be small (e.g., for a coin $S = [0, 1]$, but one needs *many* trials to see that $P(0) = P(1) = 1/2$).

Axioms:

- $0 \leq P(A) \leq 1$
- $P(S) = 1$
- If $A \cap B = \emptyset$:

$$P(A \cup B) = P(A) + P(B) \tag{109}$$

A few simple theorems:

- $P(A^c) = 1 - P(A)$
-

$$P(A \cup B) = P(A) + P(B) - P(A \cap B) \tag{110}$$

HW: *KR. p.1005, Nos. 7, 10-12*

1. *"Experimental" determination of probabilities*

see Fig. 23 and 688_probab.nb

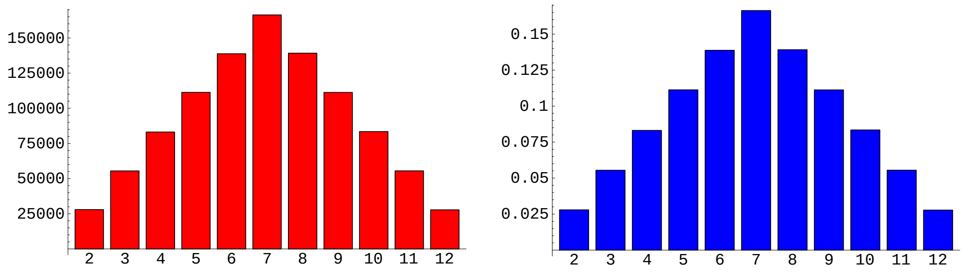

FIG. 23: Unaveraged histogram (red) and averaged (blue) after 1 million rols of 2 dice. The blue histogram represents the experimental probabilities (which are already close to theoretical expectations) with a total sum of 1.

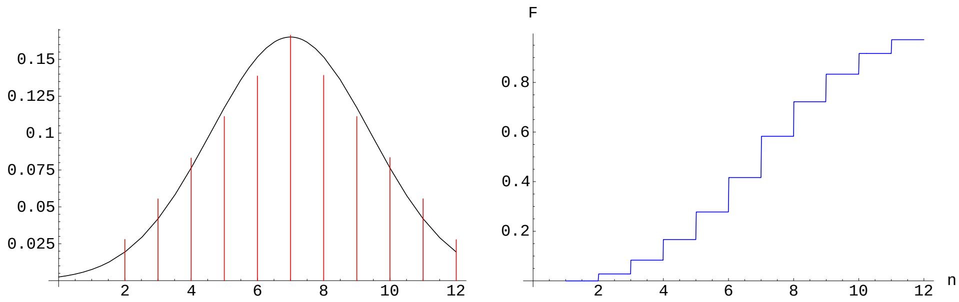

FIG. 24: Probability function (left) and cumulative distribution function (right) for rolling of 2 dice. The black curve shows the normal (gauss) approximation to the observed data.

D. Permutations, binomial coefficients and Stirling formula

in class

work-through: KR. 24.4

HW: *use Stirling formula to approximate the binomial coefficient if n, m and $n-m$ are large*

E. Discrete and continuos distributions

One-dimensional:

- Discrete: assume the elements of sample space can be numbered by an integer j; x_j are their values while p_j are the probabilites. Cumulative distribution:

$$F(x) = \sum_{x_j \leq x} p_j \tag{111}$$

- Continuous: assume the elements of sample space can be identified by a continuous variable x with a probability density $p(x)$. Cumulative distribution is given by

$$F(x) = \int_{-\infty}^{x} dx' p\left(x'\right) \tag{112}$$

Note: I use $p(x)$ instead of $f(x)$ in KR.

Primtive examples:

Discrete: "binary"

$$p_0 = p_1 = \frac{1}{2}\ , \quad F(x) = 0,\, x < 0\ , \quad F(x) = \frac{1}{2},\, 0 \le x < 1\ , \quad F(x) = 1,\, x \ge 1$$

Continuous: "uniform"

$$p(x) = \frac{1}{L},\, 0 \le x \le L\ , \quad F(x) = 0,\, x < 0\ , \quad F(x) = x,\, 0 \le x \le L\ , \quad F(x) = 1,\, x > L$$

1. *Mean and variance*

We use equivalently "bar" for averages and $\langle \ldots \rangle$ for longer expressions.

$$\bar{x} = \sum p_i x_i \ \rightarrow \ \int_{-\infty}^{\infty} x p(x)\, dx \tag{113}$$

$$\sigma^2 = \left\langle (x - \bar{x})^2 \right\rangle = \left\langle x^2 \right\rangle - \langle x \rangle^2 \tag{114}$$

