Mathematics and Modelling

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More about this document

Summary:

Here is a collection of various miscellaneous bits of mathematics useful for nuclear engineering that you need to know but may have forgotten. It is intended as refresher material, not as material for first-time learners.

Reference textbook: Chapra and Canale, Numerical Methods for Engineers, 5th edition, Publishers: McGraw Hill, ISBN 0-07-291873-X, TK345.C47, Year: 2006.

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1 Introduction

1.1 Overview

Notes on how the class will be conducted:

- short lecture
- worked examples
- hands-on
- break.

More advanced students in a given topic can help others or can try a tougher problem of the same topic.

Safe sandbox to build confidence and competence. Not intended to give you mastery, just help you on your way.

1.2 Assessment

There are two forms of assessment: formative and summative. Formative assessment is feedback during the learning process to guide the student, identify strengths and weaknesses and so on. Summative assessment is testing with some sort of grade assigned.

Herein, there will be no formal assigned grade. Assessment will be informal and formative. To the extent that is possible in the compressed nature of this course, it will be individual.

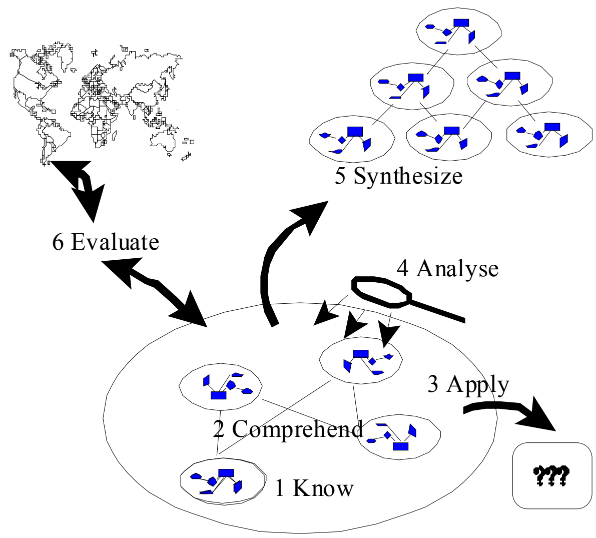
1.3 Learning Outcomes

The goal of this course is for the student to understand:

- The basic mathematical tools needed for nuclear engineering.

But what do we mean by 'understand'? See http://www.nuceng.ca/teach/teachindex.htm and read *Learning 101 - A Student Guide to Effective Learning*, especially section 3. Therein, 6 levels of understanding are enumerated:

- 1 Knowledge
- 2 Comprehension
- 3 Application
- 4 Analysis
- 5 Synthesis
- 6 Evaluation.



The first three levels are certainly required for an engineer[1]. Likely, proficiency on the analysis level is also required in most topic areas. Since the reality does not follow procedures and since procedures, even if we tried very hard to reduce reality to procedures, could not possibility cover off all possible scenarios, the engineer will be required to switch from one procedure to a more appropriate one on a regular basis. In addition, if an error was made in the execution of a procedure, the engineer would be required to recover from this error. These situations require analysis, perhaps interpolation of current practice, and, to the extent that extrapolation of current procedures are required, synthesis. Evaluation, or that 'heads up' view of life, would likely be required as a matter of course.

1.4 Why Math and Modeling

Working engineers are interested less in math for its own sake as they are interested in math as it relates to their reality. We stylize our reality by the use of models. Hence we arrive at math and modeling as a core need. But how do we achieve that?

1.5 Math Pedagogy

One does not understand math so much as one becomes familiar with it. The more you fiddle with it, the more it makes sense.

1.6 Mental Modeling Pedagogy

Modeling is pattern recognition, which is inherent in our way of thinking. So we are all capable, to some degree at least, of being able to abstract a mental model. Our lives are full of concepts

1 We can extend our coverage to scientists as well as engineers but for brevity this text will simply write 'engineers' for the sake of brevity and with out loss of generality. Apologies to those feeling slighted.

(mother, hot, cold, up, left, etc). It is a stylization of reality. A triangle is a model. They are all constructs of the mind to facilitate manipulation. An idea is a model. We lump concepts to build up a hierarchy of concepts to form more complex, layered models.

People are pattern recognition machines. We can memorize facts and images but that is of limited use in facing new situations. We need an internal representation, a mental model, that can make sense of a situation that can look beyond the image seen to model the processes and make predictions. These are abstractions of reality and allow us to interpolate and extrapolate so that we can make sense of the new images we see. We need this because the future, the new situations, are not just repeats of the past. Pure memory is of little value. It also seems that memorizing facts with no context is difficult. It is far easier to remember facts when there is a context.

Thus learning should be mental model based, not memory based. See http://teachingmath.info . In that research, it was found that mental models are learned when people try to achieve a goal and receive feedback after each effort. So, according to that research, mental models can be taught by giving students a goal to accomplish. This is goal-oriented learning. The author suggests this works because the human brain was designed to achieve goals, and thus this is a natural way for human beings to learn. Putting this all together, the natural technique for teaching mental models is goal-oriented learning. It was found that it does not work to just teach a solution because the students just memorize the procedure. Problem solving works better.

1.7 Study techniques

The student is urged to visit http://www.nuceng.ca/teach/teachindex.htm and read *Learning 101 - A Student Guide to Effective Learning* for some general tips on studying and for some insight into how it is that we learn, internalize and use knowledge and skills.

1.8 Mastery

It takes considerable effort and time to master any skill. And if you are going to work that hard and spend that much time at it, you might as well enjoy it as much as you can. Hard word and enjoyment are not contradictions. In fact, it turns out that real joy can come from the process of mastering something. For more on this, see http://www.nuceng.ca/teach/teachindex.htm and read *Mastery - proceeding with a sense of quality*. The key, and this applies to the task of learning more than anything else, is to proceed at an optimal pace – not too slow and not too fast, and to ramp up the complexity of the task as your abilities grow. It’s a mindset.

Don’t confuse speed with mastery. Deep thinking takes time. Don’t be swayed off your path by the apparent speed of others.

You need to master the prerequisites (or refresh yourself in them if you have forgotten them) before you can move on to subsequent material.

And so, we begin.

2 Engineering Concepts, Equations and Context

2.1 The Evolution of Physics

There is a rather interesting little book *The Evolution of Physics* by A. Einstein and L. Infeld (see http://www.nuceng.ca/eng2c3/eng2c3index.htm for a summary) that surveys the evolution of the concept of a "field". It is common place now to think of reality in terms of force fields, including gravity, electricity, and magnetism. But these are recent concepts, dating from the early 1800's or so. The development of the mathematics and physics in the last 200 years has been a phenomenal success…Maxwell's equations, relativity, potential and kinetic energy, and so on, all are based on the concept of a field. Yet, we still don't know what a field is and probably never will. In the end, the force field is a convenient mathematical construct whose sole justification is that it works.

And so it is with mathematics. As I said above, one does not understand math so much as one becomes familiar with it. It is astoundingly and unreasonably useful. But useful it is.

So if you have harboured deep and nagging doubts about science and mathematics, and thought that this was a personal shortcoming, then perhaps you had a good understanding of math and scientific thinking after all. This doubt is justified but we must press on regardless. This doubt raises a big of mystery and wonder to it all, making the pursuit of knowledge all the more interesting. And amazing.

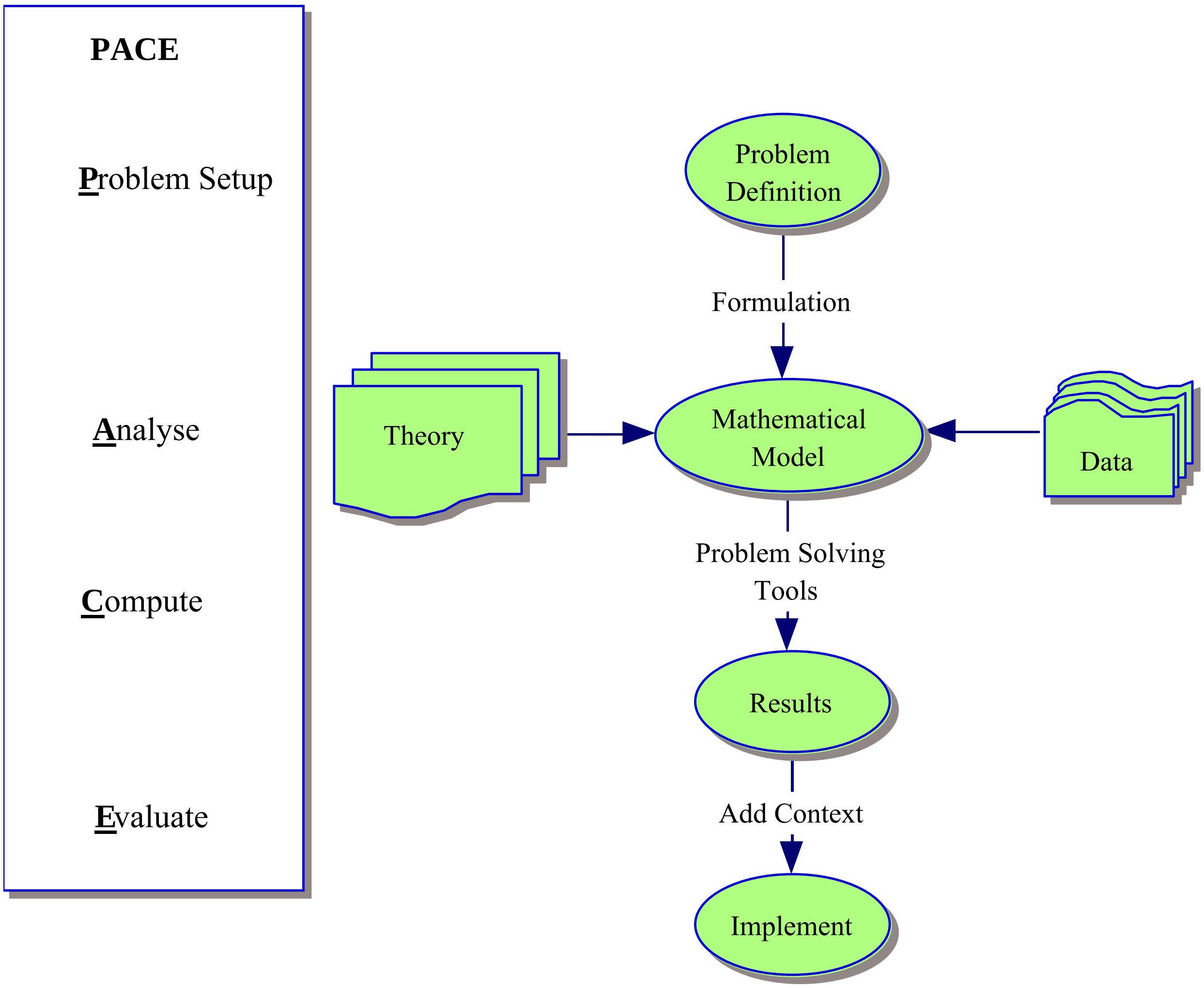
Exercises:

1. Define force. Then define the terms you used to define force.

2.2 A Simple Mathematical Model

[Reference C&C 1.1]

Typically we proceed systematically as shown below. PACE yourself!



Let's take a simple example to illustrate the above and to introduce some concepts along the way. This will be typical of the approach in this course: introduce concepts in context to link the abstract with the concrete.

2.3 Force Balance

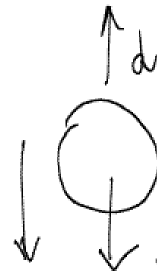
Consider a falling object:

$$F = ma$$

or

$$ma = \sum_i F_i$$

$$a = \frac{dv}{dt} \qquad v = \frac{dx}{dt}$$



$\uparrow$ drag $= F_{drag} = -cv$ or $-cv^2$ or whatever

$mg = F_{gravity}$

+ve direction

or
$$\frac{dv}{dt} = \frac{1}{m}\sum_i F_i = \frac{1}{m}(mg - cv) = g - cv/m$$

Solution:

Can sometimes do it analytically if the problem is simple enough but usually we have to use numerical techniques.

Analytical solutions are good for 'ball parking' results, scoping studies, looking for relationships and effects of the various parameters on the solution. They are often a good sanity check on numerical results.

Numerical solutions are good for more realistic assessments and have a broader applicability.

