Machine Learning lecture – recapitulation of gradients knowledge

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Takeaway:

- directional derivatives and gradient
- directional derivatives ↔ partial derivatives
- side topics in the deep learning lecture:
 - vector-valued function → Jacobi-matrix
 - chain rule with directional argument written as matrix multiplications
 - derivative of a linear function and matrix multiplications
 - derivative of a bilinear function

Limits

• a sequence $(s_n)_{n=1}^{\infty}$ converges to a value s if: for each value of $\delta > 0$ there exists an index K such that

$$|s_n - e| < \delta$$

for all indices n > K

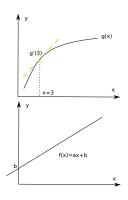
• a limit $\lim_{\epsilon \to 0} g(\epsilon)$ exists if for each sequence of numbers $(s_n)_{n=1}^{\infty}$ which converges to 0 (.i.e. $\lim_{n \to \infty} s_n = 0$) the limit of the sequence $\lim_{n \to \infty} g(s_n)$ exists and has the same value for all such sequences $(s_n)_{n=1}^{\infty}$

application: functions with kinks do not have a derivative in the point of kink

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

- intuition: slope of the function f at point x
- example: f(x) = ax + b (affine with slope a), then

$$\frac{f(x+\epsilon) - f(x)}{\epsilon} = \frac{a(x+\epsilon) + b - (ax+b)}{\epsilon}$$
$$= \frac{ax + a\epsilon + b - ax - b}{\epsilon}$$
$$= \frac{a\epsilon}{\epsilon} = a$$

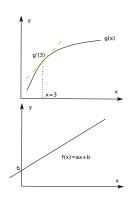




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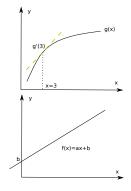
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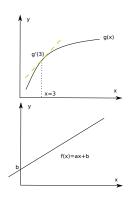
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$$= \frac{ax + a\epsilon + b - ax - b}{\epsilon}$$

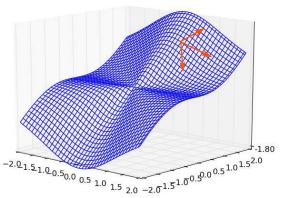
$$= \frac{a\epsilon}{\epsilon} = a$$

$$\Rightarrow \lim_{\epsilon \to 0} \frac{f(x+\epsilon) - f(x)}{\epsilon} = a$$



2-dimensions: directional derivatives

Function of 2 input variables: $f(x_1, x_2) \in \mathbb{R}^1$



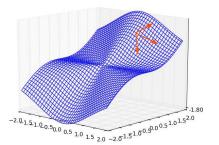
in every point (x_1, x_2) : a two dimensional vector space of directions to move from it

in every direction there is a slope - the directional derivative

n-dimensions: directional derivatives

Function of n input variables:

$$f(x_1, x_2, \ldots, x_n) \in \mathbb{R}^1$$



in every point (x_1, x_2, \dots, x_n) : a n-dimensional vector space of directions to move from it

in every direction there is a slope – the directional derivative – provides information about function value change in this direction

n-dimensions: directional derivatives and gradient

The directional derivative of function f in point x in direction v is defined as:

$$\delta_{\mathbf{v}} f(\mathbf{x}) = \lim_{\epsilon \to 0} \frac{f(\mathbf{x} + \epsilon \mathbf{v}) - f(\mathbf{x})}{\epsilon}$$

Proposition: If the function is differentiable in x, then this is equivalent to the inner product of the gradient of x in y

$$\delta_{\mathbf{v}}f(\mathbf{x}) = \nabla f(\mathbf{x}) \cdot \mathbf{v} = \sum_{d} \frac{\partial f}{\partial x_{d}}(\mathbf{x})v_{d}$$

Takeaway

- directional derivatives tell you how the function grows from x in direction v when you take an infitinely small step
- the gradient contains information about all directional derivatives, if differentiable in x
- need to define gradient, via partial derivatives

n-dimensions: the partial derivative

- consider $f: \mathbb{R}^n \to \mathbb{R}^1$, $f(\mathbf{x}) = f(x_1, \dots, x_n) \in \mathbb{R}^1$
- we can define analogously a partial derivative for variable input x_i