2. *Change of variables in continuos distributions*

$$x \ \rightarrow \ y(x)\ , \quad F\left[y(x)\right] = F(x)$$

Thus the new probability density $P(y)$ is derived from

$$P(y)\, dy = p(x)\, dx \tag{115}$$

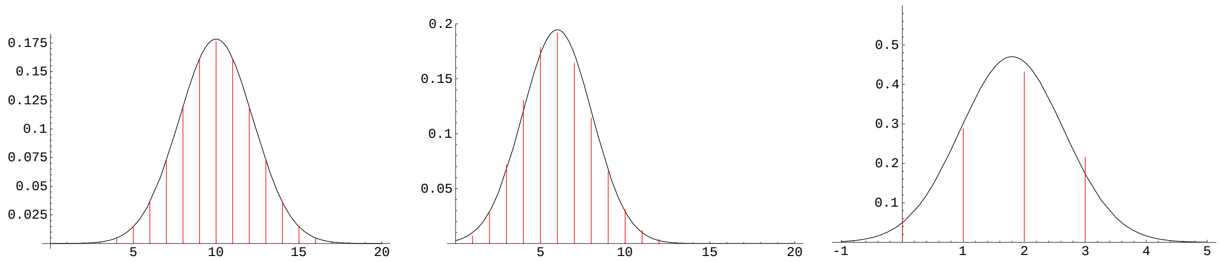

FIG. 25: Binomial probability function and approximation of the results by a gaussian curve for $n = 20\,, p = 1/2$ (left, unbiased), $n = 20\,, p = 0.3$ (middle, biased) and $n = 3\,, p = 0.6$ (right). The approximation becomes exact for $n \to \infty$ (”Limit theorem of de Moivre and Laplace”) but in practice is good starting from very modest n.

3. Binomial distribution

see 688_probab.nb

Consider a ”loaded” coin with unequal probabilities of heads and tails, p and $q = 1 - p$. Then, probability to get m heads is

$$P_m^{bin} = C_n^m p^m q^{n-m} \tag{116}$$

see Fig. 25.

HW: *(a) verify normalization*

$$\sum_{m=0}^{n} P_m^{bin} = 1$$

(b) show that

$$\bar{m} \equiv \sum_{m=0}^{n} m P_m^{bin} = pn \tag{117}$$

F. Normal distribution

see Fig. 26 and the end of 688_probab.nb.

For

$$Z = \frac{x - \bar{x}}{\sigma}$$

$$P(Z) = \frac{1}{\sqrt{2\pi}} e^{-Z^2/2} \tag{118}$$

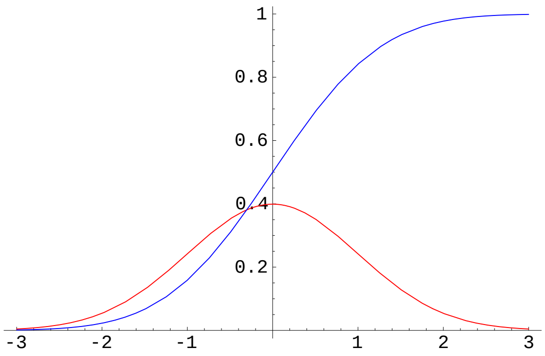

FIG. 26: Normal probability density (red) and cumulative distribution (blue).

and

$$F(Z) \equiv \int_{-\infty}^{Z} P(u)du = \frac{1}{2}\left[1 + \mathrm{erf}(Z)\right] \tag{119}$$

with

$$\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-x^2} dx \equiv 1 - \mathrm{erfc}(z) \tag{120}$$

HW: *Write the distribution in terms of x; find $\langle x \rangle$ and $\langle x^2 \rangle$*

G. Limits of the binomial distribution

1. *Poisson*

Consider $n \to \infty$, $p \to 0$ with fixed $\bar{m} = pn$. Then,

$$P_m^{bin} \approx \frac{n!}{(n-m)!\, n^m} \frac{\bar{m}^m}{m!} \left(1 - \frac{\bar{m}}{n}\right)^n = \frac{\bar{m}^m}{m!} e^{-\bar{m}} \tag{121}$$

which is the Poisson distribution, P_m. See Fig. 27 and 688_poisson.nb.

HW: *(a) verify normalization*

$$\sum_{m=0}^{\infty} P_m = 1$$

(b) find

$$\bar{m} \equiv \sum_{m=0}^{\infty} m P_m$$

(c) find

$$\left\langle m^2 \right\rangle \equiv \sum_{m=0}^{\infty} m^2 P_m$$

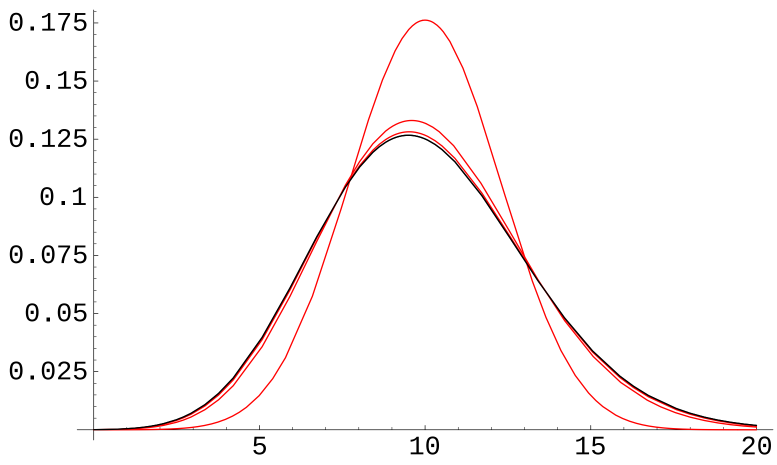

FIG. 27: Poisson distribution P_m (black) for $\bar{m} = 10$ and binomial distributions P_m^{bin} (red) with different n and $p = \bar{m}/n$. From top to bottom: $n = 20$, $n = 100$ and $n = 400$ (which practically blends with the Poisson curve)

2. Normal

Alternatively, let m be close to the average $n/2$ for $p = q = 1/2$. We will use

$$x = 2m - n$$

and further switch to scaled

$$y = x/\sqrt{n} \sim 1$$

(with this the distribution is multiplied by $\sqrt{n}$ to ensure normalization). This leads to Gaussian. Major steps:

- use Stirling approximation

$$n! \simeq \sqrt{2\pi n}\,(n/e)^n \quad , \quad n \gg 1 \tag{122}$$

  for *both* $n!$ and $(n-m)!$

- replace m by $\left(n + y\sqrt{n}\right)/2$ (and multiply by $\sqrt{n}/2$ to ensure normalization).

