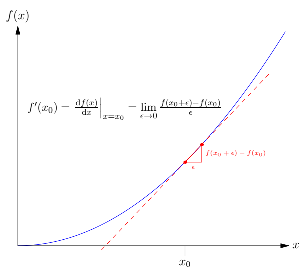
Advanced Machine Learning

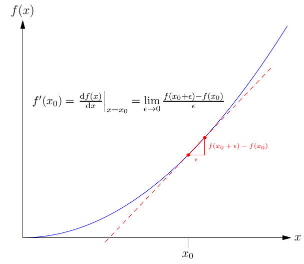
Differential Calculus



Differentiation, product and chain rules, vectors and matrices

Outline

1. **Why Calculus?**
2. Differentiation
3. Vector and Matrix Calculus



Why Calculus?

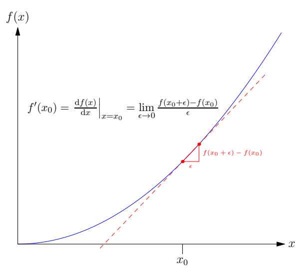
- Calculus is a fundamental tool of mathematical analysis
- In machine learning differentiation is fundamental tool in optimisation
- Integration is an essential tool in taking expectations over continuous distributions
- Both differentiation and integration crop up elsewhere
- This material will not be examined explicitly, but I assume elsewhere that you can do calculus

Back to Basics

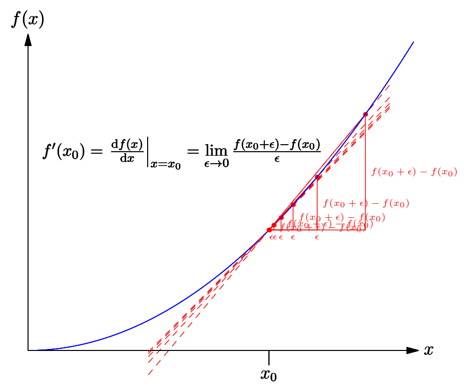
- You have all done A-level maths so should be familiar with the rules of calculus
- But, it is easy to forget the rules and sometimes we use quite sophisticated tricks
- Although the sophisticated tricks really speed up calculations, it pays to be able to understand where these tricks come from

Outline

1. Why Calculus?
2. **Differentiation**
3. Vector and Matrix Calculus



Differentiation



Polynomials

- $f(x) = x^2$

$$\frac{\mathrm{d}x^2}{\mathrm{d}x} = \lim_{\epsilon\to 0} \frac{(x+\epsilon)^2 - x^2}{\epsilon} = \lim_{\epsilon\to 0} \frac{(x^2 + 2\epsilon x + \epsilon^2) - x^2}{\epsilon}$$
$$= \lim_{\epsilon\to 0} 2x + \epsilon = 2x$$

- $(x+\epsilon)^n = (x+\epsilon)(x+\epsilon)\cdots(x+\epsilon) = x^n + n\epsilon x^{n-1} + O(\epsilon^2)$

$$\frac{\mathrm{d}x^n}{\mathrm{d}x} = \lim_{\epsilon\to 0} \frac{(x+\epsilon)^n - x^n}{\epsilon} = \lim_{\epsilon\to 0} n x^{n-1} + O(\epsilon) = n x^{n-1}$$

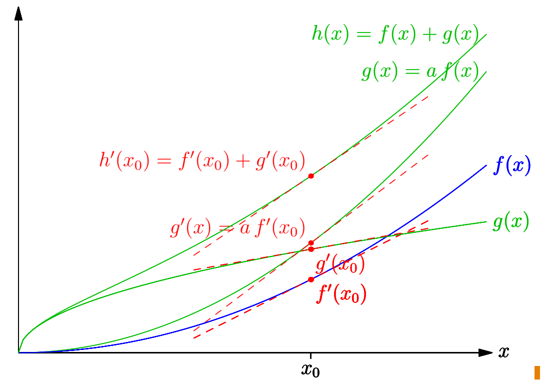
Linearity of derivatives

- Note that $f(x+\epsilon) = f(x) + \epsilon f'(x) + O(\epsilon^2)$ (from the definition of $f'(x)$)

