

COMPUTATIONAL MATHEMATICS

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Australian National University Course Overview

COURSE OUTLINE

Course modules

- Numerical linear algebra
- Function approximation
- Numerical integration and differentiation
- Modeling with and solving differential equations

Core concepts

- Mathematical (Conditioning) and Numerical Stability
- Error (accuracy)
- Cost (efficiency)
- Using software tools correctly

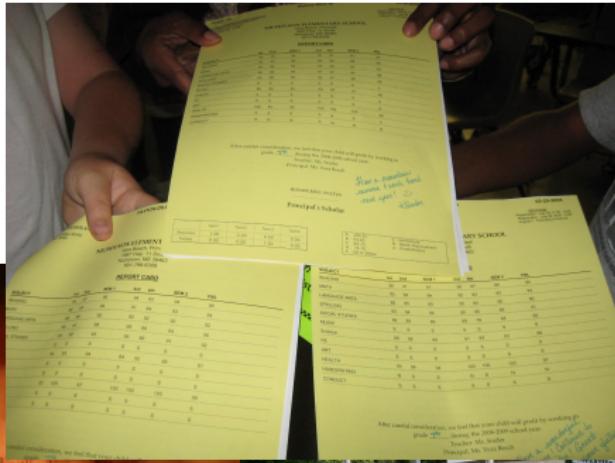
RELEVANCE



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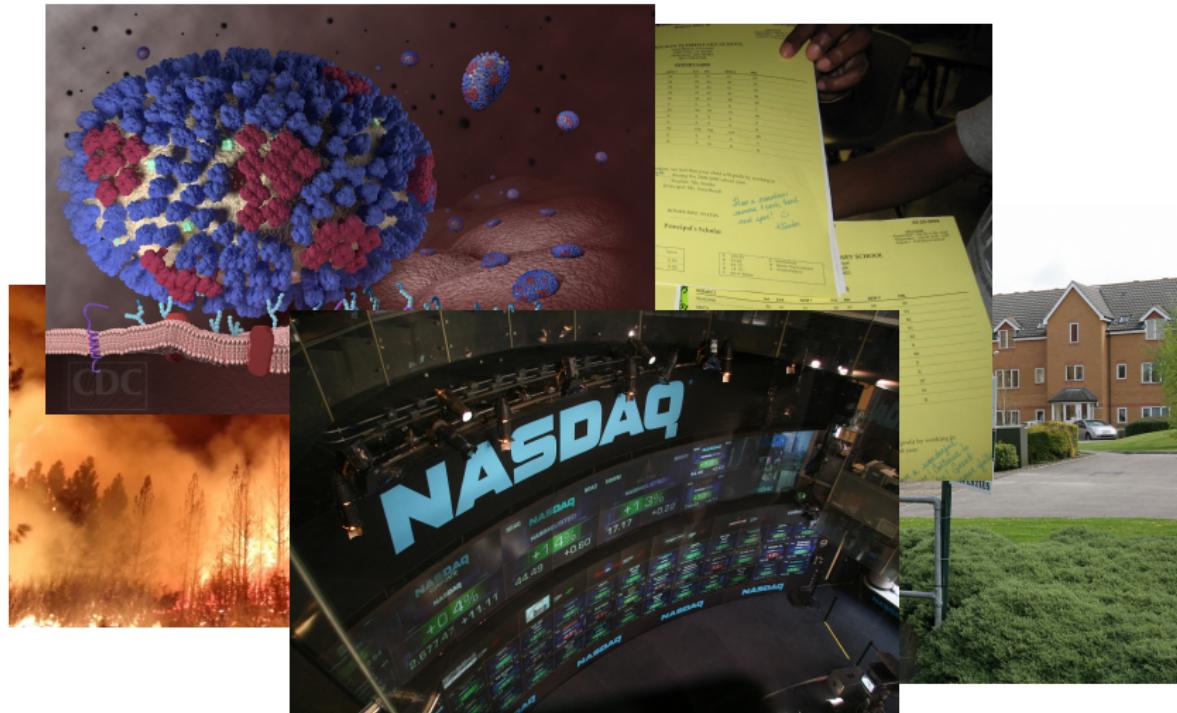
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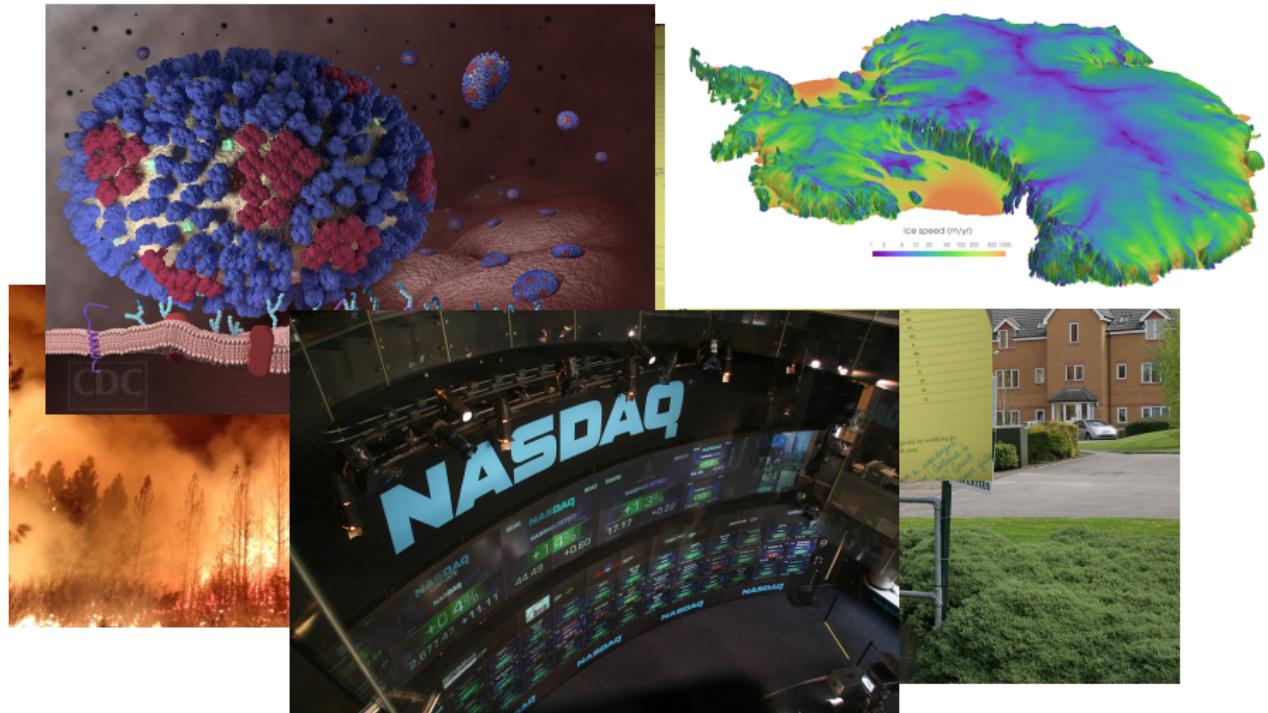
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RELEVANCE