Analytical solution

Let $v = u + b$

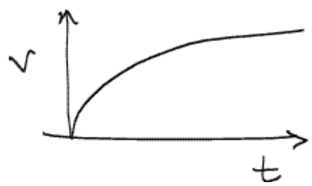
$$\therefore \frac{du}{dt} = g - \frac{cu}{m} - \frac{cb}{m} \Leftarrow \text{choose } b = gm/c$$

$$\Rightarrow \frac{du}{dt} = -cu/m \Rightarrow u = u_0 e^{-ct/m}$$

Initial condition $v_0 = 0 \quad \therefore v_0 = u_0 + b = u_0 + gm/c = 0$

$$\therefore u_0 = -gm/c$$

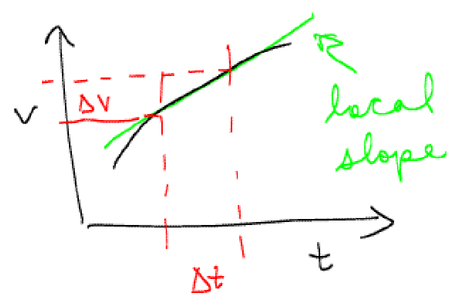
$$\therefore v = u_0 e^{-ct/m} + gm/c = \frac{gm}{c}\left(1 - e^{-ct/m}\right)$$



Numerical solution

$$\frac{dv}{dt} = g - \frac{cv}{m} \simeq \frac{\Delta v}{\Delta t} = \frac{v^{t+\Delta t} - v^{t}}{\Delta t}$$

$$\therefore v^{t+1} = v^{t} + \Delta t\left(g - \frac{cv^{t}}{m}\right)$$



Use a spreadsheet or code to solve. Try it for g = 9.8 m/s2, c = 12.5 kg/s, m = 68.1 kg for various time steps and compare to analytical solution.

Notes:

1. The nice thing about the numerical solution is that we can easily add more realism, complicated time-varying drag coefficient, etc., and still solve with ease.
2. The above numerical solution technique (Euler) is simple to implement but can lead to large errors and instabilities for larger time steps. More on this later.

Exercise:

1. What is the distance traveled? Do analytically and numerically.

2.4 Conservation Laws

[Reference C&C 1.2]

This section presents common equation types and computational situations that engineers encounter and points to what math is needed.

A basic law that comes up often is conservation:

$$\frac{dc}{dt} = \sum_1' \text{sources} - \sum_1' \text{sinks}$$

This applies to mass ← see Gd removal example.
energy
momentum

Examples

$$\frac{1}{v}\frac{\partial}{\partial t}\phi(\mathbf{r},t) \equiv \frac{\partial}{\partial t}n(\mathbf{r},t) = s(\mathbf{r},t) - \Sigma_a(\mathbf{r})\phi(\mathbf{r},t) - \nabla\bullet\mathbf{J}(\mathbf{r},t)$$

$$\frac{1}{v_g}\frac{\partial}{\partial t}\phi_g(\underline{r},t) = \underbrace{\nabla\cdot D_g(r)\nabla\phi_g(\underline{r},t)}_{\text{leakage}} - \underbrace{\Sigma_{ag}(r)\phi_g(\underline{r},t)}_{\text{loss by absorption}} - \underbrace{\Sigma_{sg}(r)\phi_g(\underline{r},t)}_{\text{removal by scattering}} + \underbrace{\sum_{g'=1}^{G}\Sigma_{sg'g}(r)\phi_{g'}(\underline{r},t)}_{\text{scattering into group g}}$$

$$+ \underbrace{\chi_g}_{\text{fraction appearing in group g}} \underbrace{\sum_{g'=1}^{G}\nu_{g'}\Sigma_{fg'}(\mathbf{r})\phi_{g'}(\underline{r},t)}_{\text{total fission production}} \underbrace{+S_g^{ext}}_{\text{external source}}$$

$$\frac{1}{v}\frac{\partial}{\partial t}\phi(\mathbf{r},t) = \nabla\cdot D(\mathbf{r})\nabla\phi(\mathbf{r},t) - \Sigma_a(\mathbf{r})\phi(\mathbf{r},t) + (1-\beta)\nu\Sigma_f(\mathbf{r})\phi(\mathbf{r},t) + \sum_{i=1}^{6}\lambda_i C_i$$

$$\frac{\partial}{\partial t}C_i(r,t) = -\lambda_i C_i(r,t) + \beta_i\nu\Sigma_f(r)\phi(r,t)$$

$$a_{1,0}\begin{pmatrix} a_{11} & a_{12} & & & & \\ a_{21} & a_{2,2} & a_{2,3} & & & \\ & & \ddots & & & \\ & & a_{PW} & a_{PP} & a_{PE} & \\ & & & & \ddots & \\ & & & & a_{N,N-1} & a_{N,N} \end{pmatrix} a_{N,N+1} \begin{pmatrix}\phi_1\\ \phi_2\\ \vdots\\ \phi_P\\ \vdots\\ \phi_N\end{pmatrix} = \begin{pmatrix}S_1\\ S_2\\ \vdots\\ S_P\\ \vdots\\ S_N\end{pmatrix}$$

Typical engineering analysis leads to conservation equations which involve:

algebraic equations → notation
→ matrix manipulation

Taylor Series ↓ numerical sol'n ←
Analytical sol'n

ODE's → Laplace Transform
→ Integration
PDE's → Differentiation (chain rule etc.)

Plus we have data analysis

Statistics → definitions, confidence intervals

Probability → binomial distribution
→ Poisson "
→ Gauss "

Signal Analysis → Fourier Series + Transforms
Convolution

Typically, we have systems of interconnected parts

Macro examples – trusses
– piping networks
– circuits

Micro examples – distributed systems (discretized)
– circulation in a tank
– heat flow in solids

In these systems there are at least one equation for each part + these equations are interconnected.

↘ leads to systems of algebraic or ODE's or PDE's

$\underline{\underline{A}}\,\underline{x} = \underline{b}$ ← This is what we invariably end up having to solve.

And so in short, the engineer needs to be fluent in the following areas:

- Algebra
- Calculus
- Vectors result from force and velocity diagrams
- Matrices result from systems of equations
- ODE – ss and transient
- PDE – ss and transient, parabolic, elliptical, hyperbolic
- Analytical and numerical - > Taylor series
- Laplace
- Fourier
- Stats
- Prob

Can only scratch the surface on these topics.
Won't do:

- error analysis
- anything in depth

The goal is just to get you back up to speed and to ensure you feel confident to tackle just about any mathematical situation that might arise on the job.

Once in a while, we'll stop to derive something because sometimes these 'not understood bits' erode your confidence.

Exercise:

What else should be on the list?

Rank them in terms of importance for work noting that it may be important not because you use it today but for how it is a basis for thinking.

Where are your weaknesses?

We need to focus on those items with a high importance : weakness ratio.

3 Vectors (Div, Curl, Grad and all that)

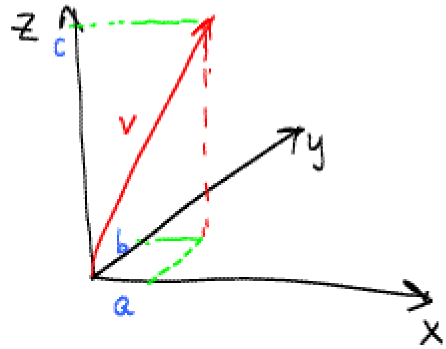
[Reference: http://epsc.wustl.edu/classwork/454/syllabus.html]

3.1 Notation

$$\underline{V} = a\hat{i} + b\hat{j} + c\hat{k}$$

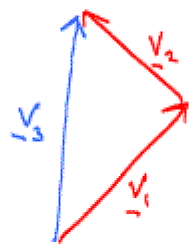
unit vectors

$$|\underline{V}| = \sqrt{a^2 + b^2 + c^2}$$



3.2 Vector Addition

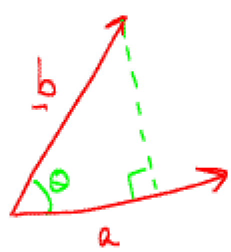
$$\begin{aligned} \underline{V}_3 &= \underline{V}_1 + \underline{V}_2 \\ &= a_1\hat{i} + b_1\hat{j} + c_1\hat{k} \\ &\quad + a_2\hat{i} + a_2\hat{j} + a_3\hat{k} \\ &= (a_1 + a_2)\hat{i} + (b_1 + b_2)\hat{j} + (c_1 + c_2)\hat{k} \end{aligned}$$



3.3 Dot product

for 2 vectors $\underline{a}$ + $\underline{b}$

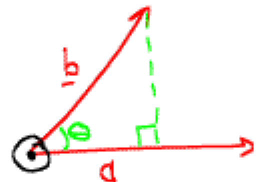
$$\underline{a} \cdot \underline{b} = \underline{b} \cdot \underline{a} = |\underline{a}||\underline{b}| \cos\theta$$
$$= \text{scalar}$$



3.4 Cross Product

$\underline{c} = \underline{a} \times \underline{b} = -\underline{b} \times \underline{a} = |a||b| \sin\theta$

Right hand rule:
$\underline{a}$ = fore finger
$\underline{b}$ = middle finger
$\underline{c}$ = thumb



$\underline{c}$ points out of page (denoted $\odot$)

$\underline{d} = \underline{b} \times \underline{a}$ points into page (denoted $\otimes$)

The result of a cross product is a vector.

We can compute $\underline{a} \times \underline{b}$ from its components as follows:

$$\underline{a} \times \underline{b} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ a_x & a_y & a_z \\ b_x & b_y & b_z \end{vmatrix}$$ ← determinant

$$= (a_y b_z - b_y a_z)\hat{i} - (a_x b_z - b_x a_z)\hat{j} + (a_x b_y - b_x a_y)\hat{k}$$

3.5 Gradient (Grad)

For some scalar $\phi(x,y,z)$ we define the gradient as:

$$\underline{F} = \frac{\partial \phi}{\partial x}\hat{i} + \frac{\partial \phi}{\partial y}\hat{j} + \frac{\partial \phi}{\partial z}\hat{k}$$
$$= \nabla \phi$$

This comes up often in engineering.
ϕ = potential
F = force (typically we define $F = -\nabla\phi$ actually)

Examples: gravity
electrical potential
pressure gradients

3.6 Divergence (Div)

The divergence of a vector is defined as:

$$\nabla \cdot \underset{\sim}{g} \equiv \left(\frac{\partial}{\partial x}\hat{i} + \frac{\partial}{\partial y}\hat{j} + \frac{\partial}{\partial z}\hat{k}\right)\cdot\left(g_x\hat{i} + g_y\hat{j} + g_z\hat{k}\right)$$

$$= \frac{\partial g_x}{\partial x} + \frac{\partial g_y}{\partial y} + \frac{\partial g_z}{\partial z}$$

This comes up when we are modelling flows through a surface of a volume:

$$\int_{\text{surface}} \underset{\sim}{g}\cdot\underline{n}\, ds = \int_{\text{volume}} \nabla\cdot\underset{\sim}{g}\, dV$$

This is the Divergence Theorem

surface normal

This is a pretty remarkable result when you think about it.

3.7 Curl

The curl of a vector is

$$\text{curl}\,\underline{V} = \nabla \times \underline{V} = \left(\frac{\partial}{\partial x}\hat{i} + \frac{\partial}{\partial y}\hat{j} + \frac{\partial}{\partial z}\hat{k}\right)\times\left(V_x\hat{i} + V_y\hat{j} + V_z\hat{k}\right)$$

$$= \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \partial/\partial x & \partial/\partial y & \partial/\partial z \\ V_x & V_y & V_z \end{vmatrix}$$

A useful theorem related to this is:

$$\oint_{l} \underline{V}\cdot d\underline{l} = \int_{s} (\nabla\cdot V)\cdot\underline{n}\, ds$$

Stokes Theorem

line integral
(called the 'circulation')

surface integral

3.8 Laplacian

The Laplacian operator is defined as

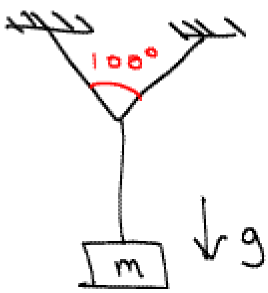
$$\nabla \cdot \nabla \equiv \nabla^2 = \left(\frac{\partial}{\partial x}\hat{i} + \frac{\partial}{\partial y}\hat{j} + \frac{\partial}{\partial z}\hat{k}\right) \cdot \left(\frac{\partial}{\partial x}\hat{i} + \frac{\partial}{\partial y}\hat{j} + \frac{\partial}{\partial z}\hat{k}\right)$$

$$= \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Thus $\nabla^2 \phi = \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2}$ (scalar)

Exercise:

Resolve forces:



What is the tension in each rope?

Ropes are of equal length?

4 Linear Algebra

[ref C&C PT3.1 Pg 217 and following].
[See Reference: http://www.cse.unr.edu/~bebis/MathMethods/ for more details]

Our motivation to study matrices is that we often end up with linear systems of equations of the form:

$$\underline{\underline{A}}\,\underline{x} = \underline{b}$$

which needs to be solved for $\underline{x}$.