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

$$\mathbf{e}_i = (0, \dots, 0, \underbrace{1}_i, 0, \dots, 0)^{\top}$$

$$\mathbf{x} + \epsilon \mathbf{e}_i = (x_1, \dots, x_{i-1}, \underbrace{x_i + \epsilon}_{i-\text{th comp.}}, x_{i+1}, \dots, x_n)^{\top}$$

• why we did not simply say f is differentiable if all its partial derivatives exist? (later)

the gradient

 define the gradient ∇f(x) of function f in x as the vector of all partial derivatives in input point x:

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

 the gradient stores information about all slopes of a function at x for every direction v away from that point.

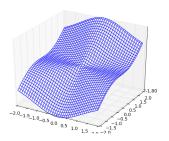
n-dimensions: differentiability

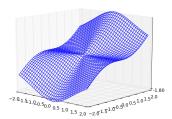
- $f: \mathbb{R}^n \to \mathbb{R}^1$, $f(\mathbf{x}) = f(x_1, \dots, x_n) \in \mathbb{R}^1$ is differentiable in input \mathbf{x} if
 - all directional derivatives (for all vector **v**) exist
 - the directional derivatives satisfy a linear relationship (with real numbers a₁, a₂)

$$\partial_{a_1\mathbf{v}_1+a_2\mathbf{v}_2}f(\mathbf{x})=a_1\partial_{\mathbf{v}_1}f(\mathbf{x})+a_2\partial_{\mathbf{v}_2}f(\mathbf{x})$$

n-dimensions: the partial derivative

- why we did not simply say f is differentiable if all its partial derivatives exist?
- f((x,y)) = $\begin{cases} \frac{y^3}{x^2+y^2} & \text{if } (x,y) \neq (0,0) \\ 0 & \text{if } (x,y) = (0,0) \end{cases}$
- both partial derivatives exist, but function has kinks in its directional derivatives







n-dimensions: vector-valued functions

$$f(x) = (f_1(x_1, ..., x_n), f_2(x_1, ..., x_n), ..., f_s(x_1, ..., x_n))$$

$$f : x \in \mathbb{R}^n \mapsto f(x) \in \mathbb{R}^s$$

Apply above for every component f_i .

Gradient becomes the Jabobi-matrix, which are the gradients of f_i concatenated.

$$\nabla f(\mathbf{x}) = \left(\nabla f_1(x), \nabla f_2(x), \dots, \nabla f_s(x)\right)$$

$$= \begin{pmatrix} \frac{\partial f_1}{\partial x_1}(x), \frac{\partial f_2}{\partial x_1}(x), \dots, \frac{\partial f_s}{\partial x_1}(x) \\ \frac{\partial f_1}{\partial x_2}(x), \frac{\partial f_2}{\partial x_2}(x), \dots, \frac{\partial f_s}{\partial x_2}(x) \\ \dots \\ \frac{\partial f_1}{\partial x_n}(x), \frac{\partial f_2}{\partial x_n}(x), \dots, \frac{\partial f_s}{\partial x_n}(x) \end{pmatrix}$$

For every component f_i one looks at its slopes in all possible directions.





Its piece of cake!

n-dimensions: derivatives as linear mappings into the space of all directional derivatives

- above counter-example (with kinks) does not satisfy the linearity!
- linear relationship means: the directional derivatives define a linear mapping $Df(\mathbf{x})[\mathbf{v}]$ in point x:

$$\mathbf{v} \mapsto \partial_{\mathbf{v}} f(\mathbf{x}),$$
 $Df(\mathbf{x})[\mathbf{v}] := \partial_{\mathbf{v}} f(\mathbf{x})$

- $Df(\mathbf{x})[\mathbf{v}]$ has two arguments
 - the point x in which the derivative is computed
 - the vector v for the direction, in which one wants to know the slope
 - the mapping $Df(\mathbf{x})[\mathbf{v}]$ is linear only in its second argument \mathbf{v} (the direction)



n-dimensions: derivatives as linear mappings into the space of all directional derivatives

What this is good for ?