Financial institutions often combine multiple stocks into one package. One may be given the total number of each stock and the total price for all stocks but not the individual stock prices.

We can determine the prices on the individual stocks given the price of each package p and number of stocks M_{ij} in each package using linear algebra. Given

$$M = \begin{bmatrix} 3 & 1 \\ 2 & 2 \end{bmatrix}, \quad p = \begin{bmatrix} 100 \\ 120 \end{bmatrix} \quad \text{we know} \quad Mc = p$$

The price of the individual stocks are

$$c = M^{-1}p = [20, 40]^T$$

How can we solve this when there are many stocks and packages?

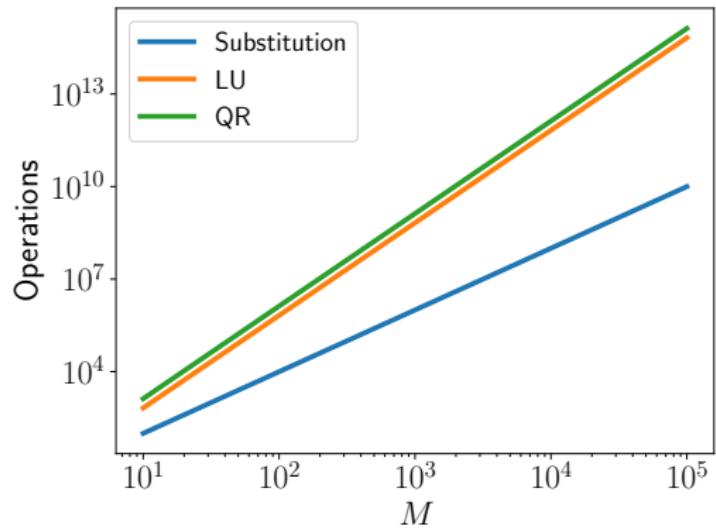
Algorithm choice depends on cost (FLOPS) and numerical stability.

