# Introduction to Matrix Calculus

Zayn Patel

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- We can define a linear map f: $R^m$ -> $R^n$ if m > n, m < n, m = n as long as the transformation matrix between these spaces m and n shares the same rank.
- When we define a matrix A, the entries of this matrix transform the standard basis vectors, this is how we get the transformation.
- Linear means the transformation satisfies the following two conditions:

$$L[v_1 + v_2] = L[v_1] + L[v_2] \textbf{ and } c[Lv] = L[cv]$$

# Brief reminders about linear transformations as matrices

- On an earlier slide we talked about *why* we can think of linear transformations as matrices. Recall:
  - Start with basis vectors
  - Some transformation (rotation by 90 degrees clockwise) has column vectors which define how these change the basis vectors
  - We put these column vectors into a matrix, A
  - We conclude that this linear transformation (rotation) is represented by the column vectors in A
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**Key idea:** We can generalize this idea to any linear transformation and represent it as a matrix. Rotations, shears, projections are easy transformations to visualize but there are many more.

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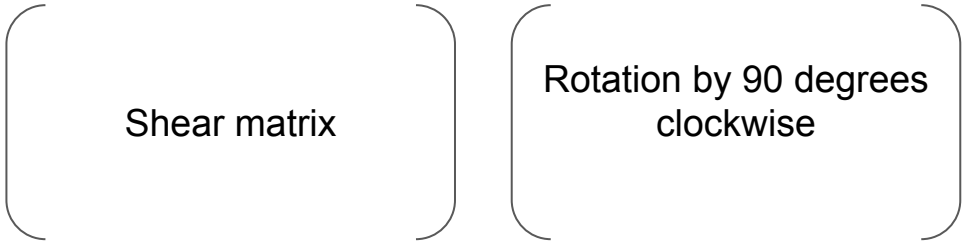
**Key idea 2:** Every time you write see a matrix or write one down you should think of it as a linear transformation instead of some m x n set of values.

# Brief reminders about linear transformations as matrices

To make this more concrete let’s think of a 2x2 rotation matrix and a 2x2 shear matrix:



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$$\begin{pmatrix} \text{Shear matrix} \end{pmatrix} \quad \begin{pmatrix} \text{Rotation by 90 degrees clockwise} \end{pmatrix}$$

Now if we apply the rotation to a vector in $R^2$ we get a new matrix, R:

$$\begin{pmatrix} \text{Rotation by 90 degrees clockwise} \end{pmatrix} \quad \begin{pmatrix} x \\ y \end{pmatrix} \quad = \quad \begin{pmatrix} \mathbf{R} \end{pmatrix}$$

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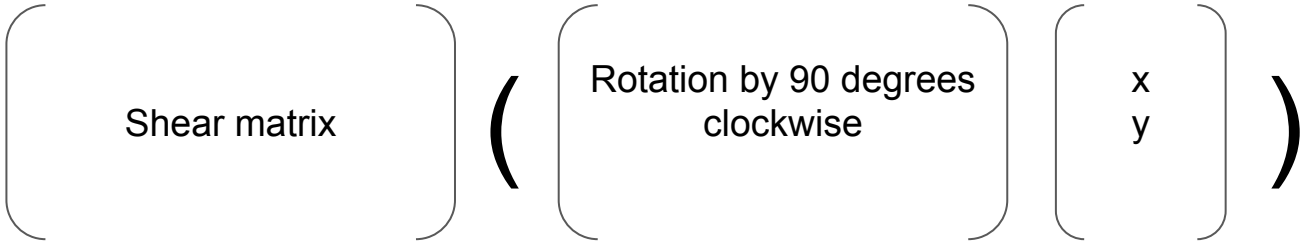
If we apply the shear to this matrix R we can look at this as:



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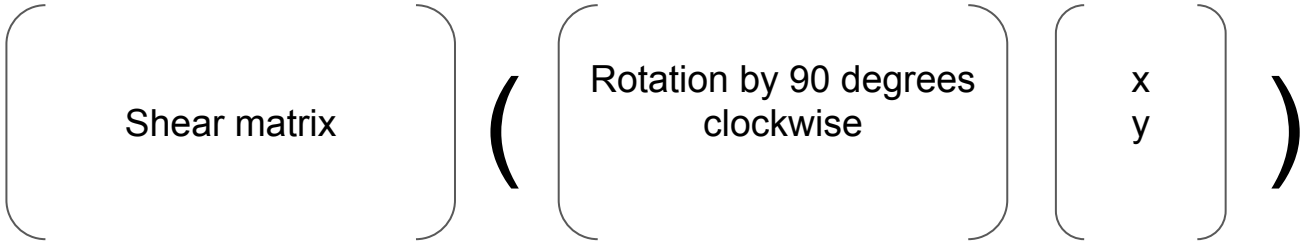