- Writing directional derivatives conveniently in matrix form
- partial derivatives $\frac{\partial f}{\partial x_i}$ are directional derivatives along canonical vectors e_i
- writing chain rule terms in matrix form

the derivative of a linear function

• let f be linear in x:

$$f(\mathbf{x}) = \mathbf{u}^{\top} \mathbf{x} = \sum_{i} u_{i} x_{i}$$

• then $\frac{\partial f}{\partial x_i}(\mathbf{x}) = u_i$ and in general

$$Df(\mathbf{x})[\mathbf{v}] = f(\mathbf{v})$$

- the derivative of a linear function is a linear function
- practical for matrix algebra!

$$f(\mathbf{x}) = \mathbf{x}^{\top} \mathbf{z}$$

$$\Rightarrow Df(\mathbf{x})[\mathbf{v}] =$$

$$f(\mathbf{x}) = \mathbf{x}^{\top} \mathbf{A}$$

$$\Rightarrow Df(\mathbf{x})[\mathbf{v}] =$$

can get all directional derivatives as matrix-multiplications (GPU-implementations!)

example
$$\mathbf{A}\in\mathbb{R}^{k imes m},\mathbf{X}\in\mathbb{R}^{m imes l},\mathbf{C}\in\mathbb{R}^{l imes r}$$

$$f(\mathbf{X})=\mathbf{A}\mathbf{X}\mathbf{C}$$
 $\Rightarrow Df(\mathbf{X})[\mathbf{V}]=$

example
$$\mathbf{A} \in \mathbb{R}^{k \times m}, \mathbf{X} \in \mathbb{R}^{m \times l}, \mathbf{C} \in \mathbb{R}^{l \times r}$$

$$f(\mathbf{X}) = \mathbf{A} \mathbf{X} \mathbf{C}$$
 linear in \mathbf{X} !!!
$$\Rightarrow Df(\mathbf{X})[\mathbf{V}] =$$

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$$f(\mathbf{X}) = \mathbf{A}\mathbf{X}\mathbf{C}$$
 linear in \mathbf{X} !!!
$$\Rightarrow Df(\mathbf{X})[\mathbf{V}] = \mathbf{A}\mathbf{V}\mathbf{C}$$

sooo easy!!!

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Chain rule

1-dim case:

$$f(x) = g(h(x))$$

$$f'(x) = g'(h(x))h'(x)$$

- $L_{g'(h(x))}[v] = g'(h(x)) * v$ is a linear mapping in v
- $f'(x) = L_{g'(h(x))}[h'(x)]$
- N-dim case: the multiplication g'(h(x)) * h'(x) will be replaced by a linear mapping in higher dimensions
- N-dim case: concatenation of linear mappings

$$f(\mathbf{x}) = g(h(\mathbf{x}))$$

$$Df(\mathbf{x})[\mathbf{v}] = Dg(h(\mathbf{x}))[Dh(\mathbf{x})[\mathbf{v}]]$$

Chain rule

N-dim case: concatenation of linear mappings

$$\begin{split} f(\mathbf{x}) &= g(h(\mathbf{x})) \\ Df(\mathbf{x})[\mathbf{v}] &= Dg(h(\mathbf{x}))[Dh(\mathbf{x})[\mathbf{v}]] \\ Dg \text{ is derivated at point } h(\mathbf{x}) \text{ in direction } \mathbf{c} &= Dh(\mathbf{x})[\mathbf{v}] \end{split}$$

Why the linear view helps here?