$$\frac{\mathrm{d}(a\,f(x) + b g(x))}{\mathrm{d}x} = \lim_{\epsilon\to 0} \frac{(a\,f(x+\epsilon) + b g(x+\epsilon)) - (a\,f(x) + b g(x))}{\epsilon}$$
$$= \lim_{\epsilon\to 0} \frac{a\epsilon f'(x) + b\epsilon g'(x) + O(\epsilon^2)}{\epsilon}$$
$$= a\,f'(x) + b g'(x)$$

- **Differentiation is a linear operation!**

Linearity in Pictures



Product Rule

- Recall $f(x+\epsilon) = f(x) + \epsilon f'(x) + O(\epsilon^2)$
- If $h(x) = f(x)g(x)$

$$\begin{aligned} h'(x) &= \lim_{\epsilon\to 0} \frac{f(x+\epsilon)g(x+\epsilon) - f(x)g(x)}{\epsilon} \\ &= \lim_{\epsilon\to 0} \frac{\left(f(x)+\epsilon f'(x) + O(\epsilon^2)\right)\left(g(x)+\epsilon g'(x) + O(\epsilon^2)\right) - f(x)g(x)}{\epsilon} \\ &= \lim_{\epsilon\to 0} \frac{\epsilon\left(f'(x)g(x) + f(x)g'(x)\right) + O(\epsilon^2)}{\epsilon} = f'(x)g(x) + f(x)g'(x) \end{aligned}$$

- This is the **product rule**

Chain Rule

- Recall $f(x+\epsilon) = f(x) + \epsilon f'(x) + O(\epsilon^2)$
- Let $h(x) = f(g(x))$
- Then

$$\begin{aligned} h(x+\epsilon) = f(g(x+\epsilon)) &= f\left(g(x) + \epsilon g'(x) + O(\epsilon^2)\right) \\ &= f(g(x)) + \epsilon g'(x) f'(g(x)) + O(\epsilon^2) \end{aligned}$$

- Thus

$$h'(x) = \lim_{\epsilon\to 0} \frac{h(x+\epsilon) - h(x)}{\epsilon} = g'(x) f'(g(x))$$

- This is the famous **chain rule**. Together with the product rule it means you can differentiate almost everything

More on chain rules

- We can also write the chain rule as

$$\frac{\mathrm{d}f(g(x))}{\mathrm{d}x} = \frac{\mathrm{d}f(g)}{\mathrm{d}g}\frac{\mathrm{d}g(x)}{\mathrm{d}x}$$

- Sometimes this is neater or easier to remember

$$\begin{aligned} \frac{\mathrm{d}\mathrm{e}^{\cos(x^2)}}{\mathrm{d}x} &= \frac{\mathrm{d}\mathrm{e}^{\cos(x^2)}}{\mathrm{d}\cos(x^2)}\frac{\mathrm{d}\cos(x^2)}{\mathrm{d}x^2}\frac{\mathrm{d}x^2}{\mathrm{d}x} \\ &= \mathrm{e}^{\cos(x^2)}\left(-\sin(x^2)\right)2x \\ &= -2x\sin(x^2)\mathrm{e}^{\cos(x^2)} \end{aligned}$$

Inverse functions

- Suppose $g(y) = f^{-1}(y)$ is the inverse of $f(x)$ in the sense that $g(f(x)) = f^{-1}(f(x)) = x$
- Using the chain rule

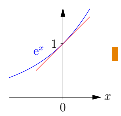
$$\frac{\mathrm{d}g(f(x))}{\mathrm{d}x} = f'(x)g'(f(x)) = 1$$

  since $g(f(x)) = x$
- So $g'(f(x)) = 1/f'(x)$
- Writing $y = f(x)$ so that $x = f^{-1}(y) = g(y)$ we find $g'(y) = 1/f'(g(y))$ that is

$$\frac{\mathrm{d}g(y)}{\mathrm{d}y} = \frac{1}{f'(g(y))} \qquad \frac{\mathrm{d}f^{-1}(y)}{\mathrm{d}y} = \frac{1}{f'(f^{-1}(y))}$$

