Introduction and Syllabus for 18.S096:

Matrix Calculus

IAP 2023

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MWF 11am–1pm in 2-190

(MIT students, comments, fixes, request for further clarifications, welcome. Please keep mathematical)

- Lectures: Jan. 18,20,23,25,27 + Feb. 1,3
    - 11am–1pm in 2-142, short break around noon
- **Two Psets:** Released Wednesday due following Wednesday (Jan 19 & 26) @ midnight on Canvas
- **3 Units**
- Prerequisite: Linear Algebra (18.06 or similar)

Some demos and hw may use julia (minimal programming experience assumed, though most LinAlg classes at MIT use a little Julia already)

Where does matrix calculus fit in?

- MIT 18.01: Scalar or Single Variable Calculus
- MIT 18.02: Vector or Multivariable Calculus

18.01 Calculus

Prereq: None
Units: 5-0-7
Credit cannot also be received for 18.01A, ES.1801, ES.18
Lecture: *TR11,F2* (2-135) **Recitation:** *MW2* (2-135)

Differentiation and integration of functions of one variable,

18.02 Calculus

Prereq: Calculus I (GIR)
Units: 5-0-7
Credit cannot also be received for 18.022, 18.02A, CC.1802, ES.1802, ES.182A
Lecture: *TR11,F2* (32-123) **Recitation:** *MW9* (2-147) or *MW10* (2-147, 2-142) or *MW11* (2-142, 2-143, 2-142, 2-136) or *MW1* (2-142, 2-136) or *MW2* (2-136) or *MW3* (2-136) ***+final***

Calculus of several variables. Vector algebra in 3-space, determinants, matrices. Vector-valued functions space motion. Scalar functions of several variables: partial differentiation, gradient, optimization techniq

Perhaps an ideal world might go Scalar, Vector, Matrix, Higher Dimensional Arrays…

(0 dimensional, 1 dimensional, 2 dimensional…)

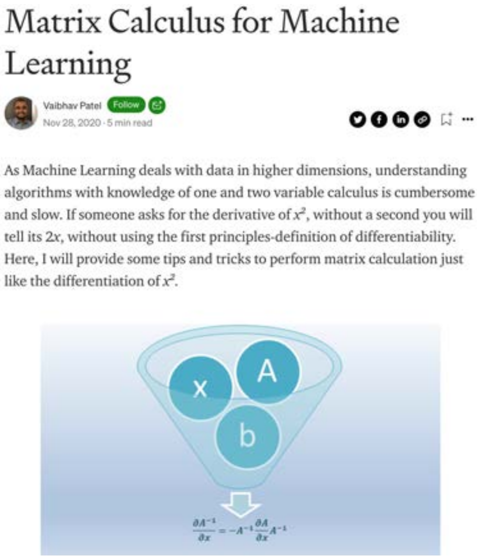
(e.g. size(scalar)=[], size(vector)=[n], size(matrix)=[m,n],...)

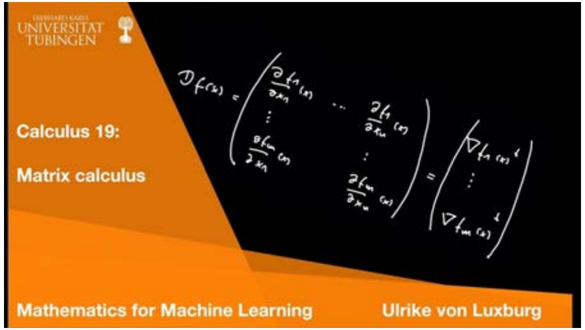
(some programming language do not implement this fully)

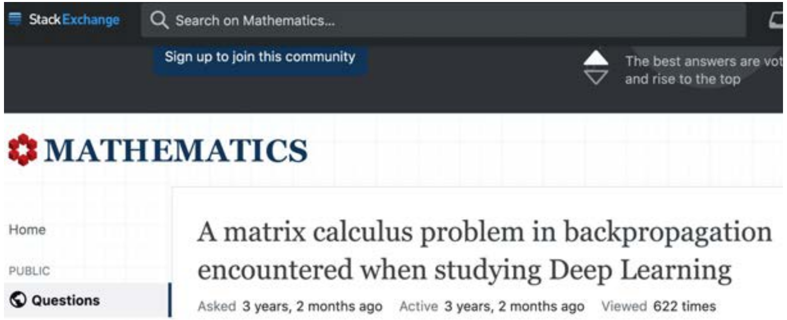
Why now?