Usually linear operations are (when looking only at one argument!):

- inner products
- matrix-vector
- matrix-matrix multiplications

Can express chain rule in terms of matrix multiplications for gradient vectors and Jacobi-matrices



N-dim case: concatenation of linear mappings

$$f(\mathbf{x}) = g(h(\mathbf{x})) = g(h_1(\mathbf{x}), \dots, h_n(\mathbf{x})), \mathbf{x} \in \mathbb{R}^k$$

$$Df(\mathbf{x})[\mathbf{v}] = Dg(h(\mathbf{x}))[\mathbf{c}], \mathbf{c} = Dh(\mathbf{x})[\mathbf{v}]$$

$$= (\nabla g_{(h(\mathbf{x}))})^{\top} Dh_{(\mathbf{x})}^{\top} \mathbf{v} \text{ as matrix multiplications}$$

$$= \mathbf{v}^{\top} Dh_{(\mathbf{x})} \nabla g_{(h(\mathbf{x}))} \text{ as matrix multiplications}$$

$$Dh_{(x)} = (\nabla h_1, \nabla h_2, \dots, \nabla h_n) \in \mathbb{R}^{k \times n}$$
 is Jacobi matrix of h in \mathbf{x} , \top is the transpose

 $D(g \circ h)(\mathbf{x})[\mathbf{v}] = \mathbf{v}^{\top} \times (\text{Jacobi of } h \text{ in } \mathbf{x}) \times (\text{Gradient of } g \text{ in } h(\mathbf{x}))$ or its transpose, bcs its a real number



$$f(\mathbf{x}) = g(h(\mathbf{x})) = g(h_1(\mathbf{x}), \dots, h_n(\mathbf{x})), \mathbf{x} \in \mathbb{R}^k$$

$$Df(\mathbf{x})[\mathbf{v}] = Dg(h(\mathbf{x}))[\mathbf{c}], \mathbf{c} = Dh(\mathbf{x})[\mathbf{v}]$$

$$= \nabla g(h(\mathbf{x})) \cdot \mathbf{c} \text{ as inner product}$$

$$= (\nabla g_{(h(\mathbf{x}))})^{\top} \mathbf{c} \text{ as matrix-vector product}$$

$$= \mathbf{c}^{\top} \nabla g_{(h(\mathbf{x}))} \text{ as matrix-vector product}$$

$$f(\mathbf{x}) = g(h(\mathbf{x})) = g(h_1(\mathbf{x}), \dots, h_n(\mathbf{x})), \mathbf{x} \in \mathbb{R}^k$$

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N-dim case: concatenation of linear mappings

$$f(\mathbf{x}) = g(h(\mathbf{x})) = g(h_1(\mathbf{x}), \dots, h_n(\mathbf{x})), \mathbf{x} \in \mathbb{R}^k$$

 $\mathbf{c} = Dh(\mathbf{x})[\mathbf{v}] = ???$ as component-wise inner products for each h_i

$$\mathbf{c} = Dh(\mathbf{x})[\mathbf{v}] = \begin{pmatrix} \nabla h_1(\mathbf{x}) \cdot \mathbf{v} \\ \nabla h_2(\mathbf{x}) \cdot \mathbf{v} \\ \dots \\ \nabla h_n(\mathbf{x}) \cdot \mathbf{v} \end{pmatrix} \text{ as comp-wise inner production}$$

$$\mathbf{c} = Dh(\mathbf{x})[\mathbf{v}] = \begin{pmatrix} \mathbf{v}^\top \nabla h_{1,(\mathbf{x})} \\ \vdots \\ \mathbf{v}^\top \nabla h_{n,(\mathbf{x})} \end{pmatrix} \text{ as matrix-vector product}$$

$$\mathbf{c}^{\top} = (\mathbf{v}^{\top} \nabla h_{1,(\mathbf{x})}, \dots, \mathbf{v}^{\top} \nabla h_{n,(\mathbf{x})})$$
 as matrix-vector product

 $\mathbf{c}^{\top} = \mathbf{v}^{\top} \left(\nabla h_{1,(\mathbf{x})}, \dots, \nabla h_{n,(\mathbf{x})} \right)$ as matrix-vector product

 $\mathbf{c}^{\top} = \mathbf{v}^{\top}$ (Jacobi-matrix of h in x) as matrix-vector product