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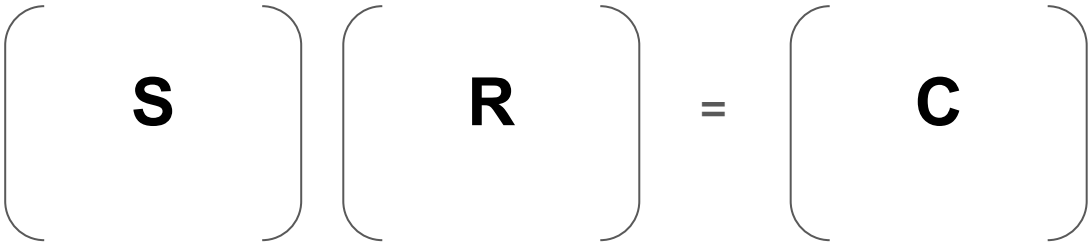

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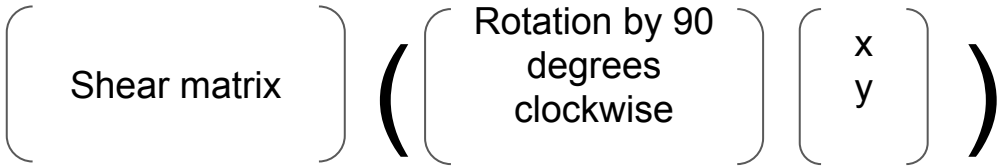


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**Key idea:** When we think of linear transformations as matrices we get **matrix multiplication as matrix composition.** We are applying one transformation to another.

# Brief reminders about linear transformations as matrices

**Key idea cont.:** If we think about the transformation on the previous slide: rotation then shear unless we had a *super special case (?) and it might still be unlikely to work* this transformation is different from shear then rotation.

So:

R @ S ≠ S @ R

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So:

R @ S ≠ S @ R

**Matrix multiplication is not communitive *because* we are applying transformations and the order of these transformations matters.**

*Note: @ is matmul notation in Python which I am using above.*

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1. We will be thinking of f'(x) as a linear operator. f'(x) will be some object[1], and it will "operate" on an object representing infinitesimal change[2] to produce an output, df. The previous slides motivate transformations from one vector space to another.

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2. While we will derive rules like the power rule and chain rule for vectors and matrices the fact that we are not working with scalars, only, for calculus means **communitivity matters**. The theory behind linear transformations built up to a nice result of why matmul does not commute.

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# Derivatives as linear operators: scalar valued functions

- The definition of the derivative we will use in this presentation is:
  $df = f(x + dx) - f(x) = f'(x)\,[dx]$

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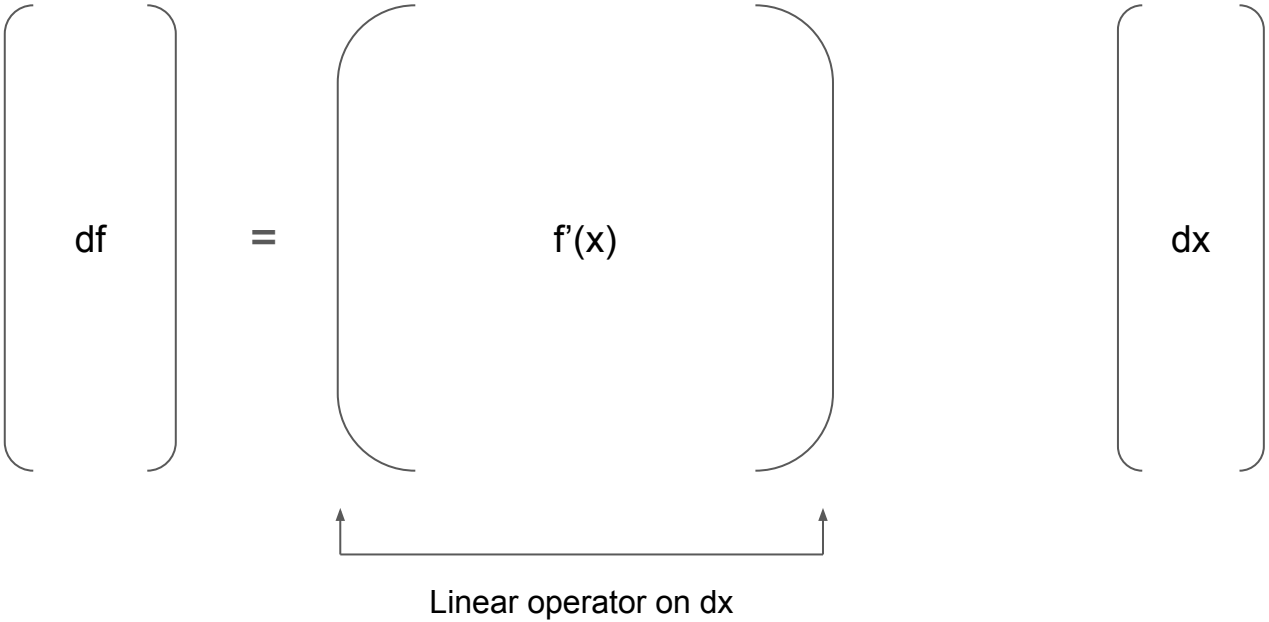
- In the definition of the derivative we defined [dx] to be a column vector. (Recall that since [dx] is a vector it represents some infinitesimal change in a direction). If we want a scalar output f'(x) needs to be in the form of a row vector. This row vector will be called $(\text{grad } f)^T$.
  - Why? Because x (input to the f'(x)) is a column vector itself. When we apply the derivative to the x we are taking *all partial derivatives of the components*. So this *is the gradient* as learned in calculus. Now because we are using vectors we transpose it so the dimensions match to get a scalar.