- Take the limit $n \to \infty$

-

$$P^{gauss}(y) = \frac{1}{\sqrt{2\pi}} e^{-y^2/2} \tag{123}$$

See the end of 688_probab.nb.

H. Central limit theorem

see p. 1057 in KR. and 688_probab.nb.

Let

$$y_n = X_1 + \ldots + X_n$$

with

$$\mu = \langle X_n \rangle \ , \ \ \sigma^2 = \left\langle (X_n - \mu)^2 \right\rangle$$

for *any* n. Then, for $n \to \infty$ the distribution for Y_n is asymptotically normal with

$$\mu_y = n\,\mu \ , \ \ \sigma_y^2 = n\sigma^2 \tag{124}$$

Note that we do not need a gaussian X, only large n(!)

For a "binary" distribution $X = \{0, 1\}$ we could see it above (in that case y_n is binomial and is known exactly). For a different X consider a inform distribution

$$p(X) = \frac{1}{\sqrt{3}} \ , \ \ 1/2 - \sqrt{3}/2 \leq X \leq 1/2 + \sqrt{3}/2$$

HW: *find* μ *and* σ^2

see Fig. 28.

I. Other continuos distributions

not in KR.

1. Exponential

$$p(x) = \frac{1}{\mu} \exp\left(-\frac{x}{\mu}\right) \tag{125}$$

with

$$\bar{x} = \mu$$

.

HW: *(a) calculate* $\langle x^2 \rangle$ *; (b) find* $F(x)$

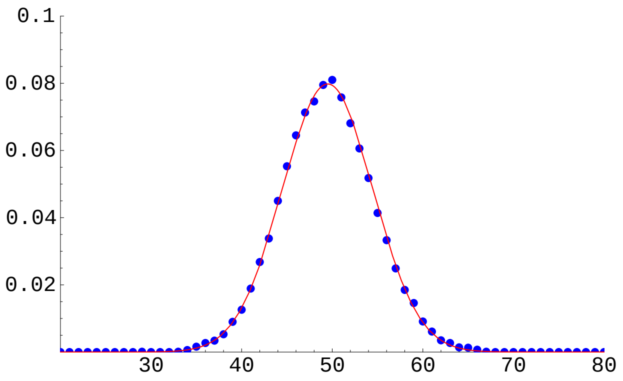

FIG. 28: Illustration of central limit theorem. A sum of a large number (100) of independent random variables has a gaussian distribution, while each individual variable can have an arbitrary non-gaussian distribution. In the example -see 688_probab.nb- individual random variables were informly distributed with an average $\mu = 1/2$ and variance $\sigma^2 = 1/4$. Points (blue) correspond to an experimental histogram after 10000 runs; the line (red) is the normal distribution with average $\mu_{100} = 100\mu - 1/2$ and variance $\sigma_{100} = \sigma\sqrt{100}$. (the $-1/2$ is due to introducing a discrete histogram).

2. *Gamma and* χ^2

$$f(x) = \lambda \exp(-\lambda x)(\lambda x)^{t-1}/\Gamma(t) \tag{126}$$

with $\lambda = 1/2$ and $t = n/2$ (integer n) this is χ^2 distribution.

HW: *(a) calculate* $\langle x \rangle$ *; (b) find* σ^2 see 688_probab.nb.

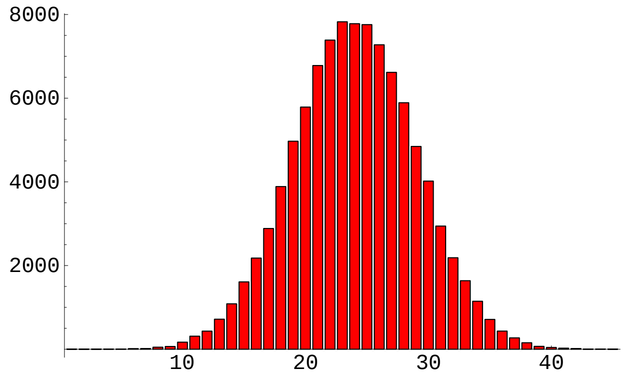

FIG. 29: The histogram of random displacements

Dr. Vitaly A. Shneidman, Phys/MtSE 688, 12th Lecture

Note: *the homework problems listed below will determine 15% of the final exam. The description should contain a clear hand-written part (in pen) and hard copies of mathematica notebooks. This homework must be submitted together with the final.*

J. Random walk and connection to the diffusion problem

Consider a random walk

$$x_{n+1} = x_n + \zeta \tag{127}$$

with $\zeta = \pm 1$ being a random variable. Consider now n random steps with $n \gg 1$ (say, 200), and repeat many times, (say, 10000).

we want to compare this to exact - see below.