N-dim case: concatenation of linear mappings

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$$f(\mathbf{x}) = g(h(\mathbf{x})) = g(h_1(\mathbf{x}), \dots, h_n(\mathbf{x})), \mathbf{x} \in \mathbb{R}^k$$

$$\begin{split} Df(\mathbf{x})[\mathbf{v}] &= Dg(h(\mathbf{x}))[\mathbf{c}], \mathbf{c} = Dh(\mathbf{x})[\mathbf{v}] \\ &= (\nabla g_{(h(\mathbf{x}))})^{\top} Dh_{(\mathbf{x})}^{\top} \mathbf{v} \text{ as matrix multiplications} \\ &= \mathbf{v}^{\top} Dh_{(\mathbf{x})} \nabla g_{(h(\mathbf{x}))} \text{ as matrix multiplications} \\ Dh_{(\mathbf{x})} &= (\nabla h_1, \nabla h_2, \dots, \nabla h_n) \in \mathbb{R}^{k \times n} \text{ is Jacobi matrix of } h \text{ in } \mathbf{x}, \\ &\top \text{ is the transpose} \end{split}$$

$$D(g \circ h)(\mathbf{x})[\mathbf{v}] = \mathbf{v}^{\top} \times (\text{Jacobi of } h \text{ in } \mathbf{x}) \times (\text{Gradient of } g \text{ in } h(\mathbf{x}))$$

Bilinear functions

consider B(·,·) to be any bilinear function of both variables.
 Let a and c be two vector-valued functions which take a vector x as input and compute a vector as output, i.e. a(x) and c(x) are vectors

$$f(\mathbf{x}) = B(\mathbf{a}(\mathbf{x}), \mathbf{c}(\mathbf{x}))$$

$$Df(\mathbf{x})[\mathbf{v}] = B(D\mathbf{a}(\mathbf{x})[\mathbf{v}], \mathbf{c}(\mathbf{x})) + B(\mathbf{a}(\mathbf{x}), D\mathbf{c}(\mathbf{x})[\mathbf{v}])$$

is sum of two terms ... each time plug in derivative in one component

Product rule - more general

All kind of matrix-matrix A * B, matrix-vector products $A\mathbf{v}$ and the like are bilinear as a function of both arguments. So apply

$$f(\mathbf{x}) = B(\mathbf{a}(\mathbf{x}), \mathbf{c}(\mathbf{x}))$$

$$Df(\mathbf{x})[\mathbf{v}] = B(D\mathbf{a}(\mathbf{x})[\mathbf{v}], \mathbf{c}(\mathbf{x})) + B(\mathbf{a}(\mathbf{x}), D\mathbf{c}(\mathbf{x})[\mathbf{v}])$$

Product rule

 1-dim case application of chain rule to the product – a bilinear mapping

$$f(x) = g(x)h(x)$$

$$f'(x) = g'(x)h(x) + g(x)h'(x)$$

$$f(\mathbf{x}) = \mathbf{a}(\mathbf{x})^{\top} \mathbf{c}(\mathbf{x})$$

$$g(\mathbf{u}, \mathbf{v}) = \mathbf{u}^{\top} \mathbf{v} \text{ bilinear in } (\mathbf{u}, \mathbf{v})$$

$$Df(\mathbf{x})[\mathbf{v}] = (D\mathbf{a}(\mathbf{x})[\mathbf{v}])^{\top} \mathbf{c}(\mathbf{x}) + \mathbf{a}(\mathbf{x})^{\top} (D\mathbf{c}(\mathbf{x})[\mathbf{v}])$$

example:
$$f(\mathbf{x}) = \mathbf{x}^{\top} \mathbf{A} \mathbf{x}$$

 $= Matmul(\mathbf{x}^{\top}, \mathbf{A} \mathbf{x}), g(\mathbf{x}) = \mathbf{A} \mathbf{x}$
 $Df(\mathbf{x})[\mathbf{v}] = Matmul(Dld^{\top}(\mathbf{x})[\mathbf{v}], \mathbf{A} \mathbf{x}) + Matmul(\mathbf{x}^{\top}, Dg(\mathbf{x})[\mathbf{v}])$