# Derivatives as linear operators: vector valued functions



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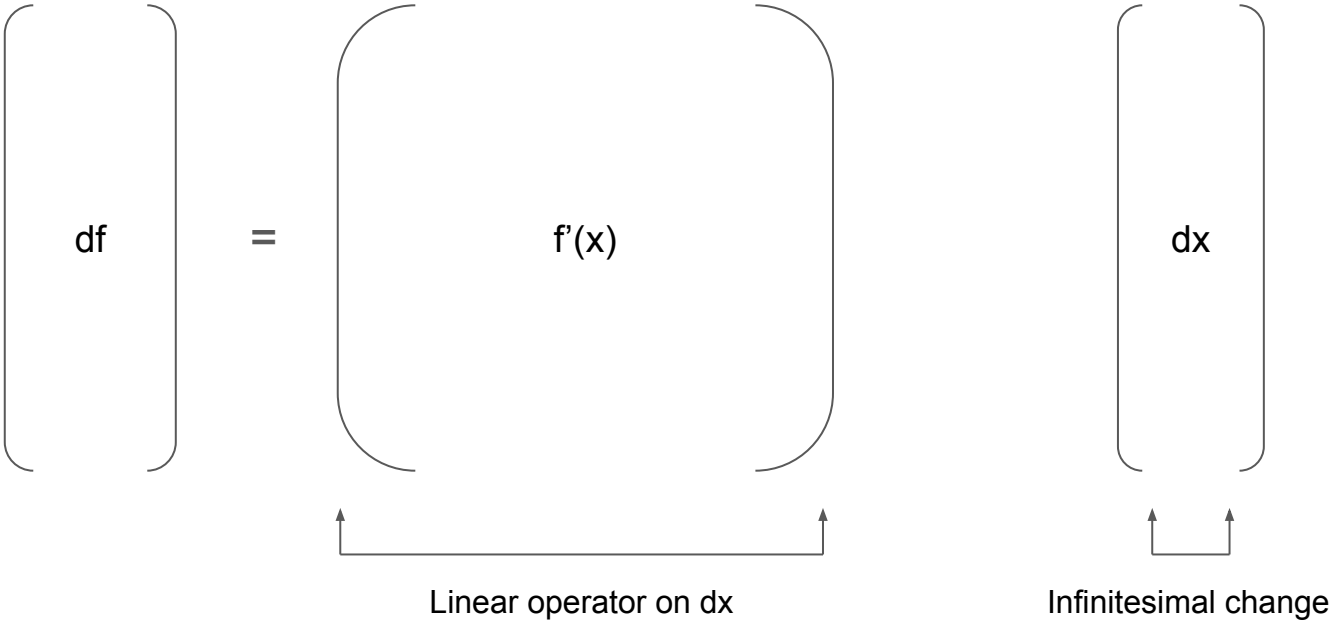

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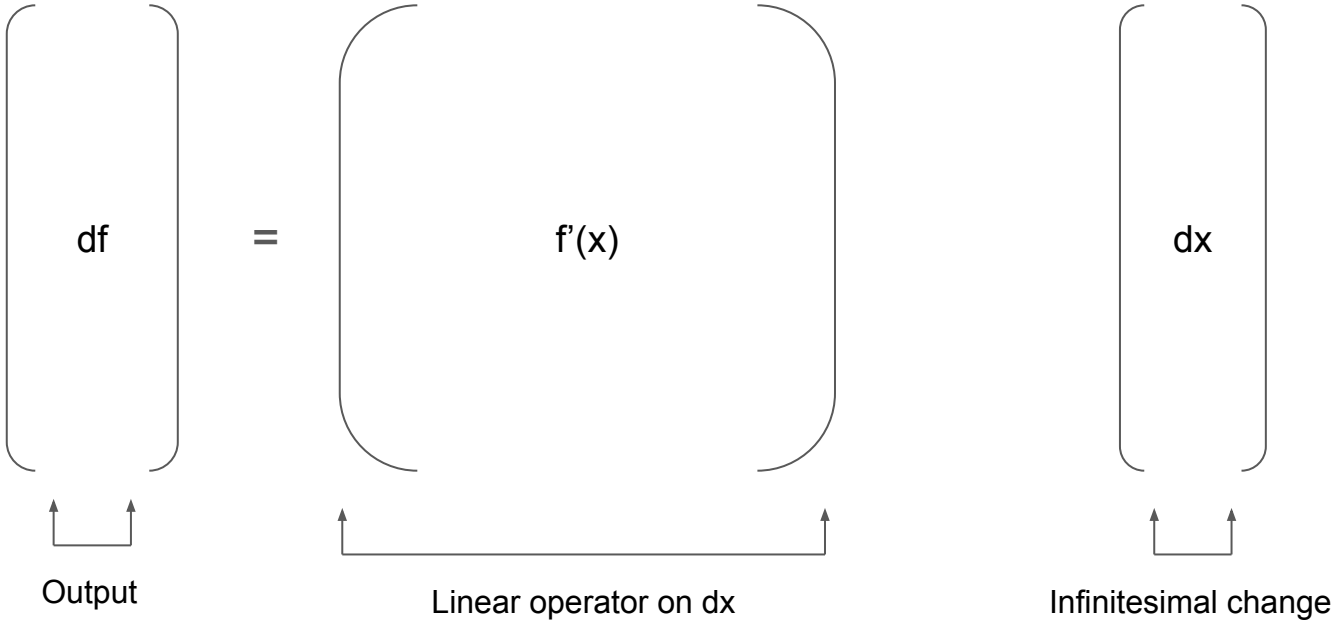