K. Exact description (Binomial distribution)

Consider a total of n steps with equal probabilities of 1/2 to go right or left. If there were m steps to the right (and $n - m$ steps left) there will be a total displacement of $m - (n - m) = 2m - n$ steps. Since the steps are taken in any order, there will be

$$C_n^m = \frac{n!}{m!(n-m)!} \tag{128}$$

possibilities to do that (a simple combinatorial problem). All in all, there will be 2^n outcomes of n steps, so that

$$\frac{1}{2^n} C_n^m$$

will give the exact probability of going $2m-n$ to the right from origin.

L. Biased random walk

p probability to go right and $q = 1-p$ - probability to go left. Then, probability to make m steps right is

$$P_m^{bin} = C_n^m p^m q^{n-m} \tag{129}$$

M. The diffusion approximation

Consider a "distribution function" f_k with $k = 0, \pm 1, \pm 2, \dots$ (analog of $2m-n$) which changes with "time" t, analog of n. One has

$$\begin{aligned} f_k(t+1) &= f_k(t) + \frac{1}{2} f_{k-1}(t) + \frac{1}{2} f_{k+1}(t) - f_k \\ &= f_k(t) + D\left[f_{k-1}(t) + f_{k+1}(t) - 2f_k(t)\right] \ , \quad D = 1/2 \end{aligned} \tag{130}$$

Considering $f_k(t)$ as a smooth function of both t and k, one has (with k replaced by x):

$$\frac{\partial f}{\partial t} = D \frac{\partial^2 f}{\partial x^2} \tag{131}$$

The solution ("Greens function") is given by

$$G(x,t) = \frac{1}{2\sqrt{\pi D t}} \exp\left\{ -\frac{x^2}{4Dt} \right\} \tag{132}$$

Correspondence with the exact (binomial) distribution is excellent - see Fig. 30.

N. Biased diffusion

Consider a biased random walk with probability p going right, and $q = 1-p$ going left on every step.

$$\frac{\partial f}{\partial t} = D \frac{\partial^2 f}{\partial x^2} + v \frac{\partial f}{\partial x} \ , \quad v = p - q \tag{133}$$

HW: *derive this*

The Green's function just drifts with time

$$G_b(x,t) = G(x - vt, t)$$

HW: check this

Again, correspondence is excellent - see Fig. 31.

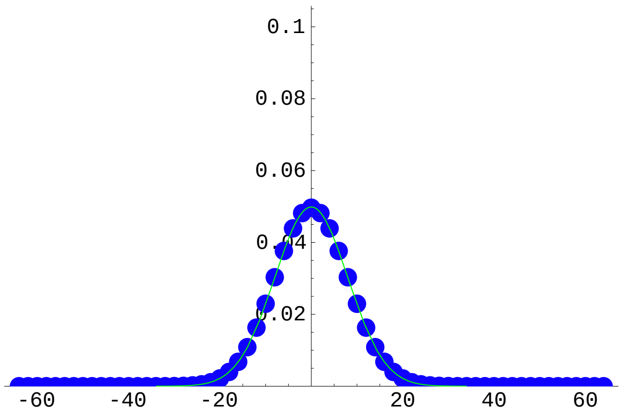

FIG. 30: Non-biased random walk (points) and the diffusion approximation

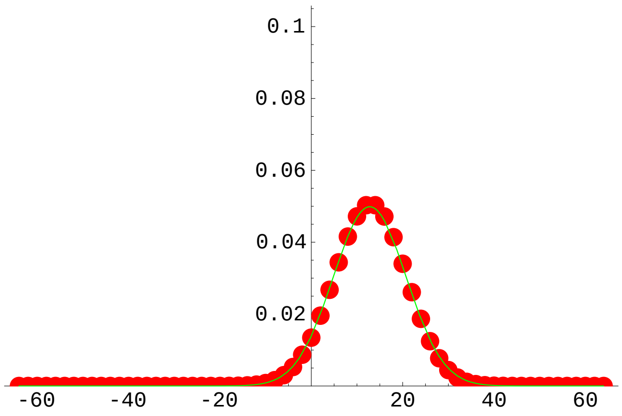

FIG. 31: Same, for a biased random walk.

O. Expectation and moments

$$E(g) \equiv \langle g(X) \rangle = \sum_i g(x_i)\, p(x_i) \;\rightarrow\; \int_{-\infty}^{\infty} g(x) p(x)\, dx \tag{134}$$

kth moment:

$$\mu_k = E\left(X^k\right) \;,\;\; \mu_1 \equiv \mu \tag{135}$$

kth *central* moment:

$$M_k = E\left((X-\mu)^k\right) \;,\;\; M_2 \equiv \sigma^2 \tag{136}$$

HW: *Show that* $\mu_0 = M_0 = 1$

Dimensionless central moments (not in KR.):

$$\gamma_k = M_k/\sigma^k \tag{137}$$

with γ_3 - "skewness" and γ_4 - "kurtosis".