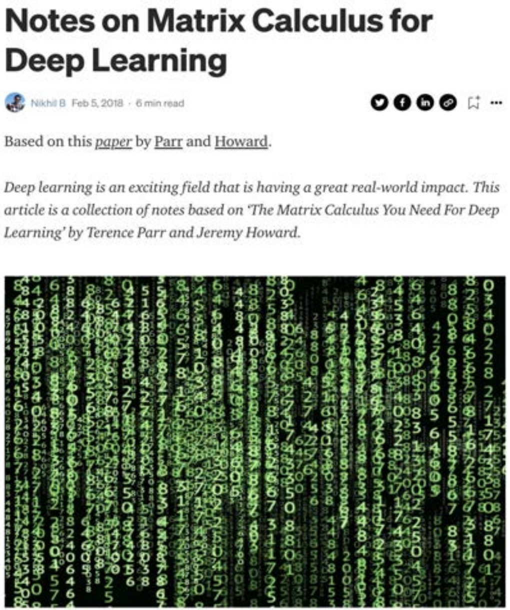
- In the last decade or two, the role of linear algebra has taken on larger importance in lots of areas including Machine Learning, Statistics, Engineering, etc.
- Warning: googling Matrix Calculus may only give a small view of the full range of the mathematics that we hope to cover example what is the derivative of X^2 when X is a square matrix? Should it be 2X? (It's not). What about X^{-1}? $-X^{-2}$? (Not quite).

Applications: Machine Learning buzzwords: parameter optimization stochastic gradient descent, autodiff, backpropagation









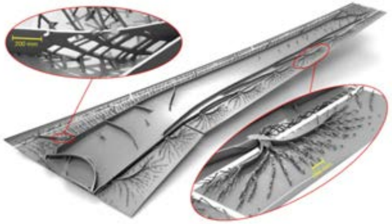
Applications: Physical Problems

Engineering optimization (structural "topology" optimization):

Find the physical structure that optimizes some objective (e.g. focusing light, minimizing drag, supporting weight, ...).

Topology-optimized aircraft wing

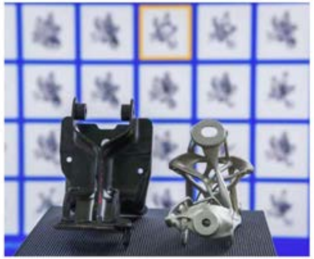
~ 10^9 parameters



Goal: maximize stiffness under external loads, utilizing limited amount of material
→ Light but strong
→ 100s tonnes of fuel saving

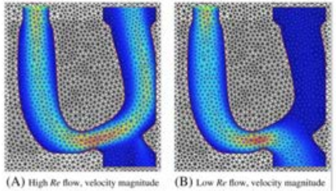
Aage, Niels, et al. "Giga-voxel computational morphogenesis for structural design." *Nature* 550.7674 (2017): 84-86.

Topology-optimized 3D-printed hip replacement (Altair)



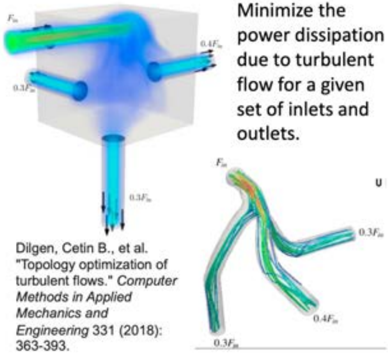
Topology-optimized 3D-printed seat bracket (General Motors)

Topology optimization with fluid dynamics



Switching flow channels for high vs. low viscosity

Zhou, Mingdong, et al. "Shape morphing and topology optimization of fluid channels by explicit boundary tracking." *International Journal for Numerical Methods in Fluids* 88.6 (2018): 296-313.