4.1 Notation and Basic Rules

We write the matrix $\underline{\underline{A}}$ as:

$$\underline{\underline{A}} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots \\ a_{21} & a_{22} & a_{23} & \cdots \\ \vdots & & & \\ & & & a_{mn} \end{bmatrix}$$

$\longrightarrow$ n columns

$\downarrow$ m rows

$(m \times n)$

$$\underline{\underline{A}} + \underline{\underline{B}} = \underline{\underline{B}} + \underline{\underline{A}}$$

Addition and subtraction are commutative

$\underline{A}$ & $\underline{B}$ must be the same size

$$\underline{\underline{A}} + \underline{\underline{B}} = \begin{bmatrix} a_{11}+b_{11} & a_{12}+b_{12} & \cdots & \cdots \\ a_{21}+b_{21} & & \cdot & \\ \vdots & & \cdot & \end{bmatrix}$$

$$k\,\underline{\underline{A}} = \begin{bmatrix} ka_{11} & ka_{12} & \cdots \\ ka_{21} & \cdots & \end{bmatrix}$$

multiplication by a scalar

$$\underline{\underline{C}} = \underline{\underline{A}}\,\underline{\underline{B}} \Rightarrow C_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj}$$

n col. n rows

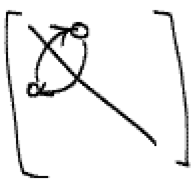
$m \times n$ $n \times l$ $m \times l$

Example:

$$\begin{bmatrix} 3 & 1 \\ 8 & 6 \\ 0 & 4 \end{bmatrix} \begin{bmatrix} 5 & 9 \\ 7 & 2 \end{bmatrix} = \begin{bmatrix} 22 & 29 \\ 82 & 84 \\ 28 & 8 \end{bmatrix}$$

(3×2) (2×2) (3×2)

<u>Transpose</u>, $\underline{\underline{A}}^T$



flip on the diagonal axis.

<u>**Exercise:**</u>

1. C&C Problem 9.2 page 261 (identify matrix types and parts).

4.2 Solution by Determinants

We introduce determinants by looking at a simple situation:

$$\left.\begin{aligned} ax + by = 0 \\ cx + dy = 0 \end{aligned}\right\} \Rightarrow \underline{\underline{A}}\,\underline{x} = 0 \tag{3.1}$$

therefore
$$y = -\frac{cx}{d} \tag{3.2}$$

$$\therefore ax - b\frac{cx}{d} = 0 \tag{3.3}$$

$$\therefore dax - bcx = 0 \tag{3.4}$$

$$\therefore (da - bc)x = 0 \tag{3.5}$$

$$\therefore da - dc = 0 \text{ if there is to be a solution where } x \neq 0. \tag{3.6}$$

We can generalize this:

$$\begin{aligned} &\text{determinant of A} = \det(\underline{\underline{A}}) = \left|\underline{\underline{A}}\right| = 0 \text{ for } x \neq 0 \\ &= ad - bc \text{ in the above particular case.} \end{aligned} \tag{3.7}$$

<u>Cramer's Rule</u> [Reference C&C 9.1.2 pg 234]

$\underline{\underline{A}}\,\underline{x} = \underline{b}$

$x_i = \dfrac{|A_i|}{|A|}$ where A_i is A with the i^{th} column replaced by $\underline{b}$

<u>Exercise:</u>

1. C&C Problem 9.6 page 262 (determinant and Cramer's rule).

4.3 Solution by Gauss Elimination

[Reference C&C 9.1 pg 231]

For $\underline{\underline{A}}\,\underline{x} = \underline{b}$

$$a_{11}x_1 + a_{12}x_2 + \cdots = b_1 \qquad (a)$$
$$a_{21}x_1 + a_{22}x_2 + \cdots = b_2 \qquad (b)$$
$$\vdots$$

Eliminate x_1 from 2nd equation by multiplying (a) by a_{21}/a_{11} and substract from (b) to give:

$$\cancel{a_{21}x_1} + a_{22}x_2 \cdots = b_2$$
$$\cancel{-a_{21}x_1} - \frac{a_{21}a_{12}}{a_{11}}x_2 \cdots = -\frac{a_{21}}{a_{11}}b_1$$

$$\Rightarrow \quad 0 + \left(a_{22} - \frac{a_{21}a_{12}}{a_{11}}\right)x_2 \cdots = b_2 - \frac{a_{21}}{a_{11}}b_1$$

- This gets rid of all terms below the diagonal.
- Can now backsubstitute to solve, starting with the last equation
- Can improve accuracy by pivoting (flipping rows to make the divisor large) to keep it diagonally dominant.

4.4 Jacobi – Richardson iterative scheme

Separate out the diagonal part:

$$\mathbf{A} = \mathbf{D} - \mathbf{B}$$

$$\begin{pmatrix} x & x & x & x \\ x & x & x & x \\ x & x & x & x \\ x & x & x & x \end{pmatrix} = \begin{pmatrix} x & & & \\ & x & & \\ & & x & \\ & & & x \end{pmatrix} - \begin{pmatrix} & x & x & x \\ x & & x & x \\ x & x & & x \\ x & x & x & \end{pmatrix} \tag{8}$$

Thus:

$$\mathbf{A}\phi = \mathbf{S} \Rightarrow \mathbf{D}\phi = \mathbf{B}\phi + \mathbf{S} \tag{9}$$

Solving for ϕ**:**

$$\phi = \mathbf{D}^{-1}\mathbf{B}\phi + \mathbf{D}^{-1}\mathbf{S} \tag{10}$$

Inverting the diagonal matrix is trivial so this solution scheme is quick to program and fast to solve per iteration. Note that you have to iterate because ϕ appears on the right hand side of the equation. So whether this turns out to be an effective scheme depends on how quickly the solution converges, ie, on how many iterations are necessary before a steady state is reached.

Written out in full, the scheme is:

$$\phi_i^{(m+1)} = \frac{1}{a_{ii}} \left[S_i - \sum_{\substack{j=1 \\ i \neq j}}^{N} a_{ij} \phi_j^{(m)} \right] \tag{11}$$

for the general matrix. In the simple two dimensional reactor case that we had before, the A matrix was quite sparse so the sum is only over 4 terms, not the whole row, ie, since:

$$a_{PN}\phi_N + a_{PW}\phi_W + a_{PP}\phi_P + a_{PW}\phi_W + a_{PS}\phi_S = S$$

we can rewrite equation 11 as:

$$\phi_P^{(m+1)} = \frac{1}{a_{PP}} \left[S_P - a_{PN}\phi_N^{(m)} - a_{PS}\phi_S^{(m)} - a_{PE}\phi_E^{(m)} - a_{PW}\phi_W^{(m)} \right] \tag{12}$$

The one and three dimensional cases should be obvious.

The iterative scheme, where the superscript represents the iteration number, is:

$\phi^{(0)} = \text{guess}$

$\phi^{(1)} = \mathbf{D}^{-1}\mathbf{B}\phi^{(0)} + \mathbf{D}^{-1}\mathbf{S}$

etc. until

$\phi^{m+1} = \phi^{m} =$ the converged ϕ

This works but converges slowly. We look for an improved scheme.

4.5 Gauss-Seidel or successive relaxation

[Reference C&C 11.2 pg 289]

In this scheme, we take advantage of the fact that as we sweep though the grid, we can use the updated values of the fluxes that we have just calculated. Thus the iteration scheme is:

$$\phi_i^{(m+1)} = \frac{1}{a_{ii}} \left[S_i - \sum_{j=1}^{i-1} a_{ij} \phi_j^{(m+1)} - \sum_{j=i+1}^{N} a_{ij} \phi_j^{(m)} \right] \tag{13}$$

or

$$\phi_P^{(m+1)} = \frac{1}{a_{PP}}\left[S_i - a_{PS}\phi_S^{(m)} - a_{PE}\phi_E^{(m)} - a_{PN}\phi_N^{(m+1)} - a_{PW}\phi_W^{(m+1)}\right] \tag{14}$$

where it is assumed that the sweep is from the north to the south, west to east, so that the north and west points have newly updated values available. Actually, programming this is quite easy: just always use the latest available values for the fluxes!

Compare this to the Jacobi-Richardson scheme just encountered. In the J-R scheme, only the old values were used.

In matrix form, the Gauss-Seidel method is equivalent to:

$$\mathbf{A} = \mathbf{L} - \mathbf{U}$$

$$\begin{pmatrix} x & x & x & x \\ x & x & x & x \\ x & x & x & x \\ x & x & x & x \end{pmatrix} = \begin{pmatrix} x & & & \\ x & x & & \\ x & x & x & \\ x & x & x & x \end{pmatrix} - \begin{pmatrix} & x & x & x \\ & & x & x \\ & & & x \\ & & & \end{pmatrix} \tag{15}$$

where **L** contains the diagonal. Thus:

$$\mathbf{A}\phi = \mathbf{S} \Rightarrow \mathbf{L}\phi = \mathbf{U}\phi + \mathbf{S} \tag{16}$$

Solving for ϕ**:**

$$\phi = \mathbf{L}^{-1}\mathbf{U}\phi + \mathbf{L}^{-1}\mathbf{S} \tag{17}$$

The iterative scheme, where the superscript represents the iteration number, is:

$\phi^{(0)} = \text{guess}$

$\phi^{(1)} = \mathbf{L}^{-1}\mathbf{U}\phi^{(0)} + \mathbf{L}^{-1}\mathbf{S}$

etc. until

$\phi^{m+1} = \phi^{m} = \text{ the converged } \phi$

L is not that hard to invert and the iteration converges more quickly that the J-R method. Overall, there is a net gain so that G-S is faster than J-R but convergence is still slow.

4.6 SOR (Successive Over-Relaxation)

If the convergence of the steady state reactor diffusion calculation is slow and if we have the change from one iteration to the next, could we not extrapolate ahead and anticipate the upcoming changes? Yes we can. The method is called the Successive Over-Relaxation (SOR) scheme. Basically the scheme is to first calculate as per Gauss Seidel and then extrapolate, ie first calculate an intermediate solution, ϕ^* as per GS:

$$\phi^* = \mathbf{L}^{-1}\mathbf{U}\phi^{(m)} + \mathbf{L}^{-1}\mathbf{S} \tag{18}$$

then weigh the intermediate solution with the old solution:

$$\phi^{(m+1)} = \omega\phi^* + (1-\omega)\phi^{(m)}, \omega \in (1-2) \tag{19}$$

Since ω is between 1 and 2, this is an extrapolation procedure. If it were between 0 and 1, it would be an interpolation procedure but we are trying to speed up the process, not stabilize it. The parameter ω is varied to give optimum convergence rate. It is suggested that you start out with ω close to 1 (ie heavy reliance on the GS solution) at the beginning and to increase ω as you become more confident that the extrapolation won't lead to overstepping the situation. Convergence rates ~100 times better than Jacobi are reported. Figure 7 illustrates this idea.

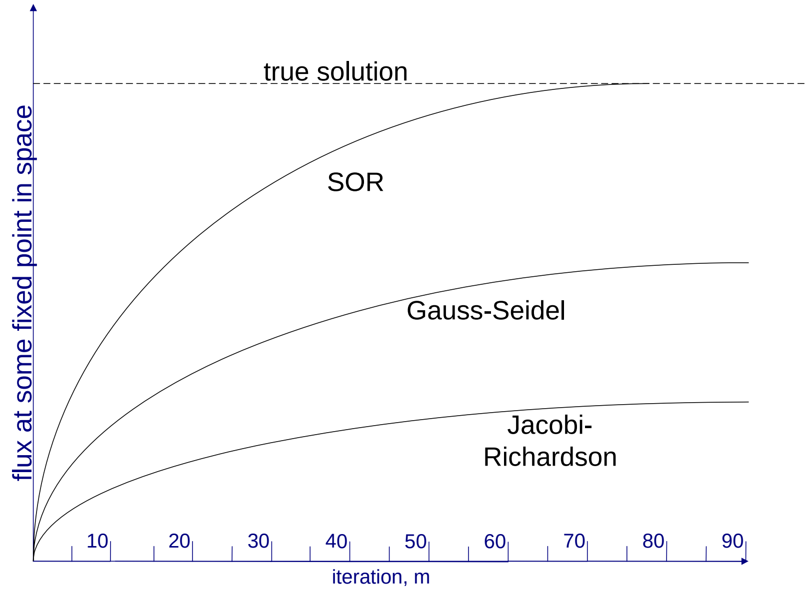


Figure 1 Convergence rate for iterative schemes.

These iterations are referred to as **inner** iterations. **Outer** or source iterations refer to varying parameters to achieve criticality and occur when the fixed source term, S, is replaced by a fission term that is proportional to the flux. More on that in a later chapter.

5 Calculus

We need to deal with rates of change, gradient induced flows, etc., inherent in differential equations. We need to be able to manipulate them.

5.1 Differentiation

[Reference C&C PT6.1 pg 569 and following]
[See also http://www.mathcentre.ac.uk/search_results.php?=1&c=1&t=26]

Some common derivatives that you should know:

$$\frac{d(\text{constant})}{dx} = 0$$

$$\frac{dx}{dx} = 1$$

$$\frac{dx^2}{dx} = 2x$$

$$\frac{dx^n}{dx} = n\frac{dx^{n-1}}{dx}$$

$$u = f_n(x), \quad \frac{du^n}{dx} = nu^{n-1}\frac{du}{dx}$$

$$\frac{d\,uv}{dx} = u\frac{dv}{dx} + v\frac{du}{dx}$$

$$\frac{d\,u/v}{dx} = \frac{1}{v}\frac{du}{dx} - \frac{u}{v^2}\frac{dv}{dx}$$

$$\frac{d\sin x}{dx} = \cos x$$

$$\frac{d\cos x}{dx} = -\sin x$$

$$\frac{d\ln x}{dx} = \frac{1}{x}$$

$$\frac{de^x}{dx} = e^x$$

Do a few exercises from the reference to refresh yourself and feel confident

5.2 Integration

[C&C PT6.1 pg 569 and following]

$$\int_a^b f(x)\,dx = F(x)\Big|_a^b = f(b) - f(a)$$

example:

$$\int_a^b x^n\,dx = \frac{x^{n+1}}{n+1}\Big|_a^b = \frac{b^{n+1}}{n+1} - \frac{a^{n+1}}{n+1}$$

$$\int u\,dv = uv - \int v\,du$$

(follows from $\frac{d\,uv}{dx} = u\frac{dv}{dx} + v\frac{du}{dx}$)

Do a few exercises from the references to refresh yourself and feel confident.