HW: *show that for normal distribution $\gamma_3 = 0$ and $gamma_4 = 3$ (for which reason $\gamma_4 - 3$ is called "excess curtosis")*

P. Distrubution of several variables

READING: KR., Ch. 24.9

Probability density

$$p(x, y)$$

which satisfies all axioms of probability. (in fact, for 2 variables Veen diagrams are the most insructive)

1. *Cumulative distribution*

$$F(x, y) \sum_{x_i \le x \, , \, y_j \le y} p\left(x_i \, , \, y_j\right) \;\rightarrow\; \int_{-\infty}^{x} \int_{-\infty}^{y} p(x, y)\, dx\, dy \tag{138}$$

2. *Multivariate Gaussian distribution*

With

$$\vec{r} = (x, y, \ldots)$$

$$p\left(\vec{r}\right) = C \exp\left(-\frac{1}{2} \vec{r} \cdot \hat{A} \cdot \vec{r}\right) \;,\;\; C = \frac{\left|\det A\right|^{1/2}}{(2\pi)^{d/2}} \tag{139}$$

where d is the dimension of r (2 in our case). [Proof in class].

3. *Covariance and correlation*

$$\mathrm{Cov}\left[X, Y\right] = E\left[\left(X - \mu_x\right)\left(Y - \mu_y\right)\right] \tag{140}$$

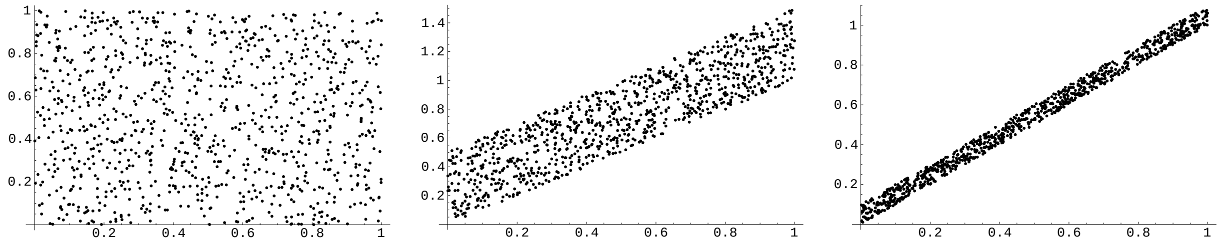

FIG. 32: Charge of pattern from non-correlated data (left) to strongly correlated data (right)

with

$$\mathrm{Cov}\,[X, X] = \sigma_x^2 \tag{141}$$

Correlation:

$$\mathrm{Corr}\,[X, Y] = \frac{\mathrm{Corr}\,[X, Y]}{\sigma_x \sigma_y} \tag{142}$$

and

$$\mathrm{Corr}\,[X, X] = \mathrm{Corr}\,[Y, Y] = 1$$

(thus, one can introduce a *correlation matrix*, $\hat{V}$.)

HW: *Construct $\hat{V}$ for a single die with X being the number on the face and Y the square of that number*

4. Statistical analog of covariance and correlation

Covariance:

$$s_{xy} = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y}) \tag{143}$$

The rest is similar. Note: a good random number generator should give practically uncorrelated results - see 688_corr.nb

5. Independent random variables

$$p(x, y) = p_1(x) p_2(y)$$

or

$$F(x,y) = F_1(x)F_2(y)$$

Then

$$E(XY) = E(X)E(Y)$$

and

$$\sigma^2 = \sigma_1^2 + \sigma_2^2$$

HW: *show that - see p. 1039 in KR. if difficulties*

Q. Modeling and analysis of data

1. Generation of random number for different distributions

Usually, the standard RNG gives a uniform density

$$p(x) = 1 \ , \quad 0 < x < 1$$

with the cumulative distribution being

$$x \ , \quad 0 \leq x \leq 1$$

Then, for another distribution with a cumulative $F(y)$ one has

$$y = F^{-1}(x)$$

Example: exponential distribution - 688_stat.nb

2. Fitting of data and LSA

Fitting to a straight line:

$$y = k_0 + k_1 x$$

with

$$k_1 = \frac{s_{xy}}{\sigma_x^2} \ , \quad k_0 = \bar{y} - k_1 \bar{x} \tag{144}$$

and s_{xy} being "sample covariance".

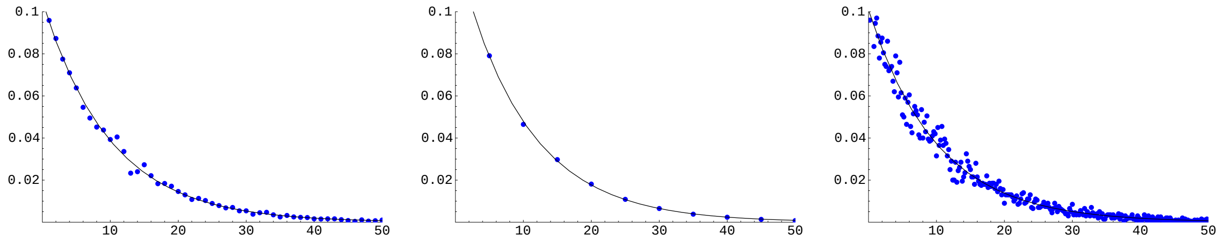

FIG. 33: "Experimental" studies of exponential distribution. 10000 data were produced by a do-it-yourself RNG obtained from a modified built-in RNG for uniform distributions (see text and 688_stat.nb) and grouped into different bins. From left to right: bin size 1, 5 and 0.2. In each case solid line is exponential approximation obtained from non-linear fit.