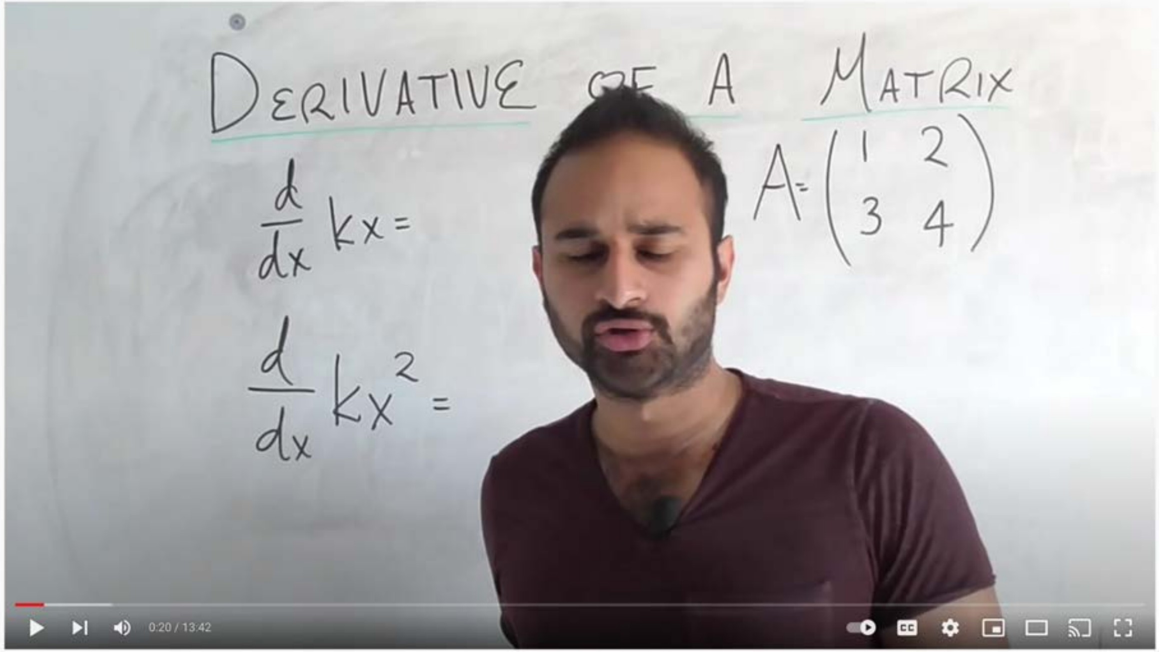
Minimize the power dissipation due to turbulent flow for a given set of inlets and outlets.

Dilgen, Cetin B., et al. "Topology optimization of turbulent flows." *Computer Methods in Applied Mechanics and Engineering* 331 (2018): 363-393.

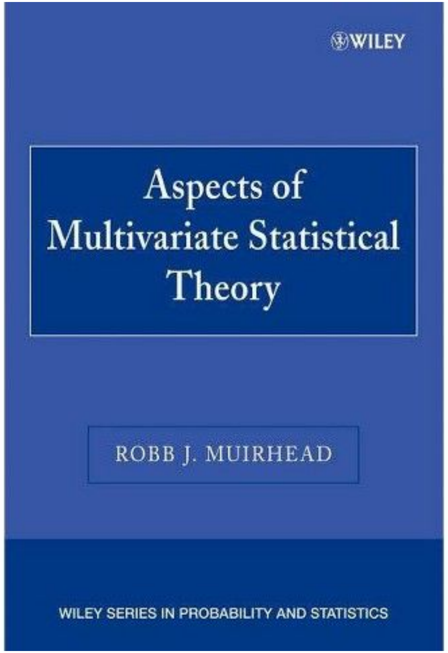
Key point is that if you have *any* complicated calculation with lots of parameters, you can compute gradient (sensitivity) of a scalar output g(u) with respect to every parameter with roughly *one* additional calculation.

Enabling factor for large-scale optimization in machine learning [g = loss function, u = network outputs, **p** = network weights & other parameters], statistics, finance, and many other fields.