5.3 Development of the Taylor Series

[Reference C&C 4.1]

Recall that we approximated

$$\frac{dv}{dt} \simeq \frac{\Delta v}{\Delta t} = \frac{v^{t+\Delta t} - v^{t}}{(t+\Delta t) - t} \Rightarrow v^{t+\Delta t} \simeq v^{t} + \Delta t \frac{dv}{dt}$$

Compare this to the Taylor Series:

$$f(x) = f(x_0) + \Delta x\, f'(x_0) + \frac{\Delta x^2}{2!} f''(x_0) + \cdots$$

We see justification for the numerical approximation and have some idea of the error.

Note that the error $\to 0$ as $\Delta x \to 0$.

'Proof' of the Taylor Series

We expand $f(x)$ as a polynomial:

$$f(x) = f(x_0) + a_1 \underset{\uparrow\\(x-x_0)}{\Delta x} + a_2 \Delta x^2 + a_3 \Delta x^3 \quad \text{—— (1)}$$

Taking the derivative:

$$f'(x) = a_1 + 2a_2(x-x_0) + 3a_3(x-x_0)^2 + \cdots$$

$$f''(x) = 2a_2 + 3\cdot 2\, a_3(x-x_0) + \cdots$$

$$f'''(x) = 3\cdot 2\, a_3 + \cdots$$

Evaluating these derivatives at $x = x_0$, we see:

$$f'(x_0) = a_1, \quad f''(x_0) = 2a_2, \quad f'''(x_0) = 3\cdot 2\, a_3, \text{ etc.}$$

Substituting back in to (1) we have:

$$f(x) = f(x_0) + f'(x_0)(x-x_0) + \frac{f''(x_0)}{2!}(x-x_0)^2 + \frac{f'''(x_0)}{3!}(x-x_0)^3 + \cdots$$

$$= \sum_{n=0}^{\infty} \frac{f^{n}(x_0)}{n!}(x-x_0)^n$$

Q.E.D.

5.4 Linearization

Sometimes our models are nonlinear. For example we had for our falling object:

$$\frac{dv}{dt} = g - \frac{c}{m} v$$

But a more realistic drag force might give:

$$\frac{dv}{dt} = g - \underbrace{\frac{c}{m} v^2}_{F_{drag}}$$

We can linearize this by using the Taylor series:

$$F_{drag}(v) = F_{drag}(v_0) + \left.\frac{\partial F_{drag}}{\partial v}\right|_{v=v_0} \underbrace{(v-v_0)}_{\Delta v} + O(\Delta v^2)$$

$$= \frac{c v_0^2}{m} + \frac{2 c v_0}{m}(v - v_0) + O(\Delta v^2)$$

$$\cong -\frac{c v_0^2}{m} + \frac{2 c v_0}{m} v$$

$$\therefore \frac{dv}{dt} = g + \frac{c v_0^2}{m} - 2\frac{c v_0}{m} v$$

We can solve this analytically as before. But this is valid only at v close to v_0. We might want to do this even though it has limitations so that we can see the analytical behaviour of a system about some operating point.

This comes up often in looking at system behaviour and our inevitable task of having to solve systems of equations. Invariably we linearize to form **Ax**=**b** so we can capitalize on the vast solution literature for such linear systems.

Exercise:

Problem C&C 4.1, page 97

6 ODE – Steady State and Transient

[Reference C&C PT7]

We have solved an example already:

$$\frac{dv}{dt} = g - \frac{c}{m}v$$

This is an example of a rate equation.

- It is 1^{st} order (i.e. involves only 1^{st} derivative)
- It is linear since it is linear in the dependent variable (v)

An example of a 2^{nd} order linear equation is

$$m\frac{dx^2}{dt^2} + c\frac{dx}{dt} + kx = 0 \qquad \text{(Spring mass system)}$$

This can be reduced to a system of 1^{st} order equations by defining

$$\left.\begin{aligned} y &= \frac{dx}{dt} \\ \therefore\ m\frac{dy}{dt} &+ cy + kx = 0 \end{aligned}\right\}$$

2 1^{st} order ODE's to be solved simultaneously

If simple enough we can solve analytically.
Typically, we solve numerically.

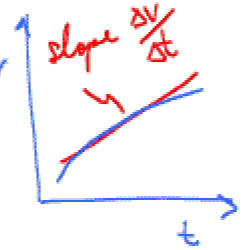
Euler's Method

Generally we have

$$\frac{dy}{dt} = f(t,y)$$

Example:

$$\underbrace{\frac{\Delta v}{\Delta t}}_{\uparrow\ \frac{dy}{dt}} = \underbrace{g - c/_m v}_{f(t,y)}$$



$$\therefore\ v^{t+\Delta t} = v^t + \Delta t \underbrace{\left(g - c/_m v^t\right)}_{\substack{f(t,y^t) \\ = \text{slope at } t}}$$

We know that our guess at the slope is in error. We can improve on it by the Predictor-Corrector method:

We have a guess at $v^{t+\Delta t}$ from above.

$$v^{t+\Delta t} = v^t + f^t \Delta t$$

We use this v at $t+\Delta t$ to estimate $f^{t+\Delta t}\left(= g - c/_m v\right)$

Thus:

$$v^{t+\Delta t} = v^t + \underbrace{\frac{\left[f(t,y^t) + f(t+\Delta t, y^{t+\Delta t})\right]}{2}}_{\text{average slope}} \Delta t$$

There are many methods that improve on this, such as the Runge Kutta family of methods.

We won't explore them here.

Stiffness

$$\frac{dy}{dt} = -1000y + 3000 - 2000e^{-t}$$

Analytical solution is

$$y = 3 - \underbrace{0.998e^{-1000t}}_{\text{rapid}} - \underbrace{2.002e^{-t}}_{\text{slow}}$$

The rapid part comes from:

$$\frac{dy}{dt} = -1000y$$

$$\therefore \quad y^{t+\Delta t} = y^t + \underbrace{\frac{dy}{dt}}_{-1000y}\Delta t$$

$$= y^t(1-1000\Delta t) \Longrightarrow \Delta t \text{ must be} \le 1/1000$$

else goes unstable

So we must use very small Δt even after the e^{-1000t} term has died out.

We can get around this by using the implicit method.

$$y^{t+\Delta t} = y^t - 1000\,\Delta t\, y^{t+\Delta t}$$

$$\Rightarrow \quad y^{t+\Delta t} = \frac{y^t}{1+1000\Delta t} \Longleftarrow \text{stable for large } \Delta t$$

Issue

- If have a system of ODE's, going implicit involves matrix inversions. This can be costly.
- Also, higher order methods exist but they are more complicated to program and each step is slower.
- Usually, the best way to get the job done in the overall engineering context is to use a simple, robust, easy to program method to minimize the time spent programming + reduce the errors. Computers are fast + cheap!

Exercise:

1. Given an initially pure radioactive sample (species N_1) that decays to N_2 which subsequently decays to N_3, write the differential equations governing the decay sequence. Set up the finite difference equations and outline a solution procedure.

7 Boundary-Value and Eigenvalue Problems

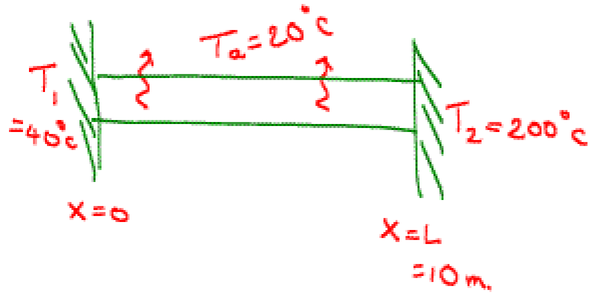
[Reference C&C 27 page 572]

So far we have looked only at initial value problems – typically transients were the initial conditions provide the constants of integration. Two other types of differential equations are boundary-value problems and eigenvalue problems.

7.1 Boundary-Value Problems

Boundary value problems are those that involve 2 or more conditions that ‘pin’ the solution down at more than one point in the solution space, for example, the temperature T at both ends of a rod, as follows.

$$\frac{d^2T}{dx^2} + h'(T_a - T) = 0$$



We try a solution of the form:

$$T = a e^{bx} + c e^{-bx} + d$$

Plugging in we find

$$a b^2 e^{bx} + c b^2 e^{-bx} + h'(T_a - a e^{bx} - c^{-bx} - d) = 0$$

For this to be true at all x,

$$a b^2 e^{bx} + h'(-a e^{bx}) = 0 \Rightarrow b^2 = a h'$$

0.01

$$\underline{T_a = d = 20}$$

$$b = \sqrt{a h'}$$

$$= \sqrt{a \times 0.01} = \underline{0.1\sqrt{a}}$$

Boundary Conditions:

$$T(0) = T_1 = a + c + 20 = 40 \Rightarrow \underline{C = 20 - a}$$

2 equations
2 unknowns

$$T(L) = T_2 = a e^{bL} + c e^{-bL} + 20 = 200$$

$$= a e^{bL} + (20 - a) e^{-bL} = 180$$

$$= a e^{\sqrt{a}} + (20 - a) e^{-\sqrt{a}} = 180$$

Solving for a gives

$$\underline{a = 73.4523}$$

Numerical solution

We define

$$\frac{dT}{dx} = z \Rightarrow \frac{dz}{dx} + h'(T_a - T) = 0$$

and start at $x = 0$ to integrate to $x = L$.
$T(0) = 40$, guess $z(0)$. ← use Euler or whatever

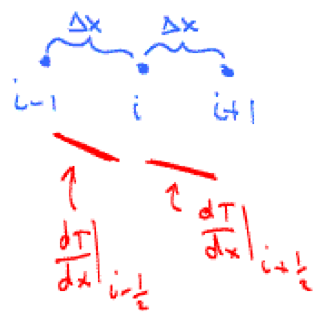
Shooting method

We won't get $T(L) = 200$ like we want.
So adjust $z(0)$ and try again.

More generally, it is best to form finite differences for $\frac{\partial^2 T}{\partial x^2}$ and set up a matrix equation.

$$\frac{d^2T}{dx^2} = \frac{d}{dx}\left(\frac{dT}{dx}\right)$$

$$\simeq \frac{\left[\left.\frac{dT}{dx}\right|_{i+\frac{1}{2}} - \left.\frac{dT}{dx}\right|_{i-\frac{1}{2}}\right]}{\Delta x}$$



$$= \frac{\frac{T_{i+1} - T_i}{\Delta x} - \frac{T_i - T_{i-1}}{\Delta x}}{\Delta x} \Rightarrow \frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2}$$

Thus $\quad T_{i+1} - 2T_i + T_{i-1} + \Delta x^2 h'(T_i - T_a) = 0$

or $\quad -T_{i-1} + (2 + h'\Delta x^2)T_i - T_{i+1} = h'\Delta x^2 T_a$

ie

$$\begin{bmatrix} \ddots & \ddots & \\ \ddots & \ddots & \ddots \\ & \ddots & \ddots \end{bmatrix} \begin{bmatrix} T_1 \\ \vdots \\ T_N \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_N \end{bmatrix}$$

left boundary condition

right B.C.

B.C.:

In the 1st equation T_{i-1} term for left boundary (T_0) is included in b_1 term

Ditto for the last equation + T_{N+1}

Solve this by Gauss-Seidel or whatever.

7.2 Eigenvalue Problems

So far we have met and solved $\underline{\underline{A}}\,\underline{x} = \underline{b}$ which has a unique solution iff $|A| \neq 0$.

But what about the case where $b = 0$?

If $|A| \neq 0$, then the only solution is $x = 0$, the trivial case.

To get a non-trivial solution for $\underline{\underline{A}}\,\underline{x} = 0$, must have $|\underline{\underline{A}}| = 0$

We usually have a free parameter to vary to force $|\underline{\underline{A}}| = 0$.

This arises in various ways. For example:

$$\frac{d\underline{Y}}{dt} = \underline{\underline{A}}\,\underline{y}$$

The solution is of the form $\underline{Y} = \underline{Y}_0\, e^{\lambda t}$

compare

$$\therefore \frac{d\underline{Y}}{dt} = \lambda \underline{Y}_0\, e^{\lambda t} = \lambda \underline{Y}$$

So we have $\lambda \underline{Y} = \underline{A}\,\underline{y}$

or $\left[\underline{A} - \lambda \underline{\underline{I}}\right] \underline{Y} = 0$ $\qquad$ $\underline{\underline{A}}$ is an $(n \times n)$ matrix

So we need λ such that $|\underline{A} - \lambda \underline{\underline{I}}| = 0$

This determinant will generate a polynomial characteristic equation in λ of degree n.