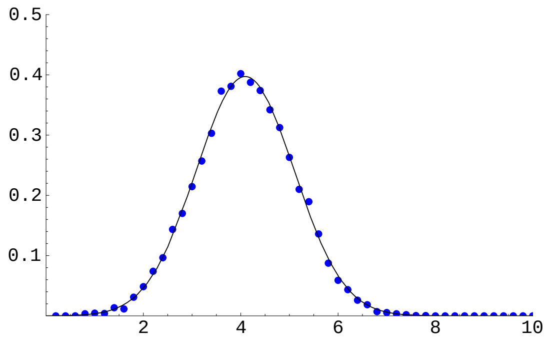

FIG. 34: Experimental studies of a normal distribution. 10000 data were produced using a RNG from standard package in Mathematica and grouped into bins. Solid line is the best non-linear fit by a gaussian curve.

In *Mathematica* linear fit is achieved using the "Fit" command with functions $\{1, x\}$. [More powers of x are possible, as well as nonpower functions, but that is non-linear fit - see 688_stat.nb].

HW: *create a list of 20 points of type* $y = ax + b$*+noise. Use "Fit" command to find a linear fit; compare coefficients to* a *and* b*.*

3. Filtering

will be discussed in class. See 688_stat.nb and Figs. 35 and 36

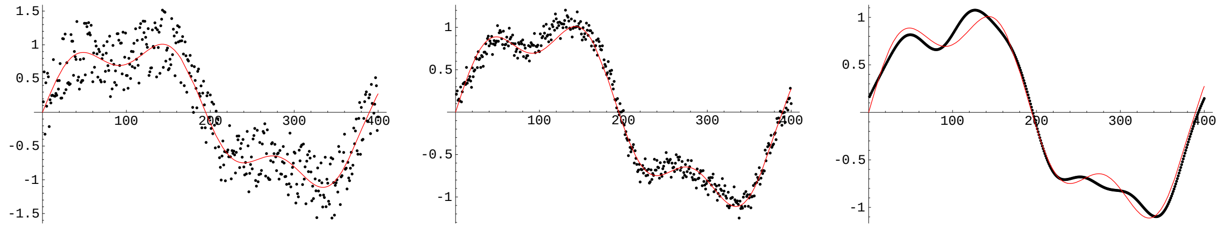

FIG. 35: A do-it-yourself Fourier filter which eliminates "noise" (in fact, any signal) with a fourier component below selected level. Red line - hidden deterministic signal, black dots - full signal after filtering: left - noise cut-off 0.1, middle - noise cut-off 0.6 and right noise cut-off 0.7

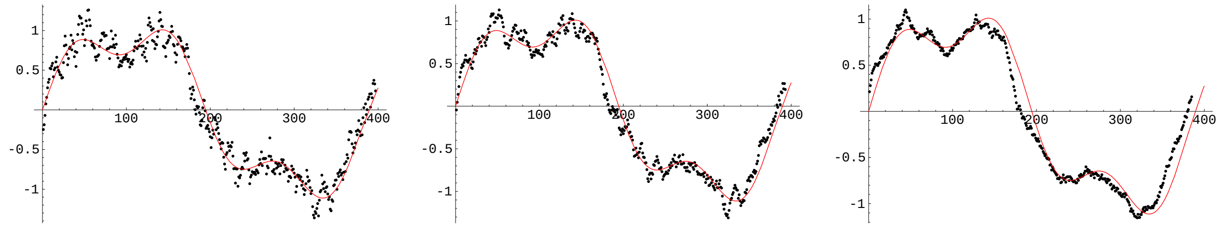

FIG. 36: Same signal as in Fig. 35 processes using the built-in moving average filter.

R. Comparing two distributions

1. χ^2-test

Let X and Y be grouped in N bins each, with $1 \leq 1 \leq N$ being the number of the bin and R_i and S_i be the number of events in a corresponding bin for X and Y, respectively. Then,

$$\chi^2 = \sum_i \frac{(R_i - S_i)^2}{R_i + S_i} \tag{145}$$

Evaluate

$$\frac{1}{\Gamma(N/2)} \Gamma\left(\frac{N}{2}, \frac{\chi^2}{2}\right) \tag{146}$$

If this is close to 1 the two distributions are close. - see 688_stat.nb. Note

- the total number of events for X and Y is not required the same (otherwise $N \rightarrow N-1$).
- bins should be filled up; 1-2 empty bins can be ok, but if a bin is empty for both X and Y will not work.

- works well if the number of bins is large
- can be used to compare with a known distribtion with S_i in the numerator replaced by a known n_i and the entire denominator replaced by the the same n_i

2. Kolmogorov-Smirnov test

$$Q_{ks}(\lambda) = 2\sum_{i=1}^{\infty}(-1)^{i-1}\exp\left(-2i^2\lambda^2\right) = 1-\theta_4\left(0, e^{-2\lambda^2}\right) \tag{147}$$

Consider two unbinned distribution with N points in each.

- Construct cummulant distributions $S_1(x)$ and $S_2(x)$
- find the maximum distance

$$D = \max_{-\infty<x<\infty} |S_1(x) - S_2(x)|$$

- Evaluate

$$Q_{ks}\left(\sqrt{N/2}D\right)$$

- If the number is close to 1 distributions are similar.

Note:

- distributions must be one-dimensional each
- can be used if disfferent number of points with $N/2 \rightarrow N_1N_2/\left(N_1+N_2\right)$
- can be used for comparison with a known distribution with $N/2 \rightarrow N$

HW: *LAST HW: (a) create 2 lists of 40 random points each with exponential distribution (see 688_stat.nb). (b) perform the χ^2-test (c) perform the KS test*
========================

APPENDIX A: A BIT OF *MATHEMATICA*

See the file 688_intro.doc for more detailed ouput, graphics, etc.