Applications: Data Science & Multivariable Statistics



Derivative of a Matrix : Data Science Basics



The Role of Automatic Differentiation

Typical differential calculus classes are mostly symbolic calculus:

- Students learn to do what mathematica/wolfram alpha readily can do

For a small portion of the class, some numerics may show up

- approximate $f'(x)$ by finite differences $(f(x+\epsilon)-f(x)) / \epsilon$ or $(f(x+\epsilon)-f(x-\epsilon)) / 2\epsilon$
- e.g. students and professors think that “sin” is actually computed using Taylor series

Today’s automatic differentiation is neither of these two things. It is more in the field of the computer science topic of compiler technology than mathematics.

However the underlying mathematics is interesting! We will learn about this in this class.

Everything is easy with scalar functions of scalars

- The derivative of a function of one variable is a function of one variable
- The linearization of a function has the form $(y-y_0) \approx f'(x_0)(x-x_0)$

  Other notations (sometimes confusing x and x_0):

  - $\delta y \approx f'(x)\ \delta x$
  - $dy = f'(x)dx$
  - $f(x)-f(x_0) \approx f'(x_0)(x-x_0)$
  - $df = f'(x)dx$ ← this one is preferred here
- Numerics are fairly trivial:

Numerical Example of what's going on in the previous slide

Suppose $f(x) = x^2$ with $(x_0,y_0)=(3,9)$ and $f'(x_0)=6$

```
f(3.0001)     = 9.00060001
f(3.00001)    = 9.0000600001
f(3.000001)   = 9.000006000001
f(3.0000001)= 9.00000060000001
```

(Notice that $\Delta y = 6\ \Delta x$)

f(3 + Δx) $\approx$ 9 + Δy = 9 + $6\ \Delta x$ ($\Delta y = f'(x_0)\ \Delta x$)

f(x)-f(3) $\approx$ 6 (x-3) $\leftarrow$ linearization of x^2 at x=3 is the "multiply by 6" function

We write:

$dy = f(x_0+dx) - f(x_0)$ where $dy = f'(x_0)dx$ or $f(x_0+dx) = f(x_0) + f'(x_0)dx$

I think of dx and dy as really small numbers; in math they are called infinitesimal.

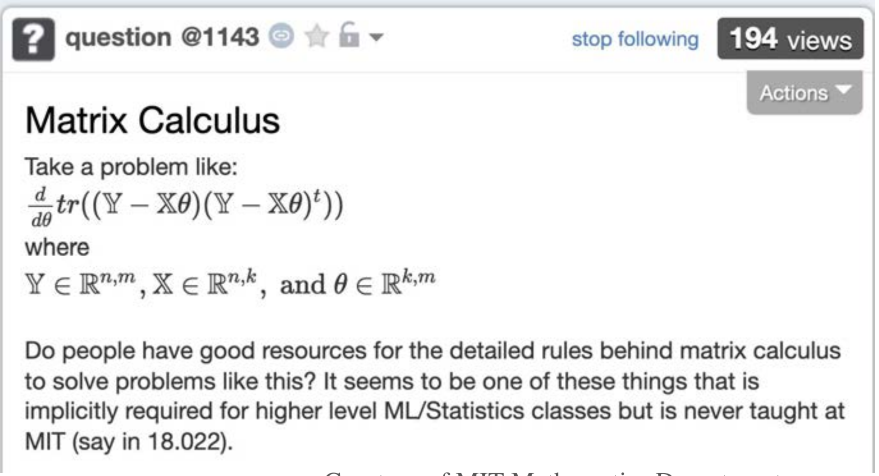
In rigorous mathematics, one takes limits.