COST

The cost of an algorithm affects best choice of algorithm?

Factorize a large matrix

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1M} \\ a_{21} & a_{22} & \cdots & a_{2M} \\ \vdots & \vdots & \ddots & \vdots \\ a_{M1} & a_{M2} & \cdots & a_{MM} \end{bmatrix}$$



Which algorithm would you choose?

CONDITIONING AND STABILITY

In 1991, a Patriot missile defense system failed to intercept an incoming Scud missile, killing 28 people.



Hours	Time Shift (s)	Range Shift (m)
0	0	0
1	.0034	7
8	.0275	55
20(a)	.0687	137
48	.1648	330
72	.2472	494
100(b)	.3433	687

(a) Continuous operation exceeding about 20 hours
— target outside range gate (b) Alpha Battery ran continuously for about 100 hours

LINEAR LEAST SQUARES PREDICTING HOUSE PRICES

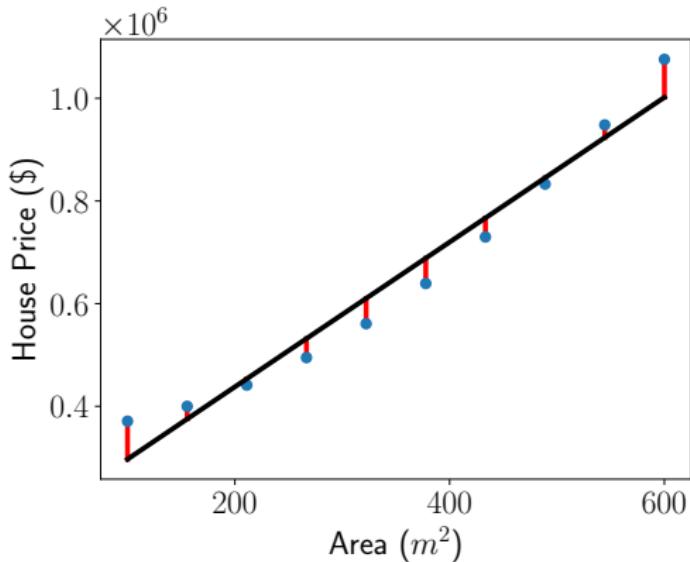
Fit data

$$(x_i, y_i)$$

with model

$$y = \beta_0 + \beta_1 x$$

$$\begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \begin{bmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_M \end{bmatrix}^{-1} \begin{bmatrix} y_1 \\ \vdots \\ y_M \end{bmatrix}$$

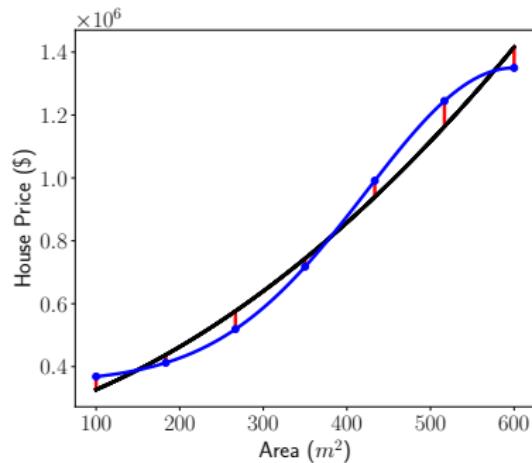
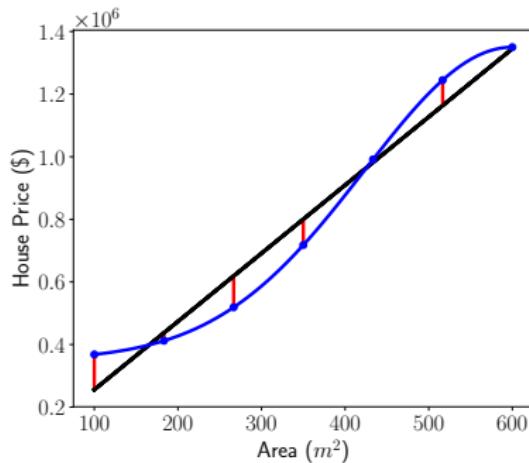


How do we deal with non-linear relationships?

Multiple independent variables (inputs x)

ACCURACY

We will learn how to measure accuracy of an approximation.