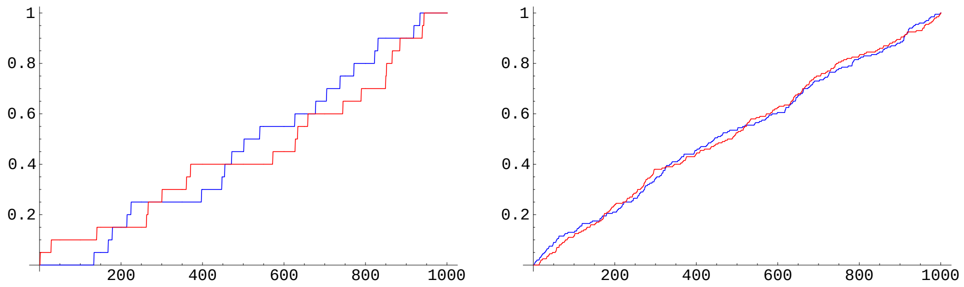

FIG. 37: Cumulative distributions used in Kolmogorov-Smirnov test for comparing two distributions. Each set of data was generated using the standard uniform RNG (so that distributions are expected identical if the number of points is large). Left - 20 points in each distribution, right - 200 points. The KS test identifies distributions with each other with confidence 0.33 for the 1st case and confidence 0.987 for the 2d.

1. Basic elementary commands

```
HELP:
 1) if you know the exact command , but want to refresh what
argument it requires, use ?.  E.g.
?Sin
2) if you approximately know the spelling, use ? with * for the
unknown part, e.g.
 ?*Plot*
gives all commands which have Plot in them
3) if you have no idea - use Help button (will not work in "math"
mode).



Frequent type- and space-saving commands:
1) % uses the last output as input.
       Similarly, %% uses the one before last output, etc. Or, %12
2) space - can be used instead of * for multiplication:
3) ; will not produce an output on the screen (but can
work with it further!)
```

(main typesaving - defining your own functions, etc. - will study later).

Saving your work:

There are two ways:

1) Save["filename", symbol] appends definitions associated with the specified symbol to a file.

if symbol includes previous definitions, will save everything which is required! "filename" usually includes .m at the end (for convenience), but you can be creative. Graphics cannot be saved this way, but you can save the last command used to generate it, and then recreate the picture upon restarting Mathematica. Files are in plain text and relatively small.

Example:

In[1]:= fig:=Plot[Sin[x]/x, {x,-8,8}] (we defined a plot function, fig)

In[2]:= Save["figSinc.m", fig] (saved this function in a file figSinc.m)

In[3]:= !!figSinc.m (this shows the contents of the file)

fig := Plot[Sin[x]/x, {x, -8, 8}]

Now, if you start a new Mathematica session, you can type

<< figSinc.m

and you will have all saved definitions. Command fig will plot your picture.

2) you save as a notebook, with all graphics you created (and all the junk). Saved files are BIG, and can quickly overflow your directory if caution is not used. Use sparingly, and only for work you feel you really need and which you cannot save using the Save command.

2. NUMBERS

```
1) Integer
2) Exact - 1/2, 10^-10, Pi, E, Sqrt[2], EulerGamma, etc.
3) approximate - 2. , 10.^-10,  pi= N[Pi,15], e=N[E,7], etc.
4) Complex numbers:
I represents the imaginary unit Sqrt[-1], e.g.
z = 2+3I and then Abs[z]=..., Arg[z]=..., etc.
5) Random numbers, e.g.
Random[]
```

3. SYMBOLIC MATH

```
Sum, e.g.:
In[74]:= Sum[i^2, {i,1,n}]
or
In[74]:= Sum[i^-2, {i, 1, Infinity}]

Derivatives and integration:
In[75]:= D[x^n,x]
            -1 + n
Out[75]= n x
In[76]:= D[%,x]
                     -2 + n
Out[76]= (-1 + n) n x
In[77]:= Integrate[%,x]
            -1 + n
Out[77]= n x

 Algebraic operations:
Expand, Factor, Collect, Simplify, etc.
```

Trigonometry:

TrigExpand and TrigReduce

Connection with exponential notations:

```
In[8]:=  ExpToTrig[Exp[I x]]
Out[8]= Cos[x] + I Sin[x]
```

or

```
In[9]:= TrigToExp[Cos[x]+I Sin[x]]
           I x
Out[9]= E
```

Power serieses:

```
In[118]:= Series[Exp[a x], {x, 0, 5}]
```

To make a polynomial by truncating a series:

```
In[119]:= Normal[%]
```

Will give a series even if there is a simple singularity (Laurent series):

```
In[1]:= Series[1/Sin[t], {t,0,2}]
        1   t       3
Out[1]= - + - + O[t]
        t   6
```

Limit:

```
In[123]:= Limit[(1+x/n)^n, n->Infinity]
           x
Out[123]= E
```

4. DEFINING YOUR OWN FUNCTIONS

```
In[1]:= f[x_]:=Sin[x]
In[3]:=Plot[f[x]/x, {x,-6,6}] (*will give a plot*)
Can define and save a plotting function:
In[23]:= plotf:=Plot[f[x]/x, {x,-6,6}]

Difference between := and =
In[19]:= r=Random[];
In[20]:= Table[r, {i,5}]
Out[20]= {0.307826, 0.307826, 0.307826, 0.307826, 0.307826}
Gives identical numbers since r was assigned a fixed value
but
In[21]:= Clear[r]; r:=Random[]
In[22]:=  Table[r, {i,5}]
Out[22]= {0.0592439, 0.981402, 0.944823, 0.0902293, 0.598816}
gives different values each time r is evaluated

A third assignment (dangerous!):
Clear[x]; f[x_]=Sin[x]
Must use Clear (!)
```

5. Graphics (2D)

Main functions: Plot, Show, ListPlot

Options: PlotStyle, AxesLabel, etc.

