Intro

•	In this video	we will take a	look at other	cases of matrix	derivatives
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Jacobian

Let's take a composition of two vector functions:

$$g(x): (x_1, ..., x_n) \to (g_1, ..., g_m)$$

$$f(g): (g_1, ..., g_m) \to (f_1, ..., f_k) \quad \text{this will be useful for RNN}$$

$$h(x) = f(g(x)): (x_1, ..., x_n) \to (h_1, ..., h_k) = (f_1, ..., f_k)$$

• The matrix of partial derivatives $\frac{\partial h_i}{\partial x_i}$ is called the Jacobian:

$$J^{h} = \begin{pmatrix} \frac{\partial h_{1}}{\partial x_{1}} & \dots & \frac{\partial h_{1}}{\partial x_{n}} \\ \vdots & \ddots & \vdots \\ \frac{\partial h_{k}}{\partial x_{1}} & \dots & \frac{\partial h_{k}}{\partial x_{n}} \end{pmatrix}$$

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• The matrix of partial derivatives $\frac{\partial h_i}{\partial x_i}$ is called the Jacobian:

$$J^h = \begin{pmatrix} \frac{\partial h_1}{\partial x_1} & \dots & \frac{\partial h_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial h_k}{\partial x_1} & \dots & \frac{\partial h_k}{\partial x_n} \end{pmatrix} \qquad \begin{aligned} J_{i,j}^h &= \frac{\partial h_i}{\partial x_j} = \\ \sum_l \frac{\partial f_i}{\partial g_l} \frac{\partial g_l}{\partial x_j} &= \sum_l J_{i,l}^f \cdot J_{l,j}^g \\ \text{Chain rule: } J^h &= J^f \cdot J^g \end{aligned}$$

Matrix by matrix derivative

Matrix product:

$$C = AB = \begin{pmatrix} a_{1,1} & a_{1,2} \\ a_{2,1} & a_{2,2} \end{pmatrix} \cdot \begin{pmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{pmatrix} = \begin{pmatrix} a_{1,1}b_{1,1} + a_{1,2}b_{2,1} & a_{1,1}b_{1,2} + a_{1,2}b_{2,2} \\ a_{2,1}b_{1,1} + a_{2,2}b_{2,1} & a_{2,1}b_{1,2} + a_{2,2}b_{2,2} \end{pmatrix}$$

• How to calculate the derivative $\frac{\partial C}{\partial A}$?

$$\frac{\partial C}{\partial A} = \left\{ \frac{\partial c_{i,j}}{\partial a_{k,l}} \right\}_{i,j,k,l}$$

This is a tensor (high-dimensional array)!

Chain rule

$$C = AB = \begin{pmatrix} a_{1,1}b_{1,1} + a_{1,2}b_{2,1} & a_{1,1}b_{1,2} + a_{1,2}b_{2,2} \\ a_{2,1}b_{1,1} + a_{2,2}b_{2,1} & a_{2,1}b_{1,2} + a_{2,2}b_{2,2} \end{pmatrix}$$

$$\frac{\partial C}{\partial A} = \begin{pmatrix} \frac{\partial c_{1,1}}{\partial A} & \frac{\partial c_{1,2}}{\partial A} \\ \frac{\partial c_{2,1}}{\partial A} & \frac{\partial c_{2,2}}{\partial A} \end{pmatrix} = \begin{pmatrix} \begin{bmatrix} b_{1,1} & b_{2,1} \\ 0 & 0 \end{bmatrix} & \begin{bmatrix} b_{1,2} & b_{2,2} \\ 0 & 0 \end{bmatrix} \\ \begin{bmatrix} 0 & 0 \\ b_{1,1} & b_{2,1} \end{bmatrix} & \begin{bmatrix} b_{1,2} & b_{2,2} \\ 0 & 0 \end{bmatrix} \end{pmatrix}$$