Exponentials

- Note that $a^{b+c} = a^b a^c$ (that is we multiply a together $b+c$ times)
- Now $\mathrm{e}^\epsilon \approx (1+\epsilon)$



- But $\mathrm{e}^{x+\epsilon} = \mathrm{e}^x\mathrm{e}^\epsilon = \mathrm{e}^x(1+\epsilon+O(\epsilon^2)) = \mathrm{e}^x + \epsilon\mathrm{e}^x + O(\epsilon^2)$

$$\frac{\mathrm{d}\mathrm{e}^x}{\mathrm{d}x} = \lim_{\epsilon\to 0}\frac{\mathrm{e}^{x+\epsilon} - \mathrm{e}^x}{\epsilon} = \lim_{\epsilon\to 0}\frac{\epsilon\mathrm{e}^x + O(\epsilon^2)}{\epsilon} = \mathrm{e}^x$$

Functions of Exponentials

- What about $f(x) = \mathrm{e}^{cx}$

$$\frac{\mathrm{d}\mathrm{e}^{cx}}{\mathrm{d}x} = \frac{\mathrm{d}\mathrm{e}^{cx}}{\mathrm{d}cx}\frac{\mathrm{d}cx}{\mathrm{d}x} = c\mathrm{e}^{cx}$$

- More generally using the chain rule

$$\frac{\mathrm{d}\mathrm{e}^{g(x)}}{\mathrm{d}x} = g'(x)\mathrm{e}^{g(x)}$$

- Also $a^{bc} = (a^b)^c$ (that is we multiply a together $b\times c$ times)

$$\frac{\mathrm{d}a^x}{\mathrm{d}x} = \frac{\mathrm{d}(\mathrm{e}^{\ln(a)})^x}{\mathrm{d}x} = \frac{\mathrm{d}\mathrm{e}^{\ln(a)x}}{\mathrm{d}x} = \ln(a)\mathrm{e}^{\ln(a)x} = \ln(a)a^x$$

Natural Logarithms

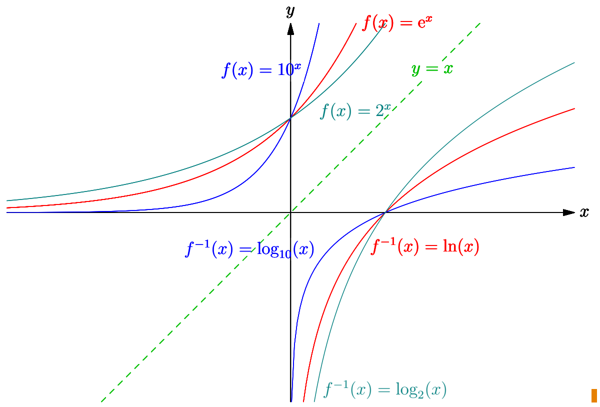
- The natural logarithm is defined as the inverse of e^x

$$\ln(\mathrm{e}^x) = x \qquad \mathrm{e}^{\ln(y)} = y$$

- Recall that if $g(y) = f^{-1}(y)$ then $g'(y) = 1/f'(g(y))$
- Consider $g(y) = \ln(y)$ and $f(x) = \mathrm{e}^x$ (with $f'(x) = \mathrm{e}^x$)

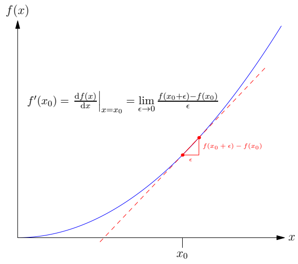
$$\frac{\mathrm{d}\ln(y)}{\mathrm{d}y} = \frac{1}{\mathrm{e}^{\ln(y)}} = \frac{1}{y}$$