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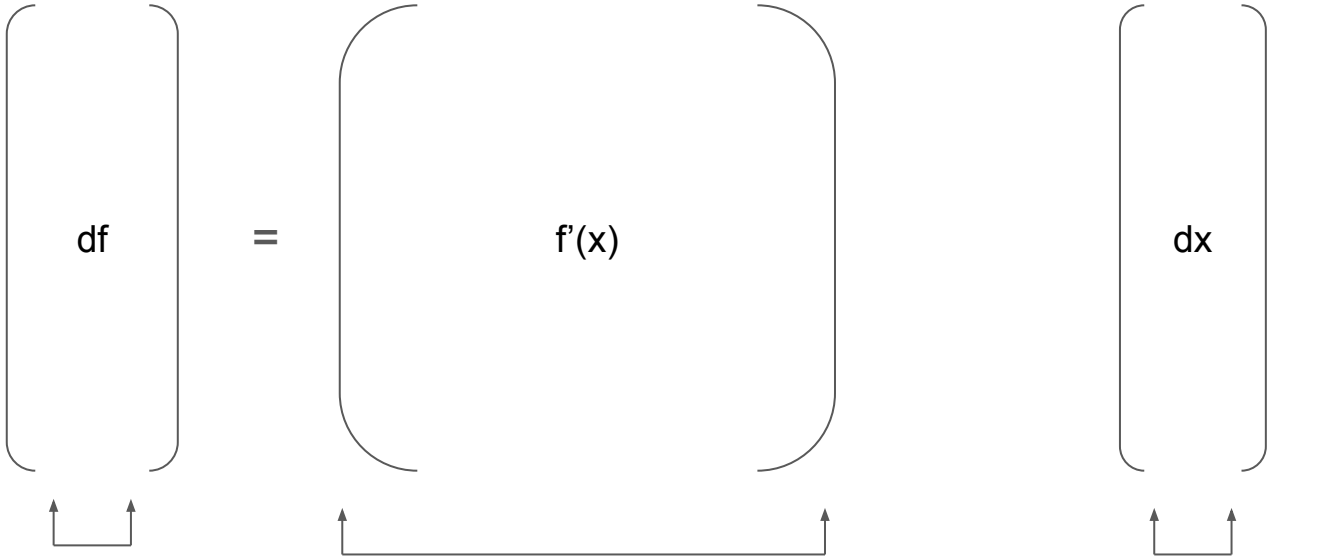

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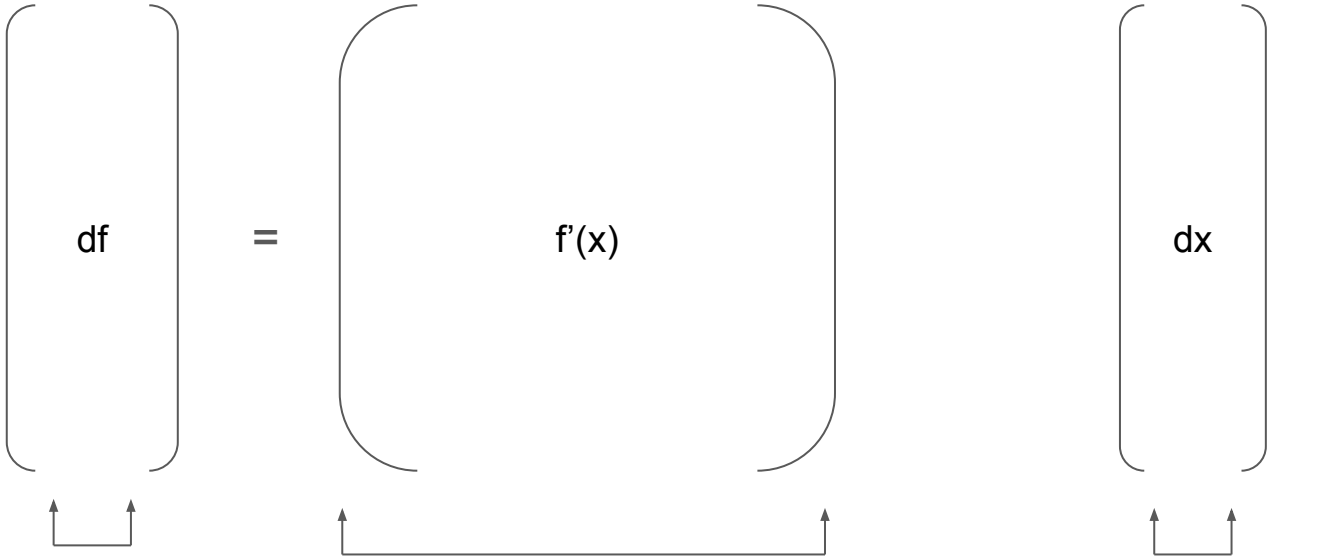

# Why the Jacobian is the linear operator for vec-valued fcn

- One perspective is dimension. If we have [dx] as a column vector with n components and [df] as a column vector with m components *then* we need a matrix (m x n) to *operate* on [dx] to produce [df]. This is **defined** to be the Jacobian.
    - Recall from Calc III that the Jacobian is a matrix with the partial derivatives w.r.t each component in each direction.