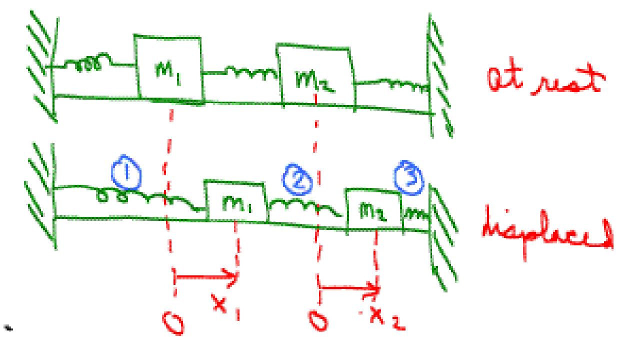
λ is called the eigenvalue

$\underline{Y}$ is called the eigenvector

Generally λ will have n values (solutions to the n^{th} degree equation).

Spring-mass Example

Consider 2 masses and 3 springs:



A force balance gives:

$$m_1 \frac{d^2 x_1}{dt^2} = -k x_1 + k(x_2 - x_1)$$

$$m_2 \frac{d^2 x_2}{dt^2} = -k(x_2 - x_1) - k x_2$$

Rearranging:

$$m_1 \frac{d^2 x_1}{dt^2} - k(-2x_1 + x_2) = 0$$

$$m_2 \frac{d^2 x_2}{dt^2} - k(x_1 - 2x_2) = 0$$

We expect oscillatory behaviour so we try

$$x_1 = A_1 \sin \omega t \quad , \quad x_2 = A_2 \sin \omega t$$

which yields:

$$\left.\begin{aligned} \left(\frac{2k_1}{m_1} - \omega^2\right) A_1 - \frac{k}{m_1} A_2 &= 0 \\ -\frac{k}{m_2} A_1 + \left(\frac{2k}{m_2} - \omega^2\right) A_2 &= 0 \end{aligned}\right\}$$

Eigenvalue problem. Need to find ω

$$\begin{bmatrix} \left(\frac{2k_1}{m_1} - \omega^2\right) & -\frac{k}{m_1} \\ -k/m_2 & \left(\frac{2k}{m_2} - \omega^2\right) \end{bmatrix} \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} = 0$$

Need to set $|\;| = 0$

$\therefore$

$$\left(\frac{2k_1}{m_1} - \omega^2\right)\left(\frac{2k}{m_2} - \omega^2\right) + k_2/m_1 m_2 = 0$$

2nd order in ω^2

ie 2 values of $\omega \Rightarrow \omega_1$, ω_2

These 2 values of ω are the fundamental vibrational modes. For $k = 200$ N/m and $m_1 = m_2 = 40$ kg we find $\omega_1^2 = 15\ s^{-2}$ & $\omega_2^2 = 5\ s^{-2}$.

Plugging ω_1^2 back into the equations of A_1 & A_2 we find $A_1 = -A_2$ (vibrating out of phase).

For ω_2^2 we find $A_1 = A_2$ (in phase).

<u>The Power Method for finding eigenvalues</u>

Power method for getting λ's.

Write $\underline{\underline{A}}\,\underline{y} = \lambda \underline{y}$.

Pick a guess at $\underline{y}$, call it $\underline{y}_0$

$\therefore$ $\underline{\underline{A}}\,\underline{y}_0$ gives the basis for a new $\lambda \underline{y}$. $(\equiv \underline{w}_1)$

Generate λ by normalizing y & putting multiplier into λ.

Iterating generates the largest λ.

$\underline{Y}_1 = \frac{1}{a_1} \underline{w}_1$ where a_1 = largest value of $\underline{w}_1$ (denoted w_k).

<u>Exercise:</u>

1. Look at 5 coupled chemical reactors (C&C page 307 Figure 12.3 for the transient situation). The equations are given on page 783 (caution: the equation for C_4 is wrong). Set up the matrix in eigenvalue form.

8 Partial differential Equations

[Reference C&C PT8]

8.1 PDE Classification

Herein we look at Partial differential Equations (PDE) in the steady state and transient modes. They are classified according to their behaviour as parabolic, elliptical, or hyperbolic.

Partial Differential Equations arise when we have 2 or more independent variables, for example in 2-D.
The most common cases we see are 2nd order, linear in 2 or 3 dimensions, steady state and transient.

ie
$$A\frac{\partial^2 u}{\partial x^2} + B\frac{\partial^2 u}{\partial x \partial y} + C\frac{\partial^2 u}{\partial y^2} + D = 0$$
can be fn (x, y, u, A, B, C)

$B^2 - 4AC$	Type	Example	
< 0	Elliptic	$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$	heated plate in steady state.
$= 0$	Parabolic	$\frac{\partial T}{\partial t} = k\frac{\partial^2 T}{\partial x^2}$	Transient propagation
> 0	Hyperbolic	$\frac{\partial^2 y}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 y}{\partial t^2}$	Wave propagation oscillation

We seldom meet hyperbolic equations so they will not be reviewed here.

8.2 Elliptic

[Reference C&C Chapter 29 page 820]

An example of the elliptic case is heat conduction in a plate:

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$

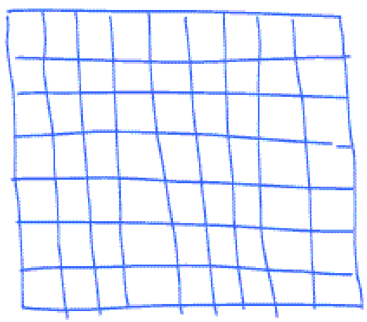
$$\rho C \cancel{\frac{\partial T}{\partial t}} = \nabla \cdot k \nabla T + \cancel{q'''}$$

S.S.

2D

k const

no heat sources



B.C.: fixed T at edges

Finite Difference

$$\frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{\Delta x^2} + \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{\Delta y^2} = 0$$

Solve by Gauss Seidel.

Possible B.C.: $\frac{\partial T}{\partial x} = 0$ (insulated case)

$T =$ given at edges

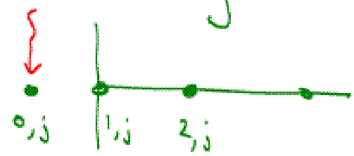
and so on.

The matrix of equations will have elements falling outside the matrix:

B.C.

$$\begin{bmatrix} \cdot \; \cdot \; \cdot & & \\ & & \\ & & \end{bmatrix} \begin{bmatrix} T \end{bmatrix} = \begin{bmatrix} 0 \end{bmatrix}$$

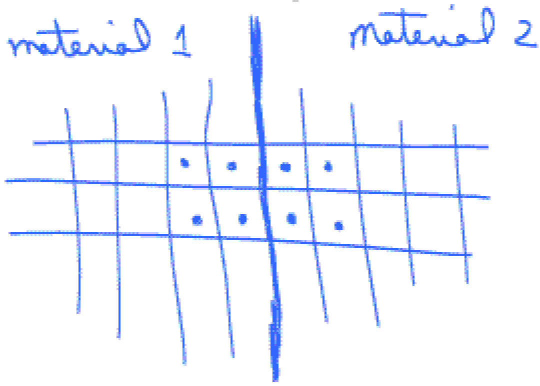
Use phantom cells outside the boundary



For $\frac{\partial T}{\partial x} = 0$ at boundary

$$\frac{T_{2,j} - T_{0,j}}{2\Delta x} = 0 \Rightarrow T_{0,j} = T_{2,j}$$

It makes more sense to use a control volume approach (nodes in the cell centers rather than the edges) for heterogeneous material.



This makes it easier to formulate equations for a node that contains only one material.

Exercise:

1. Set up the finite difference equations for steady state heat conduction in a plate where boundary temperatures are held constant (each boundary is potentially different). Limit yourself to 9 (ie 3x3) interior grid points.

8.3 Parabolic

[Reference C&C Chapter 30 page 840]

Typical of the parabolic case is the transient:

$$\rho c \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2} \qquad k' \equiv k/\rho c$$

giving

$$T_i^{t+\Delta t} = T_i^t + \frac{k'\Delta t}{\Delta x^2}\left(T_{i+1}^t - 2T_i^t + T_{i-1}^t\right) \quad \text{Explicit}$$

keep $< \frac{1}{2}$, else solution unstable

If evaluate R.H.S. at $t+\Delta t$ then the formulation is Implicit. This is stable for large Δt but involved matrix inversion (or equivalent). This can be costly and we often need a small Δt anyway so there is no gain.

If you are only interested in the S.S., it may be worth using the implicit method + large Δt. Alternatively use Gauss-Seidel in the S.S. as before.

Exercise:

1. Set up the finite difference equations for transient heat conduction in a plate where boundary temperatures are held constant (each boundary is potentially different). Limit yourself to 9 (ie 3x3) interior grid points. The initial interior plate temperature is given.

8.4 The Crank Nicolson Method

We can mix the explicit and implicit forms with the Crank-Nicolson method which is 2nd order accurate in both space and time):

$$T_i^{t+\Delta t} = T_i^{t} + \theta \frac{k\Delta t}{\Delta x^2}\left(T_{i+1}^{t} - 2T_i^{t} + T_{i-1}^{t}\right)$$
$$+(1-\theta)\frac{k\Delta t}{\Delta x^2}\left(T_{i+1}^{t+\Delta t} - 2T_i^{t+\Delta t} + T_{i-1}^{t+\Delta t}\right)$$

where θ is a weighting factor whose value is between 0 and 1, ie $\theta \in (0,1)$. Solving for the unknown $T^{t+\Delta t}$ gives you a matrix equation to solve (tri-diagonal in this case).

We can vary θ to get a blend of the explicit and implicit methods as desired. Setting $\theta = 0.5$ simulates using an evaluation of T at mid step, which is probably the most accurate value to use. Just make sure that

$$\left[T_i^{t} - \left(\theta \frac{\Delta t}{\Delta x^2}\right)\left(2T_i^{t}\right)\right] \geq 0$$

else unstable oscillations can occur.

9 Data Analysis

9.1 Motivation

[Reference C&C PT5.1 pg425]

Often we need to analyse data to
- establish a relationship (curve fit)
- interpolate
- extrapolate
- test significance of a model
- do trend analysis
- etc.

Herein we look at some basic statistics and curve fitting.

9.2 Statistics

[Reference C&C PT5.2]

Let's say we have some data, typically in the form of repeated measurements of some quantity:

$y_1, y_2, y_3 \ldots\ldots y_n$

We define:

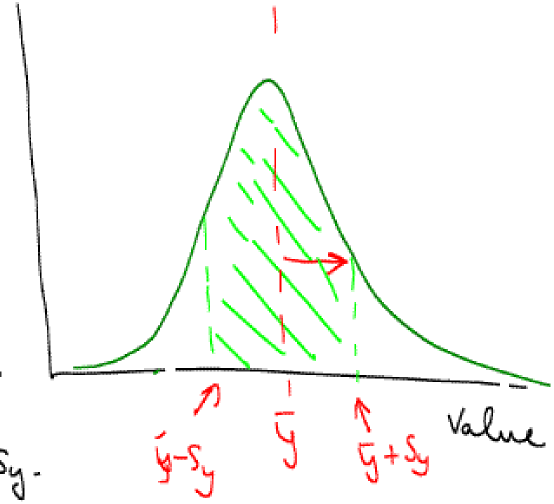
$$\bar{y} = \frac{\sum_1^n y_i}{n}$$ arithmetic mean

$$S_y = \sqrt{\frac{\sum_1^n (y_i - \bar{y})^2}{n-1}}$$ standard deviation (measure of the spread about the mean)

$$S_y^2 = \frac{\sum_1^n (y_i - \bar{y})^2}{n-1}$$ Variance $= \dfrac{\sum_1^n y_i^2 - \left(\sum_1^n y_i\right)^2 / n}{n-1}$

$$C.V. = \frac{S_y}{\bar{y}} \times 100\%$$ coefficient of variation

Data tends to cluster about the mean to form a normal distribution given enough data.



68% falls between $\bar{y}-s_y$ and $\bar{y}+s_y$.

95% " " $\bar{y}-2s_y$ and $\bar{y}+2s_y$.

We distinguish between the sample distribution from the population distribution (the entire set if we took ∞ measurements).

μ = population (or true) mean

σ = population (or true) standard deviation.

Central Limit Theorem

Suppose we take another set of measurements and compute a new $\bar{y}$ and S_y. Now we have

$\bar{y}_1 + S_{y_1}$ and $\bar{y}_2 + S_{y_2}$.

$\bar{y}_1$ will not be equal to $\bar{y}_2$ typically.