Exponentials and Logarithms



Outline

1. Why Calculus?
2. Differentiation
3. **Vector and Matrix Calculus**



Derivatives in High Dimensions

- When working with functions $f : \mathbb{R}^n \to \mathbb{R}$ in many dimensions then there will typically be different derivative in different directions
- To compute the derivative in a direction $\boldsymbol{u} \in \mathbb{R}^n$ (where $\|\boldsymbol{u}\| = 1$) at a point $\boldsymbol{x} \in \mathbb{R}^n$ we use

$$\partial_{\boldsymbol{u}} F(\boldsymbol{x}) = \lim_{\epsilon\to 0} \frac{f(\boldsymbol{x} + \epsilon \boldsymbol{u}) - f(\boldsymbol{x})}{\epsilon}$$

- If $\boldsymbol{u} = \boldsymbol{\delta}_i = (0,\ldots,0,1,0,\ldots,0)$ (i.e. $u_i = 1$) then

$$\frac{\partial f(\boldsymbol{x})}{\partial x_i} = \lim_{\epsilon\to 0} \frac{f(\boldsymbol{x} + \epsilon \boldsymbol{\delta}_i) - f(\boldsymbol{x})}{\epsilon}$$

Taylor

- If we expand $f(\boldsymbol{x} + \epsilon\boldsymbol{u})$ to first order in ϵ

$$f(\boldsymbol{x} + \epsilon\boldsymbol{u}) = f(\boldsymbol{x}) + \epsilon \boldsymbol{u}^{\mathsf{T}} \boldsymbol{g}(\boldsymbol{x}) + O(\epsilon^2)$$

then $g_i(\boldsymbol{x}) = \frac{\partial f(\boldsymbol{x})}{\partial x_i}$

- Recall we defined the vector of first order derivatives of $f(\boldsymbol{x})$ to be the gradient

$$\boldsymbol{\nabla} f(\boldsymbol{x}) = \begin{pmatrix} \frac{\partial f(\boldsymbol{x})}{\partial x_1} \\ \frac{\partial f(\boldsymbol{x})}{\partial x_2} \\ \vdots \\ \frac{\partial f(\boldsymbol{x})}{\partial x_n} \end{pmatrix}$$

- Thus

$$f(\boldsymbol{x} + \epsilon\boldsymbol{u}) = f(\boldsymbol{x}) + \epsilon \boldsymbol{u}^{\mathsf{T}} \boldsymbol{\nabla} f(\boldsymbol{x}) + O(\epsilon^2)$$

This is the start of the high-dimensional Taylor expansion

Computing Gradients 1

- We can compute the gradient by writing out $f(\boldsymbol{x})$ componentwise and performing the partial derivative with respect to x_i

$$\boldsymbol{\nabla} \boldsymbol{w}^{\mathsf{T}} \mathbf{M} \boldsymbol{w} = \begin{pmatrix} \frac{\partial}{\partial w_1} \\ \frac{\partial}{\partial w_2} \\ \frac{\partial}{\partial w_3} \\ \vdots \end{pmatrix} \sum_{i,j} w_i M_{ij} w_j = \begin{pmatrix} \sum_j M_{1j} w_j + \sum_i w_i M_{i1} \\ \sum_j M_{2j} w_j + \sum_i w_i M_{i2} \\ \sum_j M_{3j} w_j + \sum_i w_i M_{i3} \\ \vdots \end{pmatrix}$$

$$= \mathbf{M}\boldsymbol{w} + \mathbf{M}^{\mathsf{T}} \boldsymbol{w}$$

- It is tedious to compute these things component-wise, but when you need to understand what is going on then go back to the basics