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**Key idea:** First, our linear operator thinking is important because we don't care what the grad or Jacobian components are. *Just that these objects take [dx] and map it to a different vector space with [df].* Second, we can use the Jacobian to think about the chain rule for matrices (or vectors).

# *Very quick reminder*: Jacobian matrix in a picture

$$\begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}$$

Source: Wikipedia (Jacobian matrix and determinant)

# Using the Jacobian in the chain rule for matrices

Let's first derive the chain rule for functions on arbitrary vector spaces. If f(x) = g(h(x)) and g,h are matrices, x is a vector:

*df* = f(x + dx) - f(x)

= g'(h(x)) [h(x + dx) - h(x)] ←

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**Key idea:** Our output, *df* (a.k.a f'(x) dx) is an m x n Jacobian matrix. So, g'(h(x)) is an m x p Jacobian and h'(x) is a p x n Jacobian. See notebook for a numerical calculation of this product.

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$f(x) = A^2 = A * A$ ← Define function.

$f'(x) = dA\,A + A\,dA$ ← Same product rule as before but in single variable calculus the dx * x can have different orders because these commute. dA * A can't change order.

# Calculating the derivative of $A^2$ and $A^3$

Let's transition to show our second result of calculus on matrices by differentiating $A^3$.

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$f(x) = x^3 = x*(x*x)$ ← Define function.

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$f'(x) = x^2\ dx + x^2\ dx + x^2\ dx = 3x^2\ dx$ ← Final version which aligns with our "power rule"

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Matrix calculus version

$f(x) = A^3 = A*(A*A)$

$f'(x) = (A*A)' * A + dA * (A*A)$

$f'(x) = (A*dA + dA*A) * A + dA * (A*A)$

$f'(x) = A^2\, dA + A\, dA\, A + dA\, A^2$

**Key idea:** Communitivity, so far, is the key difference between single variable calculus and matrix calculus. It's why we have A dA A instead of another $A^2$ dA term.

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And we have previously shown that $f'(A)$ is $dA\,A + A\,dA$.

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Now that we have an introductory understanding of the Jacobian for $A^2$ and the Kronecker product let's state a key identity and derive it. We will use this identity to show we can write the Jacobian in Kronecker Product notation.

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**Key identity:**

$$(A \otimes B)\text{vec}(C) = \text{vec}(BCA^T)$$

*Assumption: This identity **requires** compatible sized matrices. We cannot do $BCA^T$ if the dimensions do not match.*

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$B\,(c_1, c_2, c_3, \ldots) = (Bc_1, Bc_2, Bc_3) \Rightarrow \text{vec}(BC) =$

$$\begin{pmatrix} Bc_1 \\ Bc_2 \\ \vdots \end{pmatrix}$$

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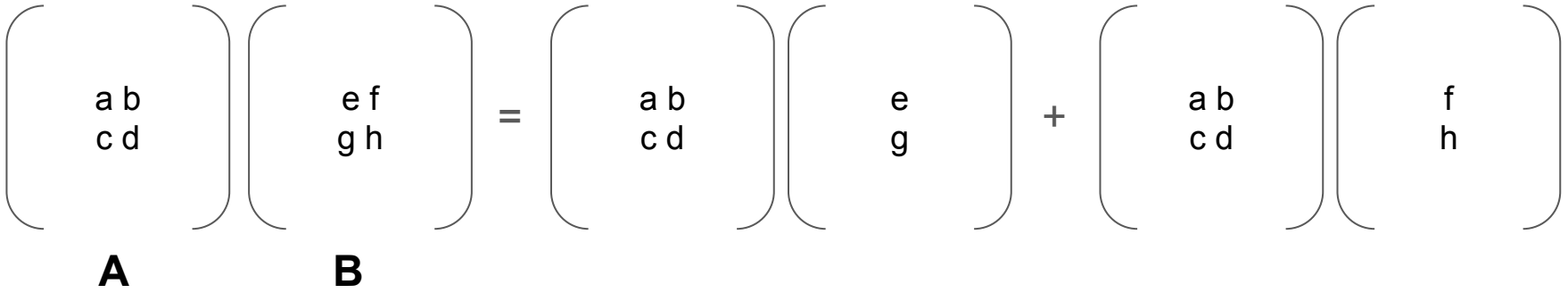
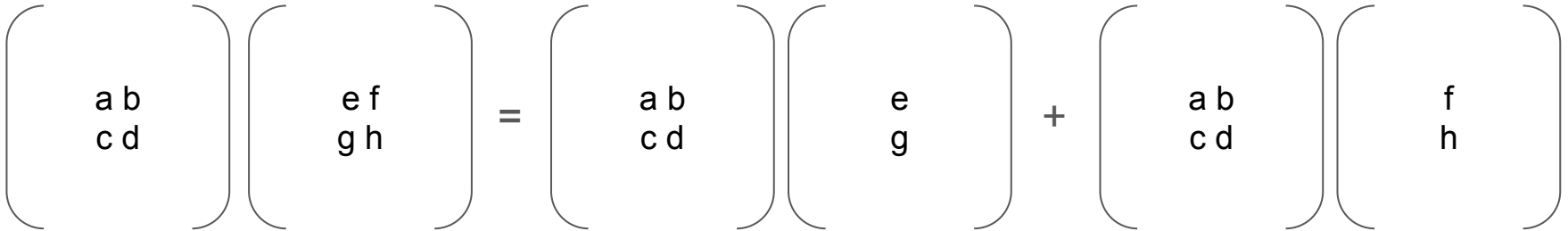