example:
$$f(\mathbf{x}) = \mathbf{x}^{\top} \mathbf{A} \mathbf{x}$$

by above rule
$$Df(\mathbf{x})[\mathbf{v}] = D(\mathbf{x}^{\top})[\mathbf{v}](\mathbf{A}\mathbf{x}) + \mathbf{x}^{\top} D(\mathbf{A}\mathbf{x})[\mathbf{v}]$$
the mapping $\mathbf{x} \mapsto \mathbf{x}^{\top}$ is linear, so $D(\mathbf{x}^{\top})[\mathbf{v}] = \mathbf{v}^{\top}$

$$\Rightarrow = \mathbf{v}^{\top} \mathbf{A} \mathbf{x} + \mathbf{x}^{\top} D(\mathbf{A}\mathbf{x})[\mathbf{v}]$$
the mapping $\mathbf{x} \mapsto \mathbf{A} \mathbf{x}$ is linear, so $D(\mathbf{A}\mathbf{x})[\mathbf{v}] = \mathbf{A}\mathbf{v}$

example:
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by above rule
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by above rule
$$Df(\mathbf{x})[\mathbf{v}] = D(\mathbf{x}^{\top})[\mathbf{v}](\mathbf{A}\mathbf{x}) + \mathbf{x}^{\top} D(\mathbf{A}\mathbf{x})[\mathbf{v}]$$
the mapping $\mathbf{x} \mapsto \mathbf{x}^{\top}$ is linear, so $D(\mathbf{x}^{\top})[\mathbf{v}] = \mathbf{v}^{\top}$

$$\Rightarrow = \mathbf{v}^{\top} \mathbf{A} \mathbf{x} + \mathbf{x}^{\top} D(\mathbf{A}\mathbf{x})[\mathbf{v}]$$
the mapping $\mathbf{x} \mapsto \mathbf{A} \mathbf{x}$ is linear, so $D(\mathbf{A}\mathbf{x})[\mathbf{v}] = \mathbf{A}\mathbf{v}$

$$\Rightarrow = \mathbf{v}^{\top} \mathbf{A} \mathbf{x} + \mathbf{x}^{\top} \mathbf{A} \mathbf{v}$$

example:
$$f(\mathbf{x}) = \mathbf{x}^{\top} \mathbf{A} \mathbf{x}$$

by above rule
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$$Df(x)[v] = \nabla f(x) \cdot v$$

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Product rule – more general

$$f(\mathbf{x}) = \mathbf{A}(\mathbf{x}) * \mathbf{C}(\mathbf{x})$$

$$Df(\mathbf{x})[\mathbf{v}] = D\mathbf{A}(\mathbf{x})[\mathbf{v}] * \mathbf{C}(\mathbf{x}) + \mathbf{A}(\mathbf{x}) * D\mathbf{C}(\mathbf{x})[\mathbf{v}]$$

Recap: Linear mapping to partial derivatives

- if f = f(u), and u is a vector, then $Df(u)[1_k] = \frac{\partial f}{\partial u_k}$
- if f = f(u), and u is a $k \times m$ matrix, then $Df(u)[1_{i,j}] = \frac{\partial f}{\partial u_{i,j}}$
- the general rule: plugging in into the linear part [·] an object which is 1 in one entry and zero otherwise, returns the partial derivative for the entry in which one has a 1
- practical example: $f(X) = u^T X v = \sum_{r,s} u_r X_{r,s} v_s$. $Df(X)[H] = u^T H v$, $\frac{\partial f}{\partial X_{i,j}} = Df(X)[1_{i,j}] = \sum_{r,s} u_r "(H = 1_{i,j})_{r,s} "v_s = u_i v_j$

I hope this messing around with gradients helps you!!



gradients are not that dangerous

Takeaway:

- directional derivatives and gradient
- directional derivatives ↔ partial derivatives
- side topics in the deep learning lecture:
 - vector-valued function → Jacobi-matrix
 - chain rule with directional argument written as matrix multiplications
 - derivative of a linear function and matrix multiplications
 - derivative of a bilinear function