Computing Gradients 2

- A slicker way is just to expand $f(\boldsymbol{x} + \epsilon\boldsymbol{u})$
- Consider $f(\boldsymbol{x}) = \boldsymbol{x}^{\mathsf{T}} \mathbf{M} \boldsymbol{x} + \boldsymbol{a}^{\mathsf{T}} \boldsymbol{x}$

$$\begin{aligned} f(\boldsymbol{x} + \epsilon\boldsymbol{u}) &= (\boldsymbol{x} + \epsilon\boldsymbol{u})^{\mathsf{T}} \mathbf{M} (\boldsymbol{x} + \epsilon\boldsymbol{u}) + \boldsymbol{a}^{\mathsf{T}} (\boldsymbol{x} + \epsilon\boldsymbol{u}) \\ &= f(\boldsymbol{x}) + \epsilon \left(\boldsymbol{u}^{\mathsf{T}} \mathbf{M} \boldsymbol{x} + \boldsymbol{x}^{\mathsf{T}} \mathbf{M} \boldsymbol{u} + \boldsymbol{a}^{\mathsf{T}} \boldsymbol{u} \right) + O(\epsilon^2) \\ &= f(\boldsymbol{x}) + \epsilon \boldsymbol{u}^{\mathsf{T}} \left(\mathbf{M} \boldsymbol{x} + \mathbf{M}^{\mathsf{T}} \boldsymbol{x} + \boldsymbol{a} \right) + O(\epsilon^2) \end{aligned}$$

using $\boldsymbol{x}^{\mathsf{T}} \mathbf{M} \boldsymbol{u} = \boldsymbol{u}^{\mathsf{T}} \mathbf{M}^{\mathsf{T}} \boldsymbol{x}$ and $\boldsymbol{a}^{\mathsf{T}} \boldsymbol{u} = \boldsymbol{u}^{\mathsf{T}} \boldsymbol{a}$

- But $f(\boldsymbol{x} + \epsilon\boldsymbol{u}) = f(\boldsymbol{x}) + \epsilon \boldsymbol{u}^{\mathsf{T}} \boldsymbol{\nabla} f(\boldsymbol{x}) + O(\epsilon^2)$ so

$$\boldsymbol{\nabla} f(\boldsymbol{x}) = \mathbf{M} \boldsymbol{x} + \mathbf{M}^{\mathsf{T}} \boldsymbol{x} + \boldsymbol{a}$$

Differentiating Matrices

- Often we have loss functions with respect to a matrix $\boldsymbol{W}$, e.g.

$$L(\boldsymbol{W}) = (\boldsymbol{a}^{\mathsf{T}} \boldsymbol{W} \boldsymbol{b} - c)^2$$

- We might want to find the minimum with respect to $\boldsymbol{W}$
- This occurs at a point $\boldsymbol{W}^*$ where $L(\boldsymbol{W})$ does not increase as we change $\boldsymbol{W}$ in any way
- That is, we seek a $\boldsymbol{W}^*$ such that, for any matrices $\mathbf{U}$

$$L(\boldsymbol{W}^* + \epsilon\mathbf{U}) - L(\boldsymbol{W}^*) = O(\epsilon^2)$$

Generalised Gradient

- We can generalise the idea of gradient to matrices

$$\frac{\partial L(\mathbf{W})}{\partial \mathbf{W}} = \begin{pmatrix} \frac{\partial L(\mathbf{W})}{\partial W_{11}} & \frac{\partial L(\mathbf{W})}{\partial W_{12}} & \ldots & \frac{\partial L(\mathbf{W})}{\partial W_{1m}} \\ \frac{\partial L(\mathbf{W})}{\partial W_{21}} & \frac{\partial L(\mathbf{W})}{\partial W_{22}} & \ldots & \frac{\partial L(\mathbf{W})}{\partial W_{2m}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial L(\mathbf{W})}{\partial W_{n1}} & \frac{\partial L(\mathbf{W})}{\partial W_{n2}} & \ldots & \frac{\partial L(\mathbf{W})}{\partial W_{nm}} \end{pmatrix}$$