# Jacobians and Kronecker Products

Just in case this isn't clear the following is a 2x2 * 2x2 example that uses the same concept as the BC case.

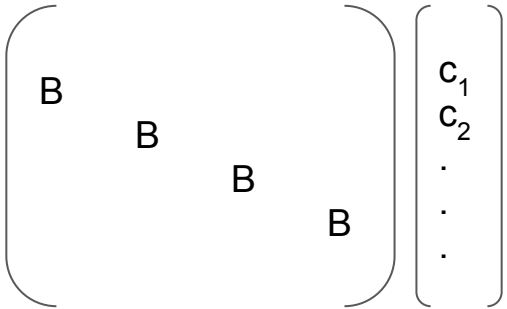



**A** **B**

**Key idea:** We take each column of B and multiply it by the matrix A. This is exactly what we are doing to compute the matrix product BC on the previous slides.

# Jacobians and Kronecker Products

Returning to the vec(BC) example we can express vec(BC) as (I $\otimes$ B) * vec(C).



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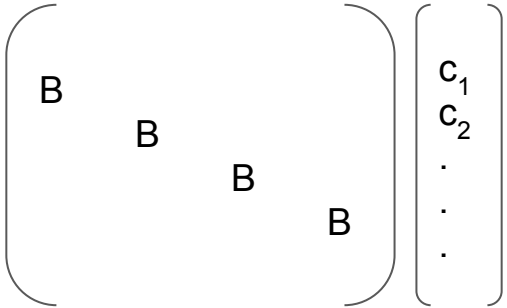


**Key idea:** Beginning with A = I and using facts about matrix product BC gives us: $(I \otimes B)vec(C) = vec(BC)$.

# Jacobians and Kronecker Products

Now let's assume B = I to understand where the $A^T$ term comes from. We will again be interested in understanding the RHS term $CA^T$, without vectorization first, then using $\text{vec}(CA^T)$ to relate it to the RHS.

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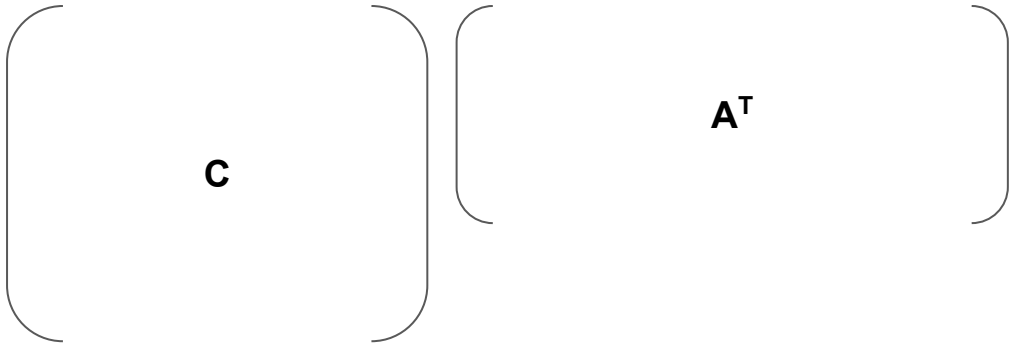

# Jacobians and Kronecker Products

Let's build our own 2x2 $CA^T$ to understand what this looks like symbolically. Then we can generalize this to arbitrarily sized C and $A^T$.

$$\begin{pmatrix} c_1 & c_2 \\ c_3 & c_4 \end{pmatrix} \begin{pmatrix} a_1 & a_3 \\ a_2 & a_4 \end{pmatrix} = \begin{pmatrix} (c_1a_1 + c_2a_2) & (c_1a_3 + c_2a_4) \\ (c_3a_1 + c_4a_2) & (c_3a_3 + c_4a_4) \end{pmatrix}$$

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**Key idea:** The first column of $CA^T$ is a linear combination of the columns of $A^T$ and the columns of C. The *coefficients* are given by the columns of $A^T$.