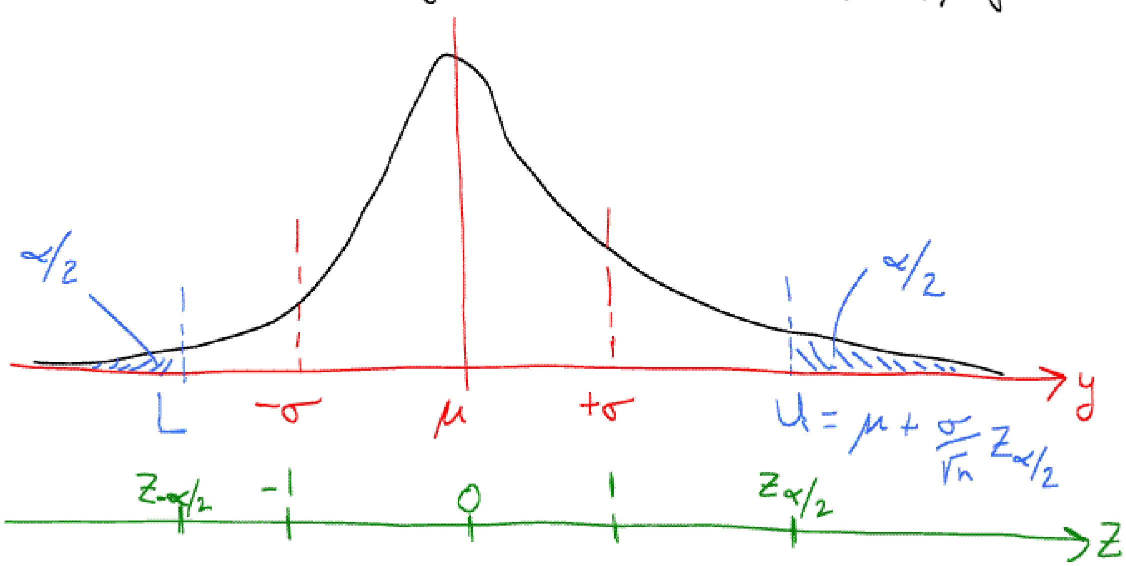
We repeat m times to give a distribution of means.

The theorem states that the distribution of means will be normal even if y is not normal.

The mean of the means should converge on μ.

The variance of this distribution of means is σ^2/n and the variable $\bar{z} = \dfrac{\bar{y}-\mu}{\sigma/\sqrt{n}}$ is standard normal.

$\bar{z}$ has a mean of 0 and variance (σ^2/n) of 1.



The probability that Z will fall in the shaded regions is α.

$Z_{\alpha/2}$ is available from tables.

Example: for $\alpha = .05$, $Z = 1.96$, ie 95% of the distribution of Z falls within ± 1.96 and 5% falls outside.

ie $Z_{-\alpha/2} < Z < Z_{\alpha/2}$ with probability $1-\alpha$.

But Z is based on σ which we don't know.

An approximation is to use

$$t = \frac{\bar{y} - \mu}{S_y/\sqrt{n}}$$ which we can look up in tables.

This gets more accurate as $n \to \infty$.

or t

On the y scale, the spread is $\frac{S_y}{\sqrt{n}} Z_{-\alpha/2}$ to $\frac{S_y}{\sqrt{n}} Z_{\alpha/2}$

Thus given the data we can calculate $\bar{y}$ and the confidence interval.

Procedure:

- Calculate $\bar{y}$ + S_y from the data

$$\bar{y} = \frac{\sum y_i}{n}, \quad S_y = \sqrt{\frac{(y_i - \bar{y})^2}{n-1}}$$

- Look up $t_{\alpha/2,\,n-1}$ in tables.

- confidence interval is $\pm\ t_{\alpha/2,\,n-1} \frac{S_y}{\sqrt{n}}$

Example

8 data points:

6.395	6.505
6.435	6.515
6.485	6.555
6.495	6.555

$\Rightarrow$ $\bar{y} = \frac{52.72}{8} = 6.59$

$S_y = 0.0899$

$t_{.05/2,\,7} = 2.36$

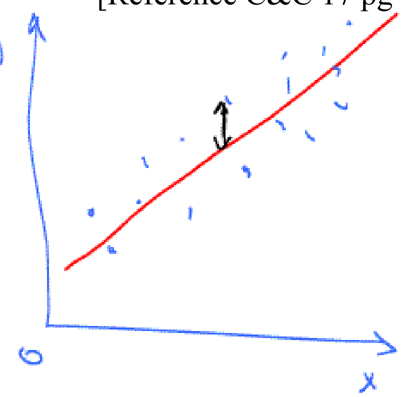
$$\therefore\ y = 6.59 \pm \left(\frac{0.0899}{\sqrt{8}} \times 2.36\right)$$

≈ 0.075

See also "The T-Test" from www.socialresearchmethods.net

9.3 Least Squares Regression

[Reference C&C 17 pg440]



Basically we want to fit the data to a given model.

Let's look at a simple case: straight line:

$$y = a_0 + a_1 x + e$$

$\nwarrow$ error

$$\therefore \; e = y - a_0 - a_1 x$$

What are $a_0 + a_1$ to minimize

$$\sum_1^n (e_i)^2 \equiv S_r = \sum_1^n (y_i - a_0 - a_1 x_i)^2 \qquad ?$$

At the minimum: $\dfrac{\partial S_r}{\partial a_0} = \dfrac{\partial S_r}{\partial a_1} = 0$ $\leftarrow$ 2 equations, 2 unknowns

$$\Rightarrow \frac{\partial S_r}{\partial a_0} = 2\sum_1^n (y_i - a_0 - a_1 x_i) = 0 \Rightarrow n a_0 + \sum_1^n x_i a_1 = \sum_1^n y_i$$

$$\frac{\partial S_r}{\partial a_1} = 2\sum_1^n (y_i - a_0 - a_1 x_i) x_i = 0 \Rightarrow \left(\sum_1^n x_i\right) a_0 + \left(\sum x_i^2\right) a_1 = \sum_1^n x_i y_i$$

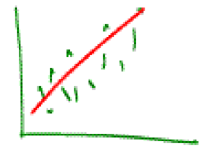
Solving gives:

$$a_1 = \frac{n \sum x_i y_i - \sum x_i \sum y_i}{n \sum x_i^2 - (\sum x_i)^2}$$

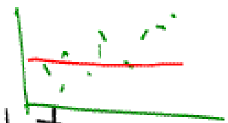
$$a_0 = \bar{y} - a_1 \bar{x} = \frac{\sum y_i}{n} - \frac{\sum x_i}{n} a_1$$

Quantification of Error

standard error: $S_{y/x} = \sqrt{\dfrac{S_r}{n-2}}$
(error compared to model)



Total sum of squares $(S_t) = \sum (y_i - \bar{y})^2$
= measure of the total variability of the data
(error compared to average)



$$r^2 \equiv \frac{S_t - S_r}{S_t} = \text{coefficient of determination}$$

$$= 1 - \frac{S_r}{S_t}$$

Perfect fit: $r^2 = 1$
no improvement: $r^2 = 0$

$r =$ correlation coefficient

So that's the general approach. But what model to use in general?

- It is best to plot the data up and eyeball the situation.
- The plot will suggest some model perhaps.
- Try semi-log plots, etc.
- Often you can do a variable transformation to get the data linearized.
- You can also do polynomial regressions, etc. Same idea, just messier.

Exercise:

1. C&C 17.4 page 471.

9.4 Binomial, Gaussian and Poisson Distributions

It is instructive to note that the normal distribution is but a special case of the Binomial distribution when the number of elements is large and the probability of the elements is random (i.e. as likely as not to be in a particular state).

If we consider a system containing elements (say gas molecules in a box or coins being flipped), we define p = probability of success (a particular outcome for a given element to be true) and q to be the probability of failure ($p+q=1$), then the Binomial distribution states that the Probability of being in a given state:

$$P_N(n) = \underbrace{\frac{N!}{n!(N-n)!}}_{\text{\# of different configurations of N elements for which n satisfy a criterion}} \underbrace{p^n q^{N-m}}_{\text{prob. that n elements satisfy a criteria \& the rest do not.}}$$

N = total # of elements

Say: "P N chose n"

If N is large, say 1000 & $p=q=0.5$ we have:

$P_{1000}(0) = 9.3\times10^{-302}$ (all tails in coin flips)

$P_{1000}(1) = 9.3\times10^{-299}$ (1 head, 999 tails)

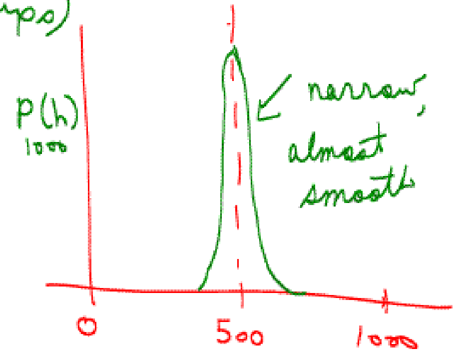
$P_{1000}(495) = 0.0240$

$P_{1000}(500) = 0.0253 \Leftarrow$ mean

⋮

$P_{1000}(1000) = 9.3\times10^{-302}$ (all heads)

All we really need is: the mean & the fluctuation



If we compute the variance:

$$\sigma^2 = \text{average of } (n-\bar{n})^2 = \sum_n{}' p_n (n-\bar{n})^2$$

$$= \sum_{n=0}^{N}{}' \left(\frac{N!}{n!(N-n)!} p^n q^{N-n}\right)(n-\bar{n})^2$$

$$= Npq$$

Note ~~that~~ $\sigma \propto \sqrt{N}$

$$\frac{\sigma}{\bar{n}} = \frac{\sqrt{Npq}}{Np} = \sqrt{q/Np} \propto \frac{1}{\sqrt{N}}$$

So the <u>relative</u> spread $\downarrow$ as $N \uparrow$

This is of interest to us in data collection since it indicates how much we might expect the fluctuations in our data to drop as we collect more.

The binomial distribution reduces to the Gaussian or normal distribution:

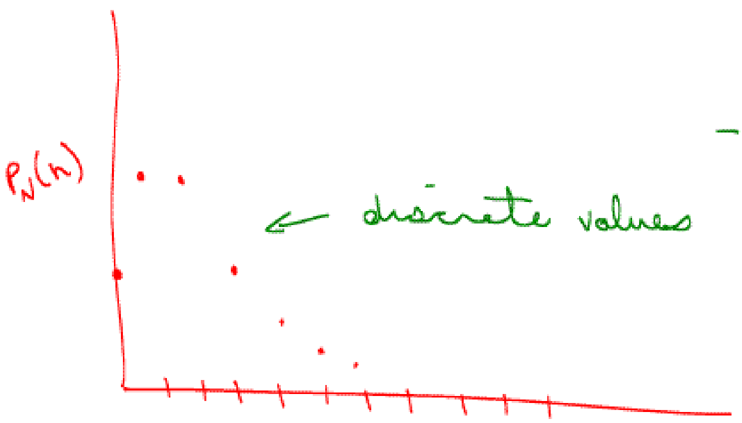
$$P(n) = \frac{1}{\sqrt{2\pi}\,\sigma} e^{-(n-\bar{n})^2/2\sigma^2}$$

Valid only for n large and $(n-\bar{n})^2 \ll \sigma^2$, ie not near the tails

The Poisson Distribution is another useful distribution derivable from the Binomial distribution under special conditions, namely ~~that~~ $p \ll 1$, ie for rare events.

It can be shown ~~that~~

$$P_n(n) \simeq \frac{(\bar{n})^n}{n!} e^{-\bar{n}}$$ Poisson Distribution.



- Becomes more symmetric as $p \uparrow$
- Still have to calculate $n!$

This might come in handy when you are counting rare events (like in long lived radioisotopes).

9.5 Bayesian Probability

Bayes Theorem proves useful in computing the effect on our estimates when new evidence comes in. Bayes Theorem is simply a restatement the fact that

$$\underbrace{P(A|B)\,P(B)} = P(AB) = P(BA) = \underbrace{P(B|A)\,P(A)}$$

equate these

Thus

$$P(A|B) = P(A)\,\frac{P(B|A)}{P(B)}$$

Example:

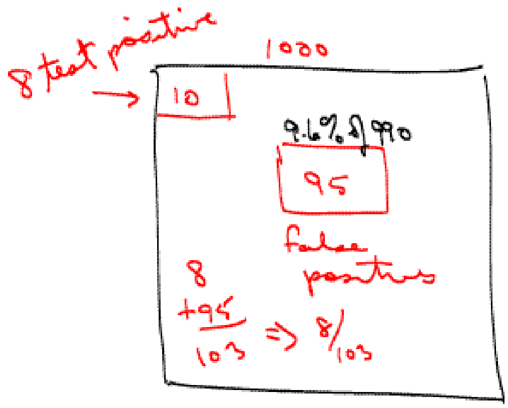
$P(A)$ = probability ~~that~~ hypothesis A is true in general.

$P(B)$ = probability ~~that test~~ B gives positive result.

$P(B|A)$ = prob. ~~that test~~ B is positive when A is true.

$P(A|B)$ = prob. that A is true given a positive test result B.