- From an identical argument we used for vectors

$$L(\mathbf{W} + \epsilon\mathbf{U}) = L(\mathbf{W}) + \epsilon \operatorname{tr} \mathbf{U}^{\mathsf{T}} \frac{\partial L(\mathbf{W})}{\partial \mathbf{W}} + O(\epsilon^2)$$

where

$$\operatorname{tr} \mathbf{U}^{\mathsf{T}} \mathbf{G} = \sum_i \left[\mathbf{U}^{\mathsf{T}} \mathbf{G} \right]_{ii} = \sum_{ij} U_{ji} G_{ji} = \sum_{ij} U_{ij} G_{ij} = \langle \mathbf{U}, \mathbf{G} \rangle$$

Example

- Suppose

$$L(\mathbf{W}) = \left(\boldsymbol{a}^{\mathsf{T}}\mathbf{W}\boldsymbol{b} - c\right)^2$$

then

$$L(\mathbf{W}+\epsilon\mathbf{U}) = \left(\boldsymbol{a}^{\mathsf{T}}(\mathbf{W}+\epsilon\mathbf{U})\boldsymbol{b} - c\right)^2 = \left(\boldsymbol{a}^{\mathsf{T}}\mathbf{W}\boldsymbol{b} + \epsilon\boldsymbol{a}^{\mathsf{T}}\mathbf{U}\boldsymbol{b} - c\right)^2$$
$$= L(\mathbf{W}) + 2\epsilon\left(\boldsymbol{a}^{\mathsf{T}}\mathbf{W}\boldsymbol{b} - c\right)\left(\boldsymbol{a}^{\mathsf{T}}\mathbf{U}\boldsymbol{b}\right) + O(\epsilon^2)$$

- Now

$$\boldsymbol{a}^{\mathsf{T}}\mathbf{U}\boldsymbol{b} = \sum_{ij} a_i U_{ij} b_j = \sum_{ij} U_{ji} a_j b_i = \mathrm{tr}\,\mathbf{U}^{\mathsf{T}}\boldsymbol{a}\boldsymbol{b}^{\mathsf{T}}$$

Thus $\frac{\partial L(\mathbf{W})}{\partial \mathbf{W}} = 2\left(\boldsymbol{a}^{\mathsf{T}}\mathbf{W}\boldsymbol{b} - c\right)\boldsymbol{a}\boldsymbol{b}^{\mathsf{T}}$

Traces

- The trace of a matrix is the sum of its diagonal elements

$$\mathrm{tr}\mathbf{A} = \mathrm{tr}\mathbf{A}^{\mathsf{T}} = \sum_i A_{ii}$$

- Clearly $\mathrm{tr}c\mathbf{A} = c\,\mathrm{tr}\mathbf{A}$
- Also $\mathrm{tr}(\mathbf{A}+\mathbf{B}) = \mathrm{tr}\mathbf{A} + \mathrm{tr}\mathbf{B}$
- We note that

$$\mathrm{tr}\mathbf{A}\mathbf{B} = \sum_{i,j} A_{ij}B_{ji} = \sum_{i,j} B_{ij}A_{ji} = \mathrm{tr}\mathbf{B}\mathbf{A}$$

- It follows that

$$\mathrm{tr}\mathbf{ABCD} = \mathrm{tr}\mathbf{DABC} = \mathrm{tr}\mathbf{CDAB} = \mathrm{tr}\mathbf{BCDA}$$

Quick Matrix Differentiation

- Let

$$\partial_{\mathbf{U}} f(\mathbf{X}) = \lim_{\epsilon\to 0}\frac{f(\mathbf{X}+\epsilon\mathbf{U}) - f(\mathbf{X})}{\epsilon} = \mathrm{tr}\mathbf{U}^{\mathsf{T}}\frac{\partial f(\mathbf{X})}{\partial \mathbf{X}}$$

- E.g.