# Jacobians and Kronecker Products

What's true in our 2x2 case is true for compatibly sized matrices C and $A^T$. So, in general, we end up with our *typical* matrix multiplication summation, **a** in this summation represents the first row of A..

$$\operatorname{vec}(CA^T) = \begin{pmatrix} \sum_j a_{1j}\vec{c}_j \\ \sum_j a_{2j}\vec{c}_j \\ \vdots \end{pmatrix} = \underbrace{\begin{pmatrix} a_{11}\,\mathrm{I} & a_{12}\,\mathrm{I} & \cdots \\ a_{21}\,\mathrm{I} & a_{22}\,\mathrm{I} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}}_{A \otimes \mathrm{I}} \underbrace{\begin{pmatrix} \vec{c}_1 \\ \vec{c}_2 \\ \vdots \end{pmatrix}}_{\operatorname{vec} C},$$

Source: Matrix Calc Notes

# Jacobians and Kronecker Products

**Key idea:** For each row in $A^T$ we take linear combinations of its columns with c's columns. This forms vec($CA^T$). In Kronecker product notation this is the same thing as ($A \otimes I$) * vec(C). We see those linear combinations are the same but vec() stacks.

$$\mathrm{vec}(CA^T) = \begin{pmatrix} \sum_j a_{1j}\vec{c}_j \\ \sum_j a_{2j}\vec{c}_j \\ \vdots \end{pmatrix} = \underbrace{\begin{pmatrix} a_{11}\,\mathrm{I} & a_{12}\,\mathrm{I} & \cdots \\ a_{21}\,\mathrm{I} & a_{22}\,\mathrm{I} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}}_{A \otimes \mathrm{I}} \underbrace{\begin{pmatrix} \vec{c}_1 \\ \vec{c}_2 \\ \vdots \end{pmatrix}}_{\mathrm{vec}\, C},$$

# Jacobians and Kronecker Products

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Let's write $d(A^2) = A\,dA + dA\,A$ as:

$d(A^2) = A\,dA\,I + I\,dA\,A$

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We want to do this because our Kronecker identity requires three matrices: B, C, and A. The identity is our method of adding another matrix without changing the algebraic structure of $d(A^2)$.

# Jacobians and Kronecker Products

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Let's write $d(A^2) = A\,dA + dA\,A$ as:

$d(A^2) = A\,dA\,I + I\,dA\,A$

Recall that in our derivation we were thinking of how the RHS $\text{vec}(BCA^T)$ related to the Kronecker notation on the LHS. At risk of sounding obvious I think we do this because $BCA^T$ is simpler to conceptualize. Most of intro linear algebra has matrix products; vec() stacks the columns of this product on each other. Kronecker notation is newer *but* since we have an equality we rearrange the RHS pieces to look like the left.

**Now, let's let dA be C in our key Kronecker identity and take $\text{vec}(dA^2)$.**

# Jacobians and Kronecker Products

Recall the key identity with dA in place of C: $(A \otimes B)\mathrm{vec}(\mathbf{dA}) = \mathrm{vec}(B\mathbf{dA}A^T)$

Now let's look at the A dA I first and ask ourselves which "Kronecker product" we should use:

$\mathrm{vec}(dA^2) = A\,dA\,I + I\,dA\,A$

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If we look at $\text{vec}(BdAA^T)$ and set $B = A$ and $A^T = I$ then we have:

$(I \otimes A)\text{vec}(dA) = \text{vec}(AdAI^T)$

Note: We know $I^T = I$ so we can avoid writing $(I^T \otimes A)\text{vec}(dA)$ on the LHS.

# Jacobians and Kronecker Products

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If we look at $\text{vec}(BdAA^T)$ and set $B = I$ and $A^T = A^T$ then we have:

$(A^T \otimes I)\text{vec}(dA) = \text{vec}(IdAA^T)$

# Jacobians and Kronecker Products

The full Kronecker product is:

$((I \otimes A) + (A^T \otimes I)) * \text{vec}(dA)$ (vec version)

$((I \otimes A) + (A^T \otimes I)) * [dA]$ (linear operator version)

**Key idea:** The Kronecker product identity abstracts away the need to compute element-wise partial derivatives using the Jacobian – giving us the *same* answer but with simpler operations.

# Jacobians and Kronecker Products in Julia

```
X^2
```

$$\begin{bmatrix} a^2 + bc & ab + bd \\ ac + cd & bc + d^2 \end{bmatrix}$$

```
# Take the Jacobian of Y, vector valued f

jac(Y, X) = Symbolics.jacobian(vec(Y), ve
```

```
jac (generic function with 1 method)
```

```
# I think we would get the same answer if
# ... of each term in X^2 are in the firs
# ... and 2,1 entry of X^2 is the second

J = jac(X^2, X)
```

$$\begin{bmatrix} 2a & b & c & 0 \\ c & a+d & 0 & c \\ b & 0 & a+d & b \\ 0 & b & c & 2d \end{bmatrix}$$

```
begin
    I2 = [1 0; 0 1]
    kron(I2,X) + kron(X', I2)
end
```

$$\begin{bmatrix} 2a & b & c & 0 \\ c & a+d & 0 & c \\ b & 0 & a+d & b \\ 0 & b & c & 2d \end{bmatrix}$$

Source: Deliverable 3

# Jacobians and Kronecker Products – Extra Fun $d(A^3)$

Recall the key identity with dA in place of C: $(A \otimes B)\text{vec}(\mathbf{dA}) = \text{vec}(B\mathbf{dA}A^T)$

On slide 43 we derived the $d(A^3)$ so I plug that result in below.

$\text{vec}(dA^3) = A^2\, dA + A\, dA\, A + dA\, A^2$

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On slide 43 we derived the $d(A^3)$ so I plug that result in below.

$\text{vec}(dA^3) = A^2\, dA + A\, dA\, A + dA\, A^2$

Just as we did before we can rewrite this with the identity matrix:

$\text{vec}(dA^3) = A^2\, dA\, I + (A\, dA\, A)\, I + dA\, A^2\, I$

# Jacobians and Kronecker Products – Extra Fun d($A^3$)

Recall the key identity with dA in place of C: $(A \otimes B)\text{vec}(\mathbf{dA}) = \text{vec}(B\mathbf{dA}A^T)$

$\text{vec}(dA^3) = A^2\, dA\, I + (A\, dA\, A)\, I + dA\, A^2\, I$

If we look at $\text{vec}(BdAA^T)$ and set $B = \mathbf{A^2}$ and $A^T = \mathbf{I}$ then we have:

$(I \otimes A^2)\text{vec}(dA) = \text{vec}(A^2 dA I^T)$

# Jacobians and Kronecker Products – Extra Fun d($A^3$)

Recall the key identity with dA in place of C: $(A \otimes B)\text{vec}(\mathbf{dA}) = \text{vec}(B\mathbf{dA}A^T)$

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If we look at $\text{vec}(BdAA^T)$ and set $B = \mathbf{A}$ and $A^T = \mathbf{A}^T$ then we have:

$(A^T \otimes A)\text{vec}(dA) = \text{vec}(AdAA^T)$

# Jacobians and Kronecker Products – Extra Fun $d(A^3)$

Recall the key identity with dA in place of C: $(A \otimes B)\text{vec}(\mathbf{dA}) = \text{vec}(B\mathbf{dA}A^T)$

$\text{vec}(dA^3) = A^2\, dA\, I + (A\, dA\, A)\, I + I\, dA\, A^2$

If we look at $\text{vec}(BdAA^T)$ and set $B = \mathbf{I}$ and $A^T = \mathbf{(A^2)^T}$ then we have:

$((A^2)^T \otimes I)\text{vec}(dA) = \text{vec}((A^2)^T dAI)$

# Jacobians and Kronecker Products – Extra Fun $d(A^3)$

The full Kronecker product is:

$((I \otimes A^2) + (A^T \otimes A) + ((A^2)^T \otimes I)) * \text{vec}(dA)$ (vec version)

$((I \otimes A^2) + (A^T \otimes A) + ((A^2)^T \otimes I)) * [dA]$ (linear operator version)

**Key idea:** The $d(A^3)$ example should feel more "plug in values" than $d(A^2)$ since we now *really understand* how to use the Kronecker identity.

# Jacobians and Kronecker Products in Julia

```
J_2 = jac(X^3, X)
```

$$\begin{bmatrix} 3a^2 + 2bc & ab + (a+d)\,b & 2ac + cd & bc \\ 2ac + cd & a^2 + (a+d)\,d + 2bc & c^2 & ac + 2cd \\ 2ab + bd & b^2 & a\,(a+d) + 2bc + d^2 & ab + 2bd \\ bc & ab + 2bd & (a+d)\,c + cd & 2bc + 3d^2 \end{bmatrix}$$

```
begin
    kron(I2, X2) + kron(X', X) + kron(X2', I2)
end
```

$$\begin{bmatrix} 3a^2 + 2bc & 2ab + bd & 2ac + cd & bc \\ 2ac + cd & a^2 + ad + 2bc + d^2 & c^2 & ac + 2cd \\ 2ab + bd & b^2 & a^2 + ad + 2bc + d^2 & ab + 2bd \\ bc & ab + 2bd & ac + 2cd & 2bc + 3d^2 \end{bmatrix}$$

**Key idea:** With some distribution in the Kronecker product solution – these are the same. We can do d($A^n$) with the same process computing the Jacobian and Kronecker products to see they are the same.

Source: Deliverable 3

# Final notes

- We can use our chain rule derivation from slide 32 to consider a function: a(b(c(x))) and take its derivative so it looks like: a’(b(c(x))b’(c(x))c’(x).
- If we cared about getting the gradient of a function (1 x n row vector):

  a’ = 1 x n

  b’ = n x n

  c’ = n x n

  We would also care about *how* we do this matrix multiplication. This is where we exploit associativity.

# Final notes

- If we cared about getting the gradient of a function (1 x n row vector):

  a’ = 1 x n; b’ = n x n; c’ = n x n

  We would also care about *how* we do this matrix multiplication. This is where we exploit associativity.

  (a’ b’) * c → (row vector * matrix) ⇒ (row vector * matrix)

  a’ (b’ c’) → (matrix * matrix) ⇒ (row vector * matrix)

  Without getting too detailed there are two observations I want to share.

  1. Associativity *matters* in ML (and all matmul) because it has different comp costs.
  2. Left to right multiplication is called *reverse mode auto differentiation (a.k.a backpropagation)*. Right to left multiplication is called *forward mode auto differentiation.*