Example: Prior knowledge of fault state = 1%. Test is accurate 80% of the time if fault state true. Test reports false positives 9.6% of the time. What is prob. of fault if Test returns true?



$$P(A|B) = \frac{\overset{0.01}{P(A)}\ \overset{0.80}{P(B|A)}}{P(B)}$$

Prob. of Testing Positive $= \underbrace{P(B|A)P(A)}_{\text{true positives}} + \underbrace{P(B|\bar{A})P(\bar{A})}_{\text{false positives}}$

$(0.8)\ (.01) + (0.096)(0.99)$

$0.008 + 0.095 = 0.103$

$P(A) = 0.01$ Prior knowledge

Test: $P(B|A) = 0.8$ ← true positive

$P(B|\bar{A}) = 0.096$ ← false positive

$$P(A|B) = P(A)\cdot\left[\frac{P(B|A)}{P(B)}\right]$$ ← original probability is modified by ratio of test showing positive given A vs test in general

$0.01 \times \frac{0.80}{0.103}$ amplification factor ~ 8

If no false positives then

$P(B) = 0.008$

∴ amplification factor of 100

⇒ $P(A|B) = 1.0$.

Makes sense since test came back positive + there are no false positives.

Conclude that in testing you want both:

(a) no missed faults (high $P(B|A)$)

(b) no false positives (low $P(B|\bar{A})$)

10 Laplace Transforms

[Reference: Kells "Elementary Differential Equations", Chapter 7]

Solving differential equations often involves transforming the dependent variable(s) to cast the equation in a form more easily solved. The Laplace Transform does just that for Ordinary Differential Equations.

We define

$$\mathcal{L}[f(t)] = \bar{f}(s) = \int_0^\infty f(t)e^{-st}\,dt$$

where f is a well behaved function. Notice that $\bar{f}(s)$ is a function of s which has dimensions of inverse time. We transform the function from the t domain to the s domain. The s may be complex.

We can see immediately that

$$\mathcal{L}[a_1 f_1(t) + a_2 f_2(t)] = a_1 \mathcal{L}[f_1(t)] + a_2 \mathcal{L}[f_2(t)]$$

Typical functions have been transformed and put in tables for convenience.

Example:

$$f(t) = e^{-at}$$

$$\therefore \quad \mathcal{L}[e^{-at}] = \int_0^\infty e^{-at}e^{-st}\,dt = \int_0^\infty e^{-(s+a)t}\,dt$$

$$= -\frac{1}{(s+a)} e^{-(s+a)t}\Big|_0^\infty = \frac{1}{s+a}$$

Note: $f(t) \Leftrightarrow \bar{f}s$ pairs are unique, so if we had (say) $\bar{f}(s) = \frac{1}{s+a}$, then $f(t)$ must be e^{-at}

Of special interest here is

$$\mathcal{L}\left[\frac{df(t)}{dt}\right] = s\bar{f}(s) - f(0)$$

This is useful when dealing with ODE's.

Proof:

$$\mathcal{L}\left[\frac{df(t)}{dt}\right] = \int_0^\infty \underbrace{\frac{df(t)}{dt}}_{dv} \underbrace{e^{-st}}_{u} dt = \underbrace{e^{-st} f(t)\Big|_0^\infty}_{0 - f(0)} + s\underbrace{\int_0^\infty f(t) e^{-st} dt}_{\bar{f}(s)}$$

[recall $\int u\,dv + \int v\,du = uv$

$\therefore \int u\,dv = uv - \int v\,du$]

$$= s f(s) - f(0)$$

I.C.

Similiarly

$$\mathcal{L}\left[\frac{d^2 f(t)}{dt}\right] = s^2 \bar{f}(s) - s f(0) - f'(0)$$

In general

$$\mathcal{L}\left[\frac{d^n f(t)}{dt}\right] = s^n \bar{f}(s) - s^{n-1} f(0) - s^{n-2} f'(0) + \cdots$$

$$- s f^{n-2}(0) - f^{n-1}(0)$$

The solution scheme is to transform the ODE to give an algebraic equation. Solve for $\bar{f}(s)$ and invert to give $f(t)$.

Example:

$$\frac{dy}{dt} + y = e^{-t}, \quad \text{I.C.: } y(0) = 5$$

$$\therefore \mathcal{L}\left[\frac{dy}{dt}\right] + \mathcal{L}[y] = \mathcal{L}\left[e^{-t}\right]$$

$$\therefore \quad s\bar{y}(s) - y(0) + \bar{y}(s) = \frac{1}{s+1}$$ ← Algebraic equation that we can manipulate

$$(s+1)\,\bar{y}(s) - 5 = \frac{1}{s+1}$$

$$(s+1)^2\,\bar{y}(s) - 5(s+1) = 1$$

$$\therefore \bar{y}(s) = \frac{1}{(s+1)^2} + \frac{5}{s+1}$$

Perform inverse transform:

$$\underline{\underline{y(t) = te^{-t} + 5e^{-t}}}$$

Often we end up with transform equations of the form

$$\bar{f}(s) = \frac{Q(s)}{P(s)} \begin{matrix} \leftarrow \text{polynomial} \\ \leftarrow \text{polynomial} \end{matrix}$$

Finding the inverse is not obvious usually.
So we use Partial Fractions to form:

$$\frac{Q(s)}{P(s)} = \frac{C_1}{r_1(s)} + \frac{C_2}{r_2(s)} + \cdots \frac{C_n}{r_n(s)} \leftarrow \text{roots}$$

We can invert these easily

Example:

$$\frac{Q(s)}{P(s)} = \frac{s^2-s-6}{s^3-2s^2-s+2} = \frac{s^2-s-6}{(s-1)(s+1)(s-2)} = \frac{C_1}{s-1} + \frac{C_2}{s+1} + \frac{C_3}{s-2}$$

Compute C_1 (multiply by $(s-1)$) to give

$$\frac{s^2-s-6}{(s+1)(s-2)} = C_1 + \frac{C_2(s-1)}{s+1} + \frac{C_3(s-1)}{s-2}$$

which must be true for all s. Setting $s=1$:

$$C_1 = \frac{1-1-6}{2 \times -1} = 3.$$

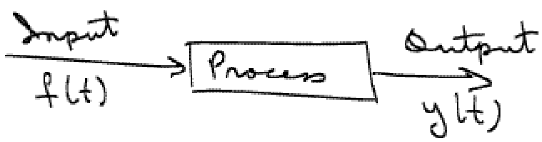
Likewise we find $C_2 = -2/3$ & $C_3 = -4/3$.

$$\therefore f(t) = 3e^{t} - \tfrac{2}{3}e^{-t} - \tfrac{4}{3}e^{2t}$$

11 Control Theory

[Reference: Chemical Process Control: An Introduction to Theory and Practice, George Stephanopoulos]

Often in engineering we have some process that gives an output, $y(t)$, from some input or forcing function, $f(t)$:



or

$$\bar{F}(s) \longrightarrow \boxed{G(s)} \longrightarrow \bar{y}(s)$$

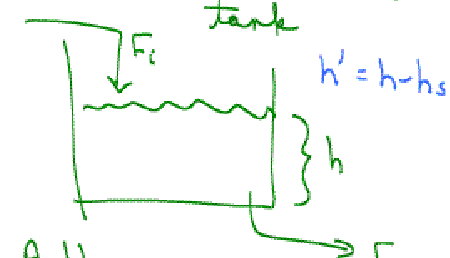
$G(s)$ is called the transfer function

A simple first order system would be

$$a_1 \frac{dy}{dt} + a_0 y = b\, f(t)$$

example $\longrightarrow$

Example: Water level in a tank



$h' = h - h_s$

$$A\frac{dh}{dt} = F_i - F_o \leftarrow h/R$$

$$\Rightarrow A\frac{dh'}{dt} = F_i' - h'/R$$

$$\therefore\ A s \bar{h}'(s) = \bar{F}_i'(s) - \bar{F}_o'(s)$$

$$= \bar{F}_i'(s) - \frac{1}{R}\bar{h}'(s)$$

$$\therefore\ \bar{h}'(s) = \frac{\bar{F}_i'(s)}{(As + 1/R)}$$

or $$\frac{\bar{h}(s)}{\bar{F}_i(s)} = \frac{1}{As + 1/R} \equiv G(s)$$

But in general we could have

$$a_n \frac{d^n y}{dt^n} + a_{n-1}\frac{d^{n-1}y}{dt^{n-1}} + \dots\dots a_1\frac{dy}{dt} + a_0 y = b f(t)$$

We define y as the deviation from steady state so that

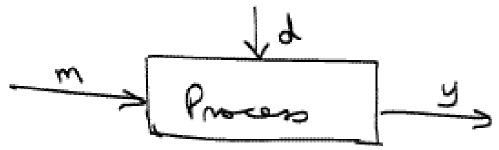
$$y(0) = \left.\frac{dy}{dt}\right|_{t=0} = \dots \left.\frac{d^{n-1}y}{dt^{n-1}}\right|_{t=0} = 0$$

Thus

$$a_n s^n \bar{y}(s) + a_{n-1}s^{n-1}y(s) \dots\dots a_1 s\bar{y}(s) + a_0 y(s) = b\bar{f}(s)$$

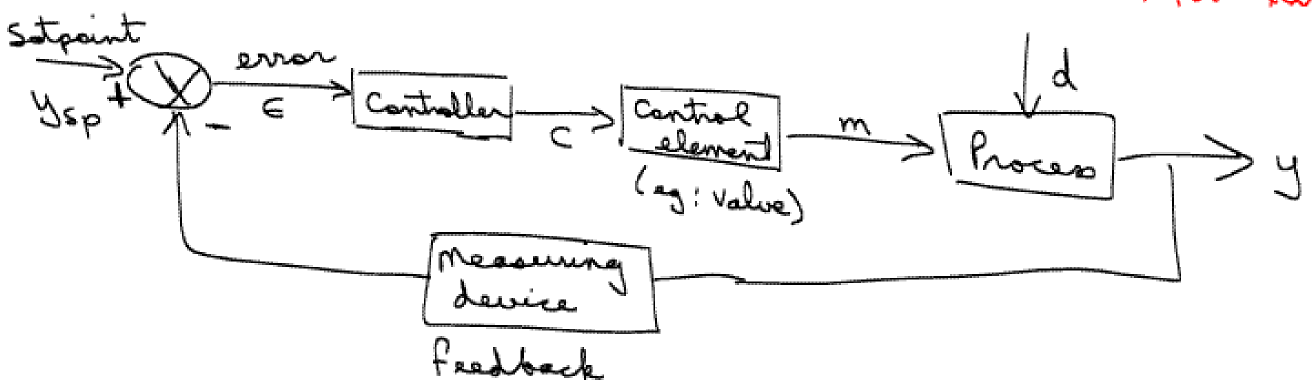
$$\therefore\ \frac{\bar{y}(s)}{\bar{f}(s)} = \frac{b}{a_n s^n + \dots a_1 s + a_0} \equiv \bar{G}(s)$$

Typically we want to control the process output $y(t)$ by manipulating some variable so that we get the desired output y_{sp} even though we have disturbances, $d(t)$.



In our water tank example, $d = F_i'$
and we control F_o' by an outlet valve, for example.

We need a controller to do that:



Types of Controllers:

P (proportional)

$$c(t) = k_c\,\epsilon(t) + C_s$$

gain   bias

deviation variables:

$$c'(t) = c(t) - C_s$$

$$\therefore\ c'(t) = k_c\,\epsilon(t)$$

$$\therefore\ \bar{G}_c(s) = \frac{\bar{C}'(s)}{\bar{\epsilon}(s)} = k_c$$

PI (proportional-integral)

$$c(t) = k_c\,\epsilon(t) + \frac{k_c}{\tau_I}\int_0^t \epsilon(t)\,dt + C_s$$

integral time constant

$$c'(t) \equiv c(t) - C_s \Rightarrow c'(t) = k_c\,\epsilon(t) + \frac{k_c}{\tau_I}\int_0^t \epsilon(t)\,dt$$

$$\therefore\ \bar{C}'(s) = k_c\,\bar{\epsilon}(s) + \frac{k_c\,\bar{\epsilon}(s)}{\tau_I s}$$

$$\therefore\ \bar{G}_c(s) = \frac{\bar{C}'(s)}{\bar{\epsilon}(s)} = k_c\left(1 + \frac{1}{\tau_I s}\right)$$

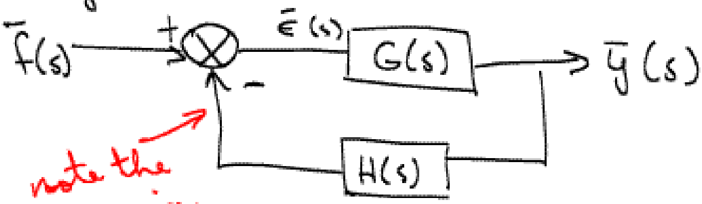
PID (proportional-integral-differential)

$$c(t) = k_c\,\epsilon(t) + \frac{k_c}{\tau_I}\int_0^t \epsilon(t)\,dt + k_c\,\tau_D\frac{d\epsilon}{dt} + c_s$$

$$\Rightarrow \quad \bar{G}_c(s) = k_c\left(1 + \frac{1}{\tau_I s} + \tau_D s\right)$$