Demo

http://www.matrixcalculus.org/

Notation: Elementwise vector or matrix product. We will use x.*y, they use x⊙y

- [2,3].*[10,11] = [20,33]
- trace(A) = tr(A) = the sum (a scalar) of the diagonal elements of matrix A
- Some limitations:
  - matrixcalculus.org will not display derivatives that involve more than 2 dimensions:
    - e.g. a derivative of a matrix with respect to a vector or a matrix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Actions

Matrix Calculus

Take a problem like:

$$\frac{d}{d\theta} tr((\mathbb{Y} - \mathbb{X}\theta)(\mathbb{Y} - \mathbb{X}\theta)^t))$$

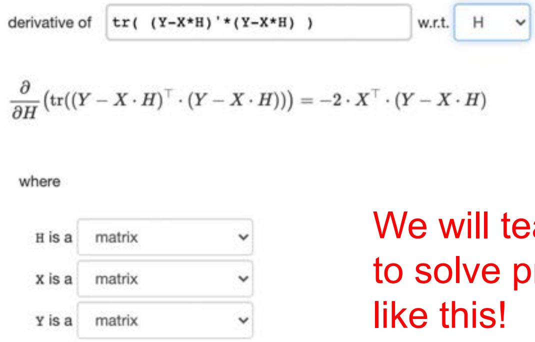
where

$$\mathbb{Y} \in \mathbb{R}^{n,m}, \mathbb{X} \in \mathbb{R}^{n,k}, \text{ and } \theta \in \mathbb{R}^{k,m}$$

Do people have good resources for the detailed rules behind matrix calculus to solve problems like this? It seems to be one of these things that is implicitly required for higher level ML/Statistics classes but is never taught at MIT (say in 18.022).

Courtesy of MIT Mathematics Department.

If we differentiate a scalar function of a matrix
Answer is a matrix: - 2 X' (Y-Xθ)



We will teach you to solve problems like this!

Format of the first derivative, explicit notation:

input ↓ \ output →	scalar	vector	matrix
scalar	scalar	vector (e.g. velocity)	matrix
vector	gradient = vector (or column vector) Notation: ∇f $f'(x)$ = row vector $df = f'(x)dx$	matrix (Jacobian matrix)	higher order array
matrix	matrix	higher order array	higher order array

Format of the first derivative, implicit view: **linear operator**

$d(x^3) = 3x^2\,dx$ scalar in, scalar out (multiply the infinitesimal scalar dx by $3x^2$)
$d(x^Tx) = 2x^Tdx$ scalar in, vector out (take the dot product of the infinitesimal vector dx with the vector 2x)
$d(X^2) = XdX + dX\,X$ matrix in, matrix out (multiply the infinitesimal matrix dX by matrix X on each side and add)

You will learn to do all of these in great detail – the purpose of this slide is just to plant the notion of **linearization**.

Let's check the linearization numerically

$f(x) = x^T x$

$x_0 = [3;4] \implies f(x_0)=x_0^T x_0 = 25$

$dx = [0.001;0.002] \implies (3.001)^2+(4.002)^2 = 25.022005$

$2x_0^T dx = 2\,[3;4]^T[0.001;0.002] = 0.022$

Notice that $f(x_0 + dx) \approx f(x_0) + 2x_0^T dx = 25+0.022$

Matrix and vector product rule

$d(AB) = (dA)B + A(dB)$ is still correct but generally the products do not commute

However if x is a vector:

$d(x^Tx) = dx^Tx + x^Tdx$ and since vector dot products commute (a dot b is b dot a), we in this special case can write $d(x^Tx) = (2x)^Tdx$.

Example: x=[1;2;3;4] ; dx=rand(4)/100000;

```
(x+dx)'*(x+dx) - x'x  # this is d(x'x)

(2x)'*dx  # this is approximately the same as d(x'x)
```

Note: the way the product rule works for vectors and matrices is that transposes "go for the ride"

Examples:

1. $d(u^Tv) = du^Tv + u^Tdv$ but note $du^Tv = v^Tdu$ because dot products commute
2. $d(uv^T)=duv^T + udv^T$

For the explicit form we want derivatives of **all outputs** w.r.t. to **all inputs**.

How many parameters are needed? If there are n inputs and m outputs

Answer:

Second derivatives (a few words for starters)

Explicit form: The second derivative of a *scalar valued* function of a *vector* is represented explicitly as a symmetric **matrix** known as the **Hessian** of the function.

Implicit form: *All* second derivatives are what is known in advanced linear algebra as a quadratic form (or a symmetric **bilinear form**).