$$\partial_{\mathbf{U}}\mathrm{tr}\mathbf{AXB} = \lim_{\epsilon\to 0}\frac{1}{\epsilon}\mathrm{tr}\mathbf{A}\left(\mathbf{X}+\epsilon\mathbf{U}\right)\mathbf{B} - \mathrm{tr}\mathbf{AXB}$$
$$= \mathrm{tr}\ \mathbf{AUB} = \mathrm{tr}\ \mathbf{B}^{\mathsf{T}}\mathbf{U}^{\mathsf{T}}\mathbf{A}^{\mathsf{T}} = \mathrm{tr}\ \mathbf{U}^{\mathsf{T}}\mathbf{A}^{\mathsf{T}}\mathbf{B}^{\mathsf{T}}$$

thus

$$\frac{\partial\,\mathrm{tr}\mathbf{AXB}}{\partial \mathbf{X}} = \mathbf{A}^{\mathsf{T}}\mathbf{B}^{\mathsf{T}}$$

Log Determinants

- We often come across logarithms of determinants of matrices, $\log(|\mathbf{M}|)$
- For GP we want to choose $\mathbf{K}$ to maximise the marginal likelihood, $\log\left(|\mathbf{K}+\sigma^2\mathbf{I}|\right)$
- To find the derivative of $\log(|\mathbf{X}|)$ we consider

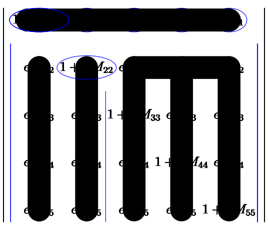
$$\log(|\mathbf{X}+\epsilon\mathbf{U}|) = \log\left(|\mathbf{X}(\mathbf{I}+\epsilon\mathbf{X}^{-1}\mathbf{U})|\right)$$
$$= \log\left(|\mathbf{X}||\mathbf{I}+\epsilon\mathbf{X}^{-1}\mathbf{U}|\right)$$
$$= \log(|\mathbf{X}|) + \log\left(|\mathbf{I}+\epsilon\mathbf{X}^{-1}\mathbf{U}|\right)$$

  - Using $|\mathbf{AB}| = |\mathbf{A}||\mathbf{B}|$
  - Using $\log(ab) = \log(a) + \log(b)$

Determinants

$$|\mathbf{I}+\epsilon\mathbf{M}| = \begin{vmatrix} 1+\epsilon M_{11} & \epsilon M_{12} \\ \epsilon M_{21} & 1+\epsilon M_{22} \end{vmatrix} = (1+\epsilon M_{11})(1+\epsilon M_{22}) - \epsilon^2 M_{21}M_{12}$$
$$= 1 + \epsilon(M_{11}+M_{22}) + O(\epsilon^2)$$

$|\mathbf{I}+\epsilon\mathbf{M}| =$



$= \ldots -\epsilon\, M_{41}\, C_{41} + \epsilon\, M_{51}\, C_{51}$

Putting it Together

- Recall

$$\log(|\mathbf{X}+\epsilon\mathbf{U}|) - \log(|\mathbf{X}|) = \log\left(|\mathbf{I}+\epsilon\mathbf{X}^{-1}\mathbf{U}|\right)$$
$$= \log\left(1+\epsilon\,\mathrm{tr}\ \mathbf{X}^{-1}\mathbf{U} + O(\epsilon)^2\right)$$
$$= \epsilon\,\mathrm{tr}\ \mathbf{X}^{-1}\mathbf{U} + O(\epsilon)^2$$
$$= \epsilon\,\mathrm{tr}\ \mathbf{U}^{\mathsf{T}}\left(\mathbf{X}^{-1}\right)^{\mathsf{T}} + O(\epsilon)$$

using $\log(1+x) = x + \frac{x^2}{2} + \cdots$

- Thus $\partial_{\mathbf{U}}\log(|\mathbf{X}|) = \mathrm{tr}\ \mathbf{U}^{\mathsf{T}}\left(\mathbf{X}^{-1}\right)^{\mathsf{T}}$
- Or

$$\frac{\partial \log(|\mathbf{X}|)}{\partial \mathbf{X}} = \left(\mathbf{X}^{-1}\right)^{\mathsf{T}}$$

Summary

- With care you can differentiate most expressions
- The chain and product rule are incredibly powerful tools
- We can generalise differentiation to vectors and matrices
- There are a number of surprisingly useful results see **The Matrix Cookbook**
- Next stop: integration