Must find a compromise between cost and accuracy.

Stability affects accuracy

ORDINARY DIFFERENTIAL EQUATIONS

VIRAL DYNAMICS

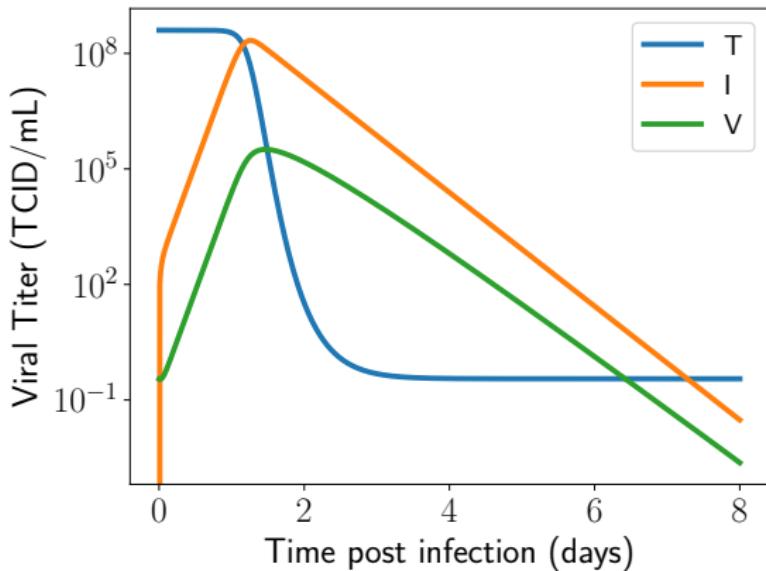
$$\frac{dT}{dt} = -\beta TV$$

$$\frac{dI_1}{dt} = \beta TV - \delta I$$

$$\frac{dV}{dt} = pI - cV$$

$$T(0) = 4 \times 10^8, I(0) = 0$$

$$V(0) = 3.5 \times 10^{-1}$$

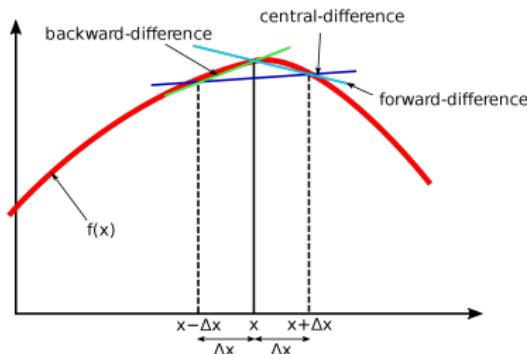


T is the number of uninfected target cells, I is the number of productively infected cells, and V is the infectious-viral titer expressed in TCID/ml of nasal wash.

PARTIAL DIFFERENTIAL EQUATIONS

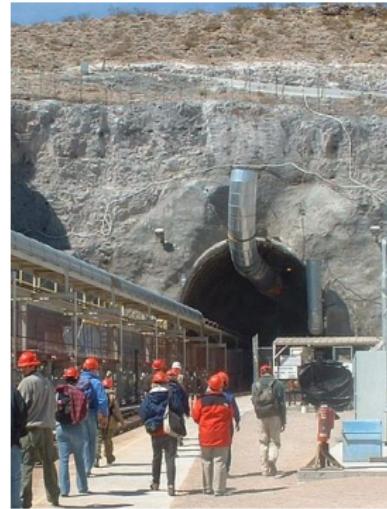
GROUNDWATER FLOW

Modelling Storage of Hazardous Material



$$\frac{df(x)}{dx} = \lim_{\Delta x \rightarrow 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

$$\frac{\partial u(x,t)}{\partial t} = a \frac{\partial u(x,t)}{\partial x} + k \frac{\partial^2 u(x,t)}{\partial x^2} + f(x,t)$$



Cost and accuracy and stability are all very important here.

COURSE OUTLINE

- Representing numbers numerically on a computer
- Matrix factorizations - condition numbers; cost vs stability
- Linear least-squares - using matrix factorizations; linear and polynomial bases; univariate and multivariate
- Interpolation - error and convergence; Lagrange interpolation and stability; tensor-product interpolation
- Numerical integration - low-order methods; Gaussian quadrature
- Numerical differentiation - Taylor approximation; finite difference methods; polynomial methods
- Ordinary differential equations (ODE) - formulation; time-stepping methods; numerical stability
- Partial differential equations (PDE) - formulation; steady state and transient equations; mesh convergence