<u>Aside</u>

You will find it handy to be able to quickly simplify block diagrams. One common occurance is the simple feedback system:



note the minus sign

$\bar{\epsilon} = \bar{f} - H\bar{y}$ (dropping the (s) for simplicity)

$\bar{y} = G\bar{\epsilon}$

$\therefore\ \bar{y} = G(\bar{f} - H\bar{y})$

$\quad = G\bar{f} - GH\bar{y}$

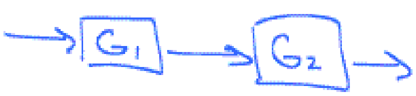
$\therefore\ \bar{y}(1+GH) = G\bar{f}$

$\therefore\ \dfrac{\bar{y}}{\bar{f}} = \dfrac{G}{1+GH}$

So we can replace the above by

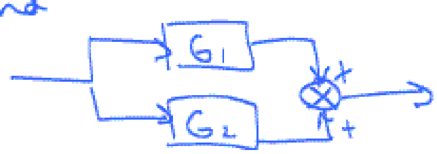
$\Leftarrow$

Also note ~~that~~



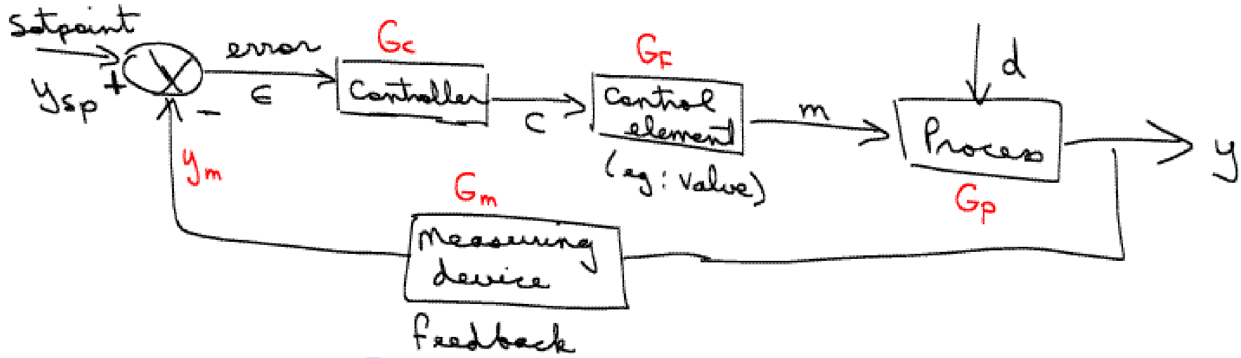
is equivalent to

and



is equivalent to

Getting back to our general controlled process



$\bar{y} = G_p \bar{m} + G_d \bar{d}$ ($\bar{y}$ means $\bar{y}(s)$ etc)

sub back in

$\bar{y}_m = G_m \bar{y}$

$\bar{\epsilon} = \bar{y}_{sp} - \bar{y}_m$

$\bar{c} = G_c \bar{\epsilon}$

$$\bar{m} = G_F \bar{c} = G_F G_c \bar{\epsilon} = G_F G_c (\bar{y}_{sp} - \bar{y}_m)$$

$$= G_F G_c (\bar{y}_{sp} - G_m \bar{y})$$

$$\therefore \bar{y} = \underbrace{G_p G_F G_c}_{\equiv G} (\bar{y}_{sp} - G_m \bar{y}) + G_d d$$

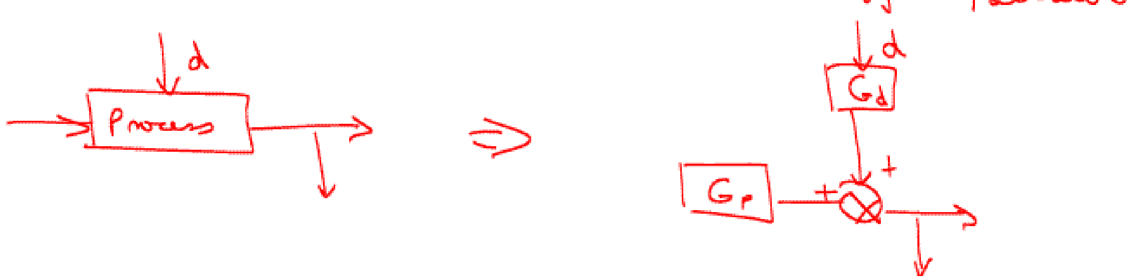
$$\therefore \bar{y}(s) = \underbrace{\frac{G \bar{y}_{sp}}{(1 + G G_m)}}_{1} + \underbrace{\frac{G_d d}{(1 + G G_m)}}_{2}$$

Note : $\bar{y}(s)$ is composed to two parts:

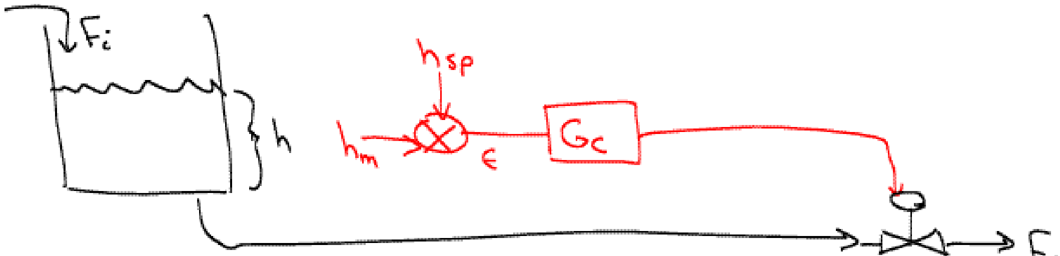
1 - Response to setpoint changes ← Servo action

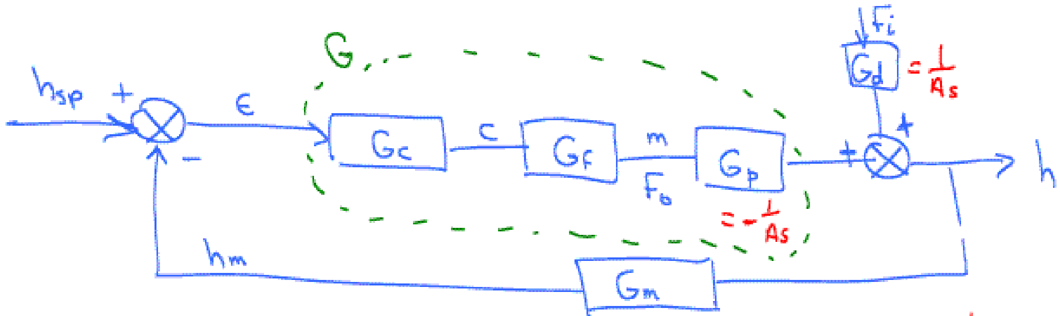
2 - Response to disturbances ← Regulation action

So in the above diagram we should modify as follows:



Example: Water tank – outlet flow control





Process: $A\frac{dh'}{dt} = F_i' - F_o' \Rightarrow \bar{h}' = \underbrace{\frac{1}{As}}_{G_d}\bar{F}_i - \underbrace{\frac{1}{As}}_{G_p}\bar{F}_o$ note '−'

Controller: PI $\therefore$ $G_c = k_c\left(1+\frac{1}{\tau_I s}\right)$

Valve: $G_f = \frac{k_v}{\tau_v s+1}$ (1st order system)

Measurement device: $G_m = \frac{k_p \alpha}{\tau^2 s^2 + 2\zeta\tau s + 1}$ (2nd order)

Note: if the valve was on the inlet then
$G_p = \frac{1}{As}$
$G_d = -\frac{1}{As}$
All else is the same.

We plug the above into:

$$\bar{y} = \underbrace{G_p G_f G_c}_{\equiv G}(\bar{y}_{sp} - G_m \bar{y}) + G_d d$$

$$\bar{y}(s) = \frac{G\bar{y}_{sp}(s)}{(1+GG_m)} + \frac{G_d d(s)}{(1+GG_m)}$$

to get the system response.

12 Worked Examples

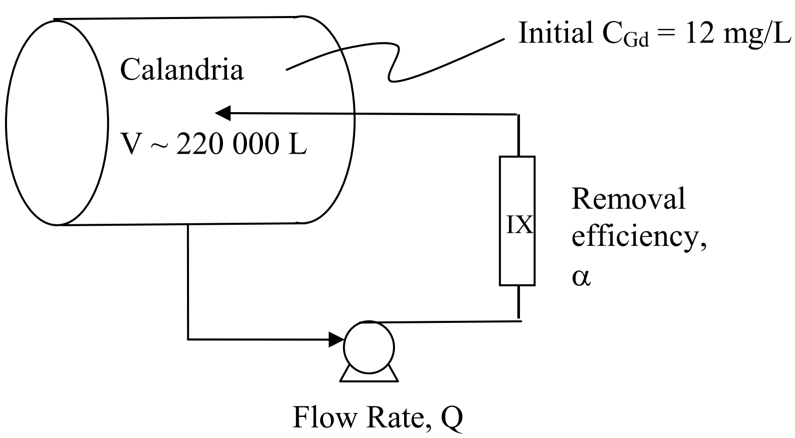
12.1 Tank Problem

The moderator in your CANDU unit has been poisoned with gadolinium nitrate due to activation of shut-down system two (SDS-2). The plant manager asks you to quickly calculate how long it will take to clean up the moderator. A rough schematic of the system is shown below.

Q1. Develop a mathematical expression describing the concentration of GdNO3 in the moderator with time based on the schematic below.

Q2. Given:
flow rate through the ion exchange columns, Q = 2,300 L/min
initial concentration of GdNO3, Co = 12 mg/L
volume of D_2O in the calandria, V = 220 000 L
removal efficiency of the ion exchange columns, α = 95%

Calculate how long it will take to get the GdNO3 concentration below 0.01 mg/L in order to begin plant start-up activities.



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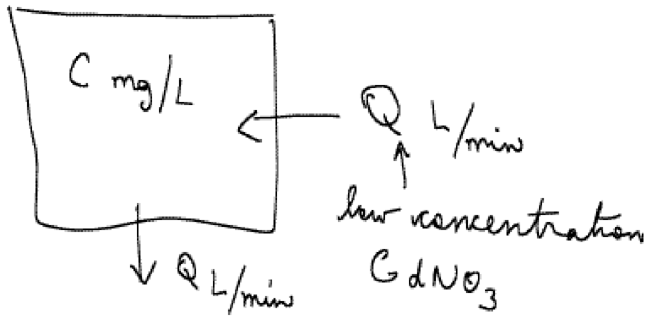
Tank Problem

We want concentration C of $GdNO_3$ in calandria as a function of time.



$C = \text{Mass}/\text{Volume} = m/V$

V is fixed.

Thus if we know mass, we know C !

Mass balance:

$$\frac{dm}{dt} = \text{mass flow in} - \text{mass flow out}$$

$= V\frac{dc}{dt}$

$= (1-\alpha)CQ$

$= CQ \quad \text{mg}/_{L} \cdot {}^{L}/_{\text{min}} = \text{mg}/_{\text{min}}$

This is what is left in the stream after it exits from IX col.

$$\therefore V\frac{dc}{dt} = (1-\alpha)CQ - CQ = -\alpha CQ$$

This makes sence; αCQ is the rate of removal.

$$\therefore \frac{dc}{dt} = -\frac{\alpha Q}{V}C \equiv -C/\tau \qquad \left(\tau \equiv \frac{V}{\alpha Q}\right)$$

Solving ↓

$$\frac{dc}{c} = -\frac{1}{\tau}dt \Rightarrow \ln c = -t/\tau + \text{const.}$$

I.C.: $C(0) = C_0 = 12 \text{ mg/L}$.

$$\therefore \ln C_0 = 0 + \text{const} \Rightarrow \ln c/c_0 = -t/\tau$$

$$\Rightarrow \boxed{C = C_0 e^{-t/\tau}}$$

What is time when $C = 0.01 \text{ mg/L}$?

$$-\ln\left(\frac{.01}{12}\right) \times \tau = t$$

$$\tau = V/\alpha Q = \frac{220{,}000}{0.95 \times 2300}$$

$$= 100.68 \text{ min.}$$

$$t = -(-7.09) \times 100.68 = 11.89 \text{ hr}$$

$$= \underline{\underline{11 \text{ hr } 54 \text{ minutes}}}$$

13 Appendices

13.1 Bessel Functions

$$\text{J} = \text{Bessel function of the first kind} \tag{3.20}$$

$$\begin{aligned} \text{Y} &= \text{Neuman} = \text{N}_\nu(\text{x}) \\ &= \text{Bessel function of the second kind} \\ &= \frac{\cos(\nu\pi)\text{J}_\nu(\text{x}) - \text{J}_{-\nu}(\text{x})}{\sin(\nu\text{x})} \end{aligned} \tag{3.21}$$

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Revision history:
Revision 0, 2009.08.08, initial creation.

Source document archive location: See page footer.

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Notes: