Computing Derivatives of Matrix and Tensor Expressions

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Friedrich-Schiller-University Jena, Germany

April 9th, 2021

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Matrix calculus

Example:

- $f(x) = x^\top A x$

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Matrix calculus

Example:

- $f(x) = x^\top A x$
- $\frac{df}{dx} = ?$

.

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Matrix calculus

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- $f(x) = x^\top A x$
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Matrix calculus

Example:

- $f(x) = x^\top A x$
- $\frac{df}{dx} = Ax + A^\top x$
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.

Matrix calculus

Example:

- $f(x) = x^\top A x$
- $\frac{df}{dx} = Ax + A^\top x$
- $\frac{d^2 f}{dx^2} = A + A^\top$

.

Matrix calculus

Example:

- $f(x) = x^\top Ax$
- $\frac{df}{dx} = Ax + A^\top x$
- $\frac{d^2f}{dx^2} = A + A^\top$

No general and coherent theory known!

Matrix calculus?

- wikipedia

Matrix calculus?

- wikipedia
- matrix cookbook

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- Matrix Differential Calculus with Applications in Statistics (Magnus and Neudecker)

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Contain only collection of recipes / lookup tables.

Matrix calculus – software?

- Mathematica

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Cannot perform matrix calculus.

Matrix calculus

MatrixCalculus.org

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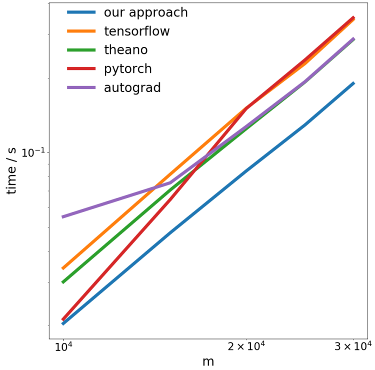
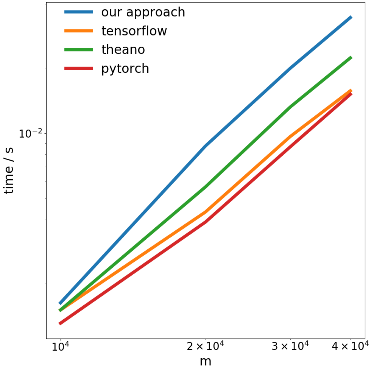
Running times

$$\text{gradient of } f(x) = x^\top A x$$



CPU



GPU

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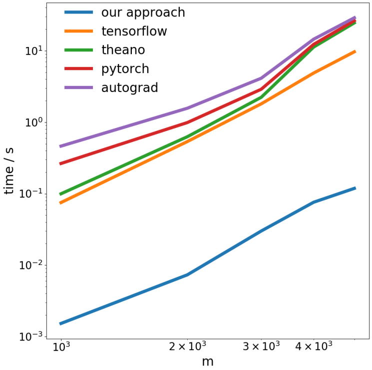
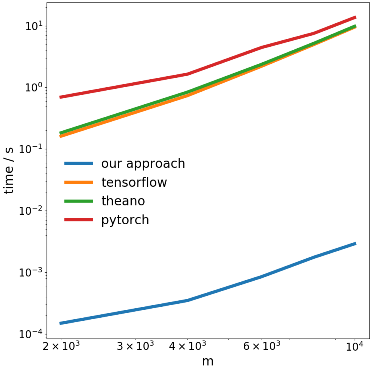
Running times

Hessian of $f(x) = x^\top A x$



CPU $\sim$ 100x



GPU $\sim$ 1000x

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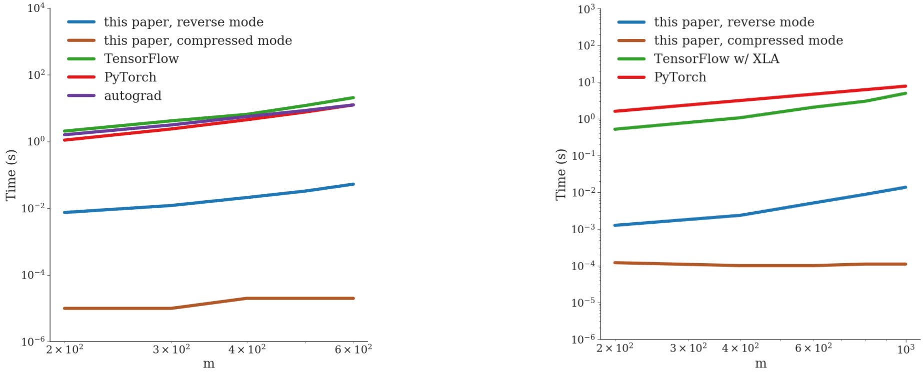
Running times

$$\text{Hessian of } f(U) = \|T - UV^\top\|_2^2$$

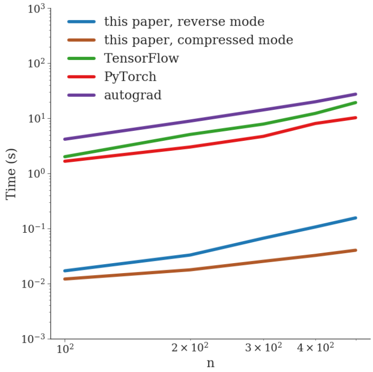


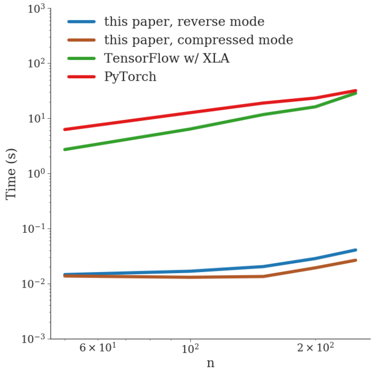
CPU $\sim$ 100x

GPU $\sim$ 1000x

Running times

Hessian of neural net (10 dense layers w/ ReLU, softmax cross-entropy)





CPU $\sim$ 100x

GPU $\sim$ 1000x

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Algorithmic Details

Derivatives

Symbolic Differentiation vs. Automatic Differentiation

Derivatives

$$f(a) = \log(\sin(a^2))$$

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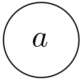
evaluation



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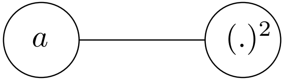

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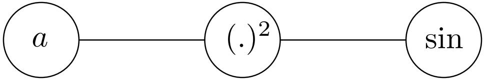

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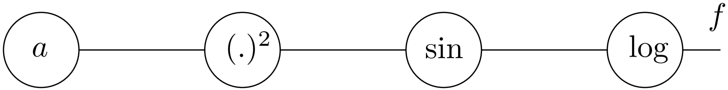

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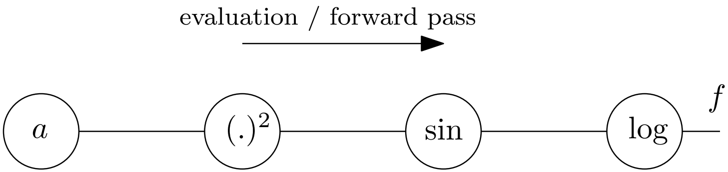

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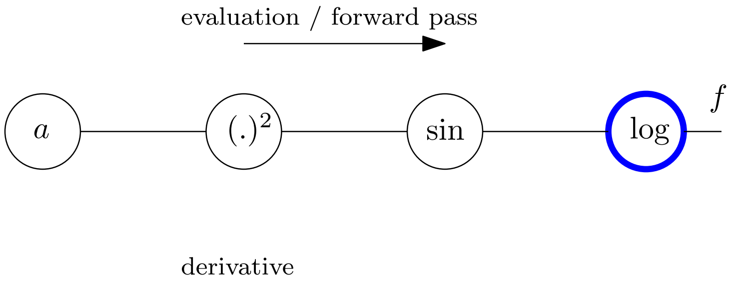

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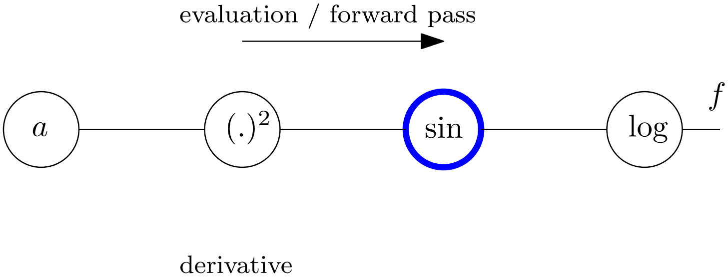

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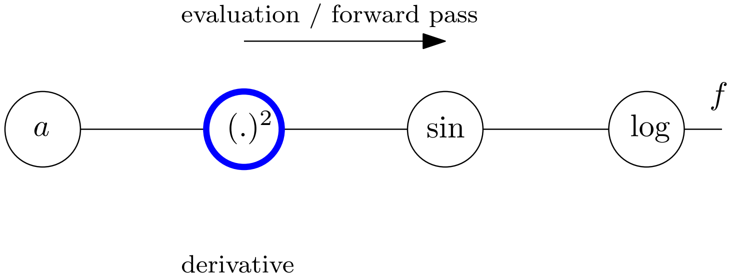

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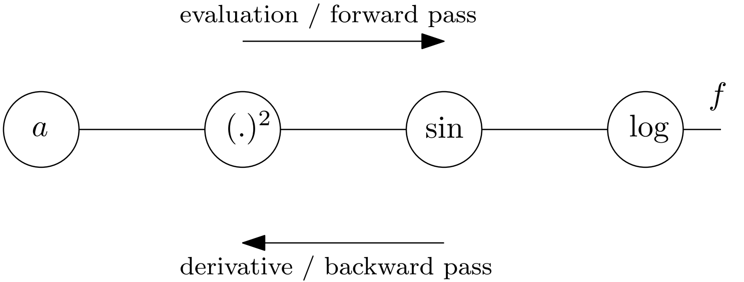

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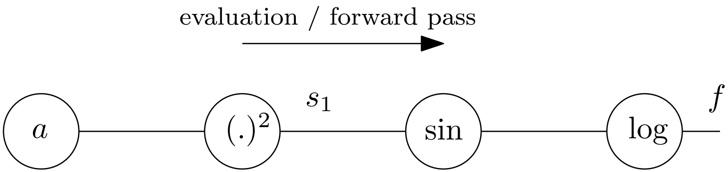

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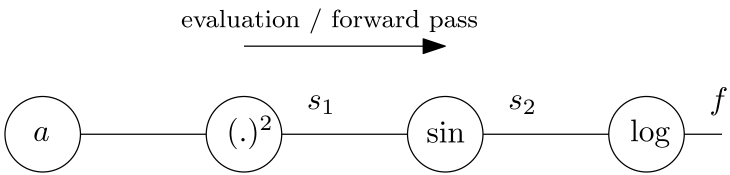

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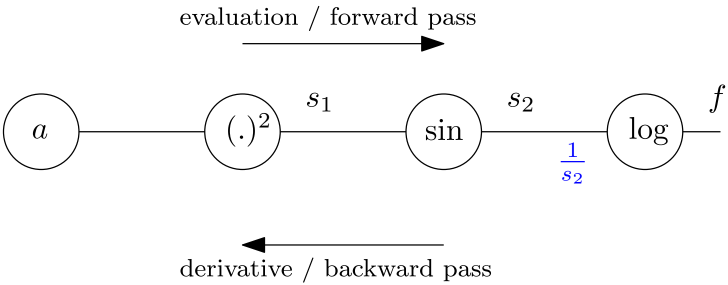

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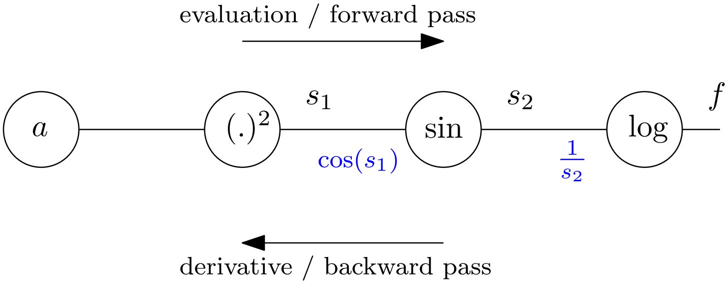

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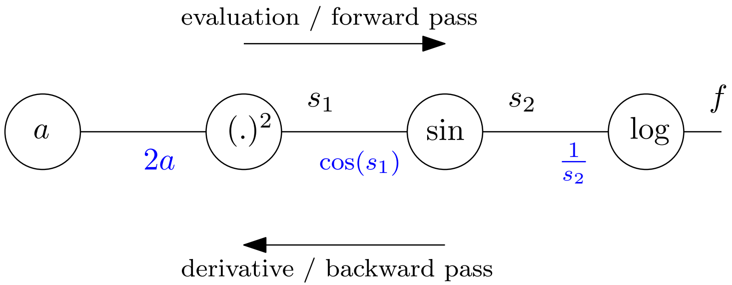

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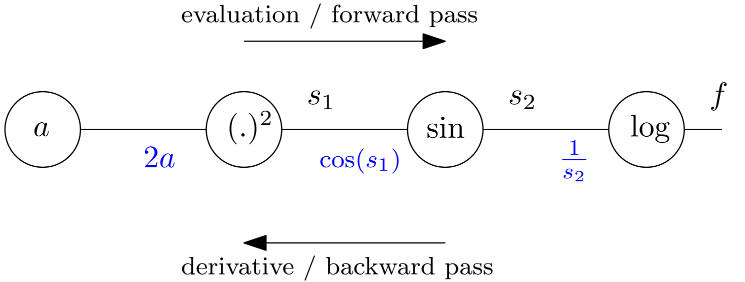

backpropagation / reverse mode autodiff

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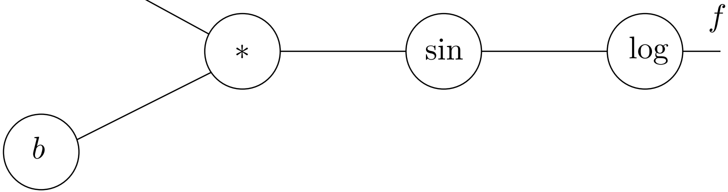

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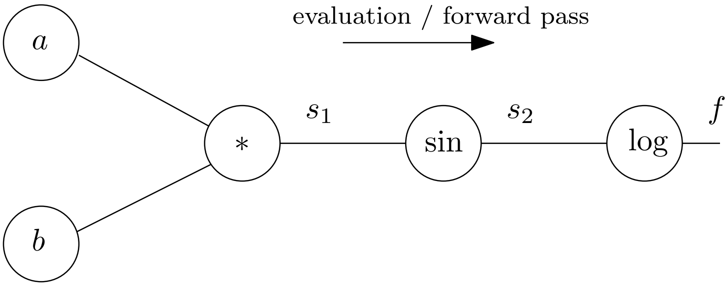

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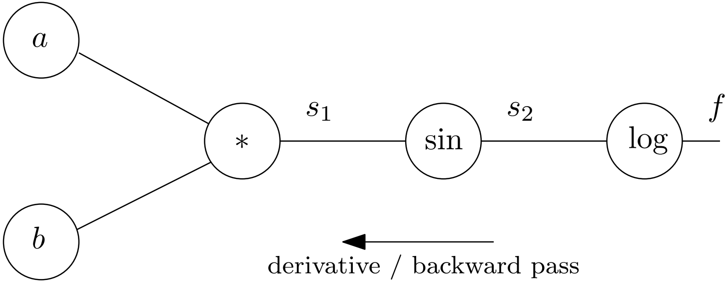

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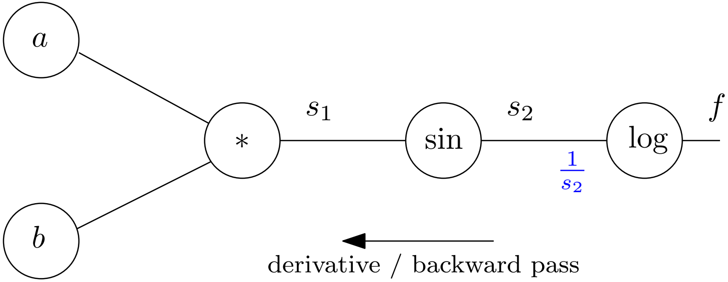

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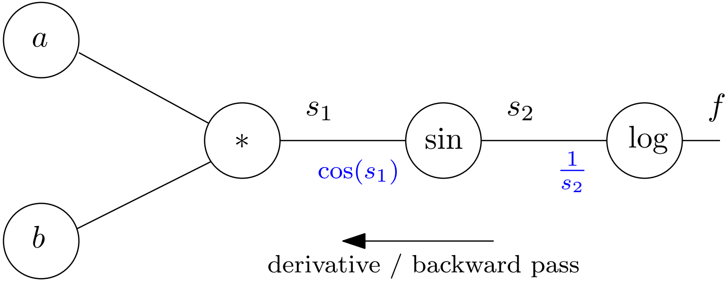

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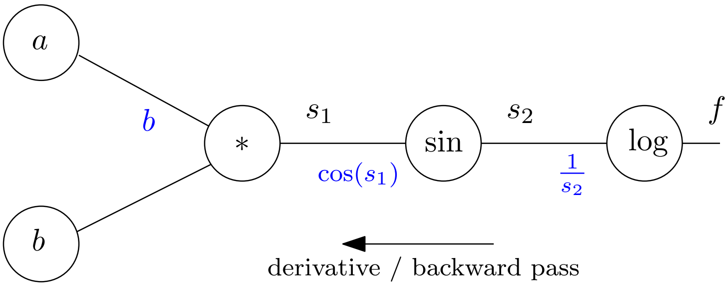

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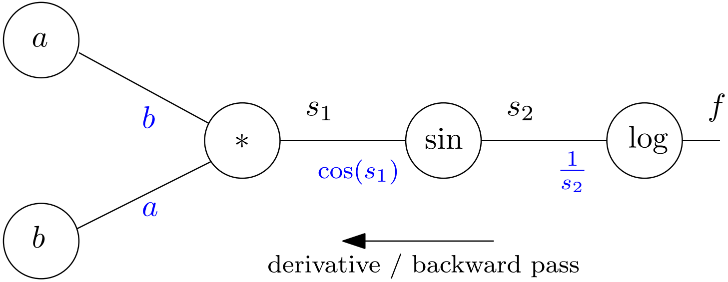

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Warning: my personal view!

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common claim: symbolic differentiation suffers from expression swell

Matrix Calculus

Matrix Case

Neural Net, 1 Layer

$$L(x, W, b, y) = \left\|\sigma(x^\top W + b^\top) - y^\top\right\|^2 \qquad x \in \mathbb{R}^n, y \in \{0, 1\}^d$$

Neural Net, 1 Layer

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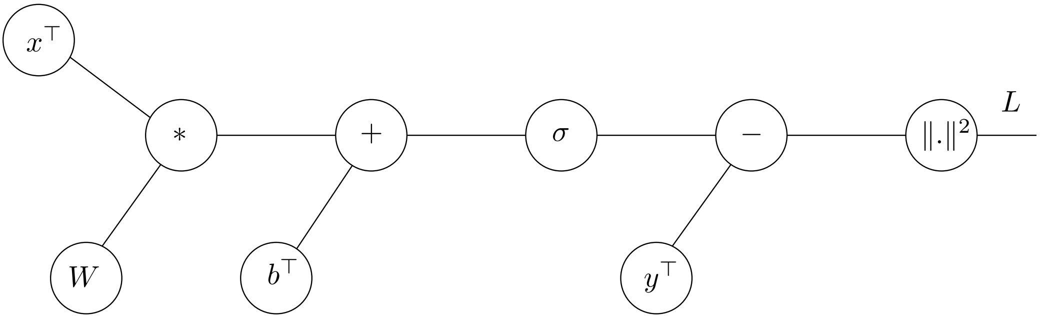

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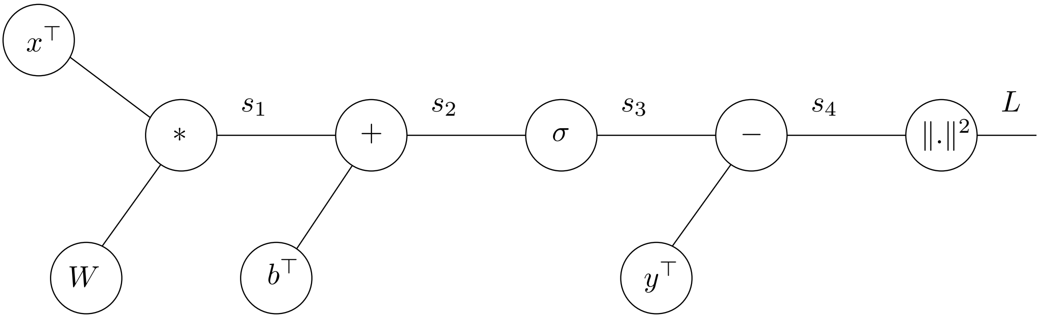

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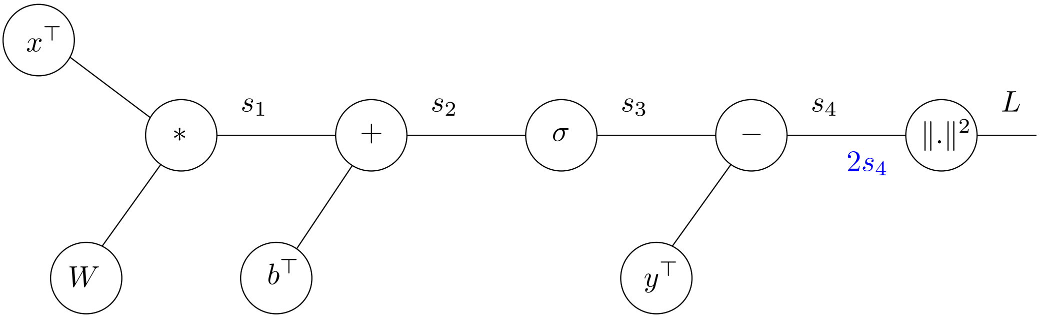

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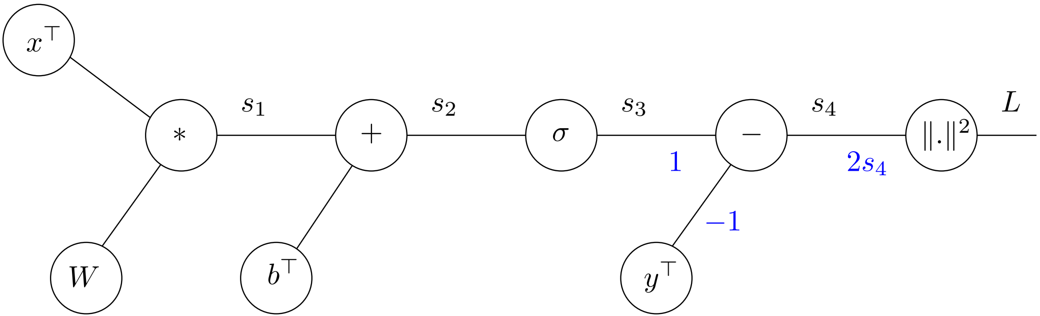

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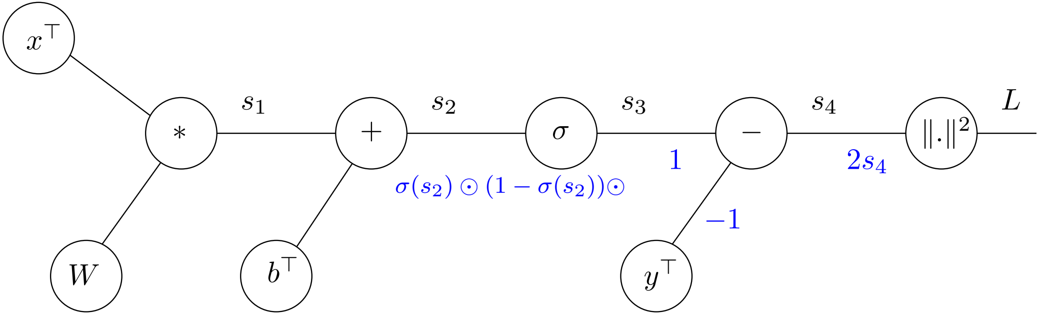

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Neural Net, 1 Layer

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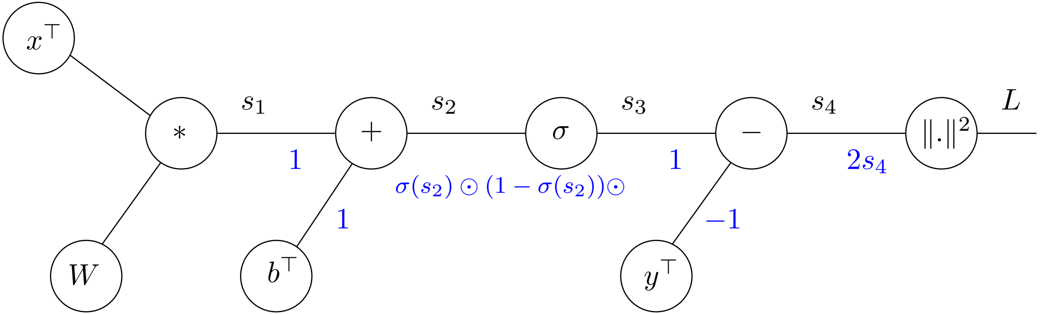

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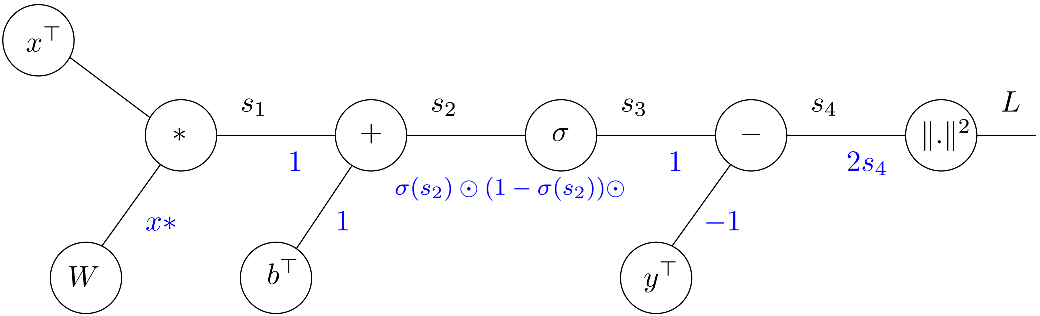

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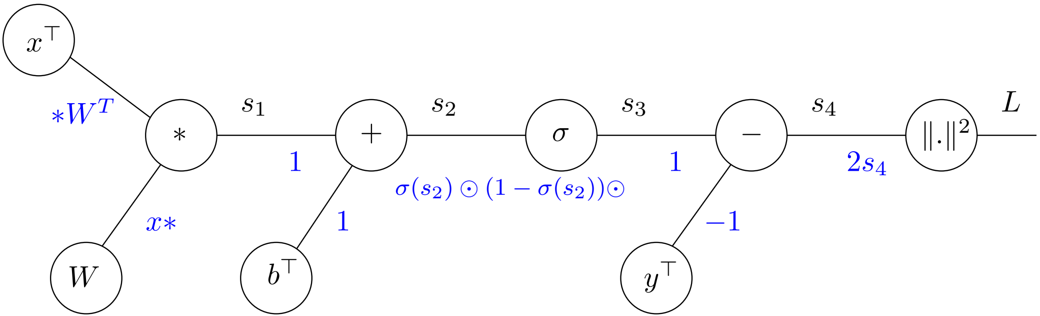

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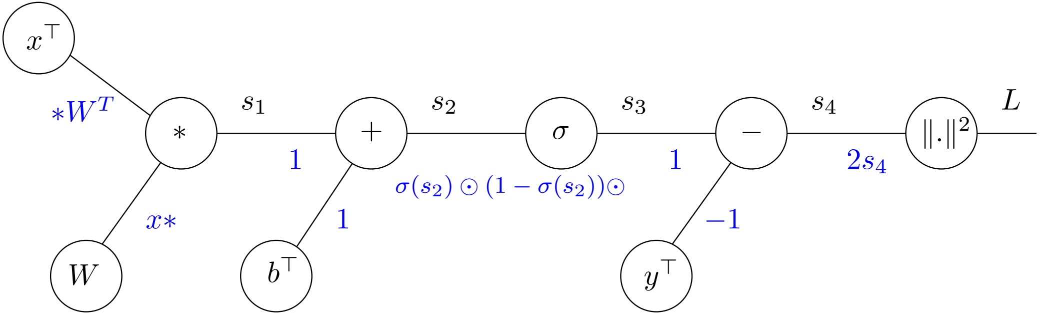

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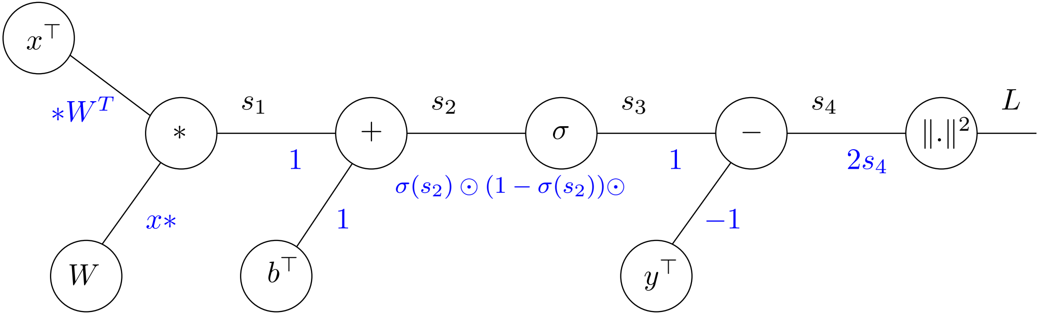

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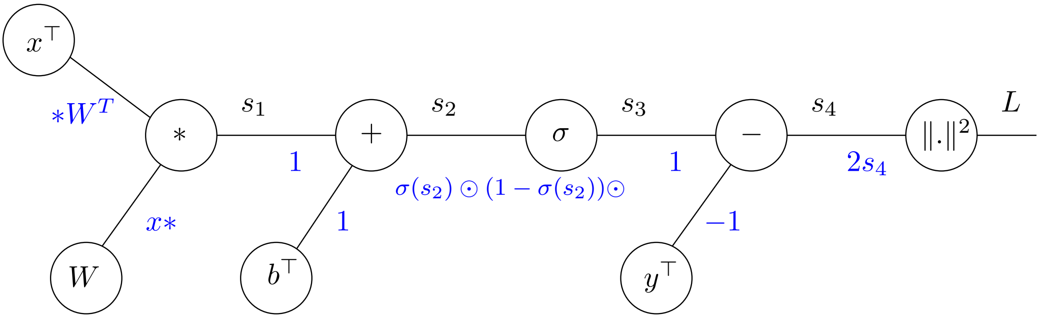

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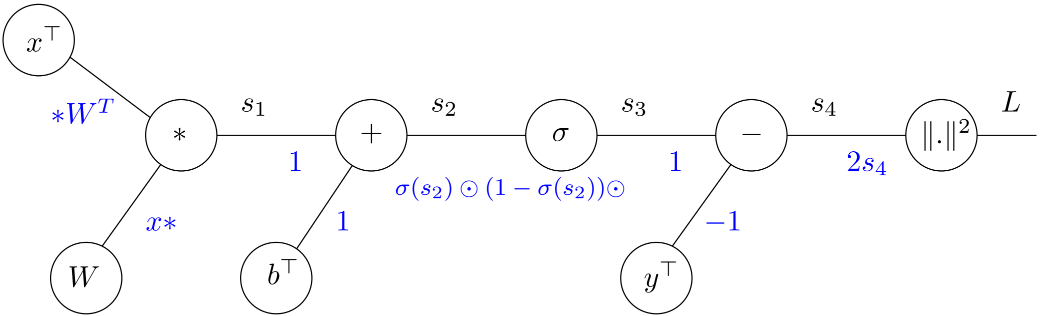

Matrix Calculus

Matrix case is identical to scalar case, except for the type of multiplications in the derivative.

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Matrix Calculus

Matrix case is identical to scalar case, except for the type of multiplications in the derivative.

This is the root of all the trouble with matrix calculus.

Matrix Calculus – Matrix Notation

First attempt: Use matrix notation for matrix calculus.

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- led to buggy implementation in SymPy

Matrix Calculus – Ricci Notation

Use Ricci notation for matrix calculus.

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- first usable algorithm for matrix calculus

Details – Elements of Ricci calculus

matrix notation	Ricci notation
a	a
x	x^i
$x^\top$	x_i
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$\mathbb{I}$	δ^i_j

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Details – Elements of Ricci calculus

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$$A_{ij} \quad B^i_{jk} \quad C^{il}_{jk}$$

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Details – Elements of Ricci calculus

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Ax	$A^i_j \, x^j$
$y^\top x$	$y_j \, x^j$
AB	$A^i_j \, B^j_k$
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Ricci notation is commutative.

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gradient of $f(x) = x^\top A x$

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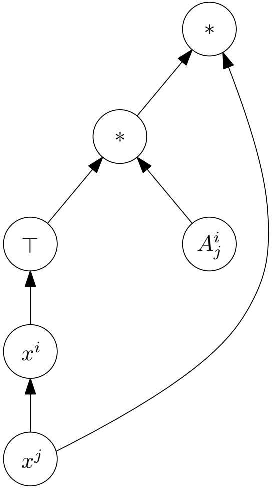

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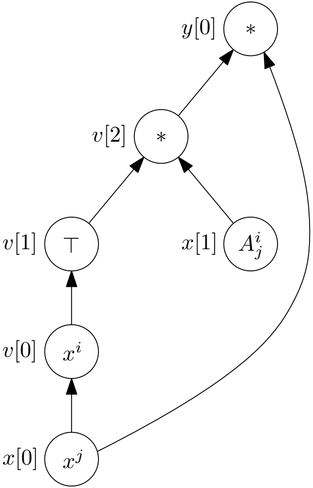

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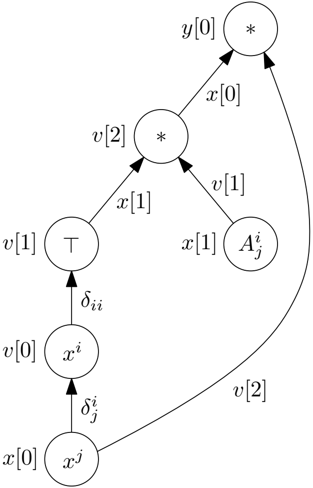

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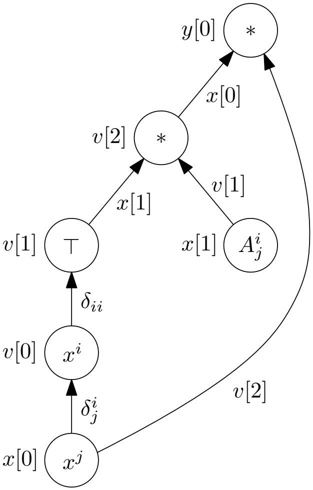

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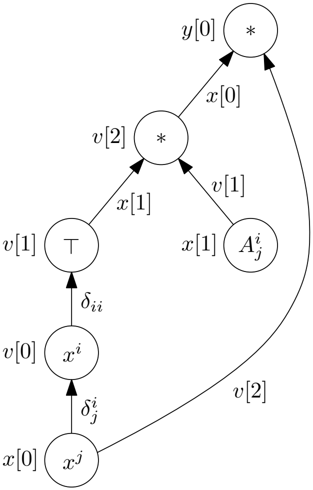

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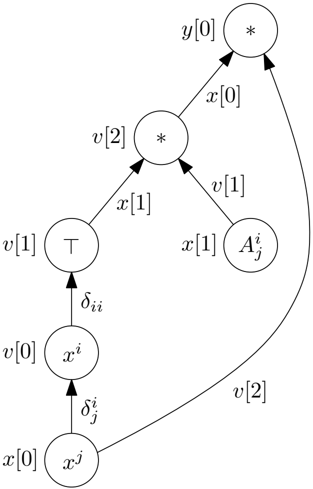

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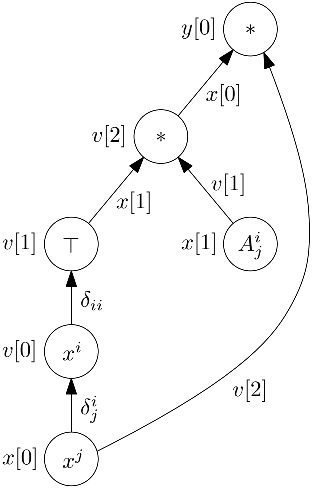

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