Text, arrows, etc.

Plot[f, {x, xmin, xmax}] generates a plot of f as a function of x from xmin to xmax. Plot[{f1, f2, ... }, {x, xmin, xmax}] plots several functions.

PlotRange is an option for graphics functions that specifies what points to include in a plot.

Show[graphics, options] displays two- and three-dimensional graphics, using the options specified. Show[g1, g2, ...] shows several plots combined.

Dashing[{r1, r2, ... }] is a two-dimensional graphics directive which specifies that lines which follow are to be drawn dashed, with successive segments of lengths r1, r2, ... (repeated cyclically).

Examples:

```
In[12]:= Clear[plo]
In[13]:= plo[n_]:=Plot[Sin[n x]/x, {x,-2,2}, PlotRange -> {-1,2},
PlotStyle -> Dashing[{0.01*n, 0.02}]]
In[15]:= sho:=Show[Table[plo[n], {n,1,3}]]
In[16]:= sho (*will give graphics*)
```

AxesLabel -> {x, y} will label each axes.

Plotting discrete data points:

ListPlot[{y1, y2, ... }] plots a list of values. The x coordinates for each point are taken to be 1, 2, ...

ListPlot[{{x1, y1}, {x2, y2}, ... }]
   plots a list of values with specified x and y coordinates.

Example:

```
In[21]:= list=Table[Sin[i/100.]+.1*Random[], {i,100}];
In[22]:= ListPlot[list]
Out[22]= -Graphics-
```

Main extra options:e.g., PlotStyle -> PointSize[0.02], or PlotJoined->True

Parametric plot:

ParametricPlot[{fx, fy}, {t, tmin, tmax}] produces a parametric plot with x and y coordinates fx and fy generated as a function of t. Example:

```
In[2]:= x[phi_]:=Cos[phi];
In[3]:= y[phi_]:=Sin[phi];
In[4]:= ParametricPlot[{x[phi],y[phi]}, {phi, 0, 2Pi}]
 -Graphics- (not a circle on the screen)
(*by default, AspectRatio ->GoldenRatio;
need to use Show[%, AspectRatio -> Automatic]*)
```

Arrow: need to use a package.

```
<<Graphics`Arrow` (*note direction of quotes!*)
e.g.,
arr = Graphics[Arrow[{0,0}, {1.1}, HeadLength ->0.03]];
(*HeadLength is optional*)
Show[Plot[-x, {x,-1.5,1.5}], arr]
```

PlotLabel:

can be simple text, PlotLabel -> "mypicture" or

Labels as parameters:

```
plo[n_] := Plot[x^n, {x, 0, 1}, PlotLabel ->n] (*no quotes
now!!!*)

(*suppose we like what we see and want to create, a
postscript file, e.g. t.ps *)
disp[n_]:=Display["t.ps", plo[n], "EPS"]
(*now disp[3] will create t.ps, as a GOOD postscript
which is outside of Mathematica and can be further used
independently*)
```

Hiding graphics:

use DisplayFunction->Identity

Then will give output Graphics on the screen (if no errors), but no picture. Used mostly to avoid intermediate plots. Restore picture in Show using DisplayFunction->$DisplayFunction. Example:

```
In[13]:= plo[n_]:=Plot[Sin[n x]/x, {x,-2,2}, PlotRange -> {-1,2},
PlotStyle ->Dashing[{0.01*n, 0.02}], DisplayFunction->Identity ]
In[14]:= plo[1]
Out[14]= -Graphics-
In[15]:= Show[Table[plo[n], {n,1,3}],
DisplayFunction->$DisplayFunction]
```

Graphics Primitives:
Line[{pt1, pt2, ... }] is a graphics primitive which represents a line joining a sequence of points.
Point[coords] is a graphics primitive that represents a point.
Circle[{x, y}, r] is a two-dimensional graphics primitive that represents a circle of radius r centered at the point x, y.
Polygon, etc. use with Graphics, similar to Arrow

Color:
RGBColor[red, green, blue] is a graphics directive which specifies that graphical objects which follow are to be displayed, if possible, in the color given."
Example: plotting 2 different Bessel functions with red and green:

```
In[1]:= Plot[{BesselI[1, x], BesselI[2, x]}, {x, 0, 5},
 PlotStyle -> {RGBColor[1, 0, 0], RGBColor[0, 1, 0]}]
```

or, same thing:

```
In[2]:= red=RGBColor[1, 0, 0]; green=RGBColor[0, 1, 0];
In[3]:= Plot[{BesselI[1, x], BesselI[2, x]}, {x, 0, 5},
 PlotStyle -> {red, green}]
```

see file 688_intro.doc for 3D and more advanced graphics.