Possible notation

• Let's say we have $\frac{\partial L}{\partial C} = \begin{bmatrix} \alpha & \beta \\ \gamma & \eta \end{bmatrix}$

$$\begin{split} \frac{\partial L}{\partial A} &= \sum_{i,j} \frac{\partial L}{\partial c_{i,j}} \frac{\partial c_{i,j}}{\partial A} = \alpha \frac{\partial c_{1,1}}{\partial A} + \beta \frac{\partial c_{1,2}}{\partial A} + \gamma \frac{\partial c_{2,1}}{\partial A} + \eta \frac{\partial c_{2,2}}{\partial A} = \\ & \begin{bmatrix} \alpha b_{1,1} + \beta b_{1,2} & \alpha b_{2,1} + \beta b_{2,2} \\ \gamma b_{1,1} + \eta b_{1,2} & \gamma b_{2,1} + \eta b_{2,2} \end{bmatrix} \end{split}$$

What's bad about it

Our chain rule is a linear combination of matrices:

$$\frac{\partial L}{\partial A} = \sum_{i,j} \frac{\partial L}{\partial c_{i,j}} \frac{\partial c_{i,j}}{\partial A} = \alpha \frac{\partial c_{1,1}}{\partial A} + \beta \frac{\partial c_{1,2}}{\partial A} + \gamma \frac{\partial c_{2,1}}{\partial A} + \eta \frac{\partial c_{2,2}}{\partial A} = \begin{bmatrix} \alpha b_{1,1} + \beta b_{1,2} & \alpha b_{2,1} + \beta b_{2,2} \\ \gamma b_{1,1} + \eta b_{1,2} & \gamma b_{2,1} + \eta b_{2,2} \end{bmatrix}$$

Crunching a lot of zeros:

$$\frac{\partial C}{\partial A} = \begin{pmatrix} \frac{\partial c_{1,1}}{\partial A} & \frac{\partial c_{1,2}}{\partial A} \\ \frac{\partial c_{2,1}}{\partial A} & \frac{\partial c_{2,2}}{\partial A} \end{pmatrix} = \begin{pmatrix} \begin{bmatrix} b_{1,1} & b_{2,1} \\ 0 & 0 \end{bmatrix} & \begin{bmatrix} b_{1,2} & b_{2,2} \\ 0 & 0 \end{bmatrix} \\ \begin{bmatrix} 0 & 0 \\ b_{1,1} & b_{2,1} \end{bmatrix} & \begin{bmatrix} b_{1,2} & b_{2,2} \\ 0 & 0 \end{bmatrix} \end{pmatrix}$$

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- Performance issues
 - e.g. no such operation in BLAS

What's bad about it

Our chain rule is a linear combination of matrices:

$$\frac{\partial L}{\partial A} = \sum_{i,j} \frac{\partial L}{\partial c_{i,j}} \frac{\partial c_{i,j}}{\partial A} = \alpha \frac{\partial c_{1,1}}{\partial A} + \beta \frac{\partial c_{1,2}}{\partial A} + \gamma \frac{\partial c_{2,1}}{\partial A} + \eta \frac{\partial c_{2,2}}{\partial A} = \begin{bmatrix} \alpha b_{1,1} + \beta b_{1,2} & \alpha b_{2,1} + \beta b_{2,2} \\ \gamma b_{1,1} + \eta b_{1,2} & \gamma b_{2,1} + \eta b_{2,2} \end{bmatrix}$$

• We know how to compute $\frac{\partial L}{\partial A}$ skipping $\frac{\partial C}{\partial A}$ tensor computation:

$$\frac{\partial L}{\partial C} = \begin{bmatrix} \alpha & \beta \\ \gamma & \eta \end{bmatrix} \qquad B^T = \begin{pmatrix} b_{1,1} & b_{2,1} \\ b_{1,2} & b_{2,2} \end{pmatrix}$$

From MLP lecture:
$$\frac{\partial L}{\partial A} = \frac{\partial L}{\partial C} B^T = \begin{bmatrix} \alpha & \beta \\ \gamma & \eta \end{bmatrix} \begin{pmatrix} b_{1,1} & b_{2,1} \\ b_{1,2} & b_{2,2} \end{pmatrix} -$$

We're still fine

 Thankfully, in deep learning frameworks we need to calculate gradients of a scalar loss with respect to another scalar, vector, matrix or tensor.

This's how tf.gradients() in TensorFlow works.

 Deep learning frameworks have optimized versions of backward pass for standard layers.

Summary

 For vector functions chain rule says that you need to multiply respective Jacobians.

Matrix by matrix derivative is a tensor

Chain rule for such tensors is not very useful in practice

 Thankfully, in deep learning frameworks we usually need to track gradients of a scalar loss with respect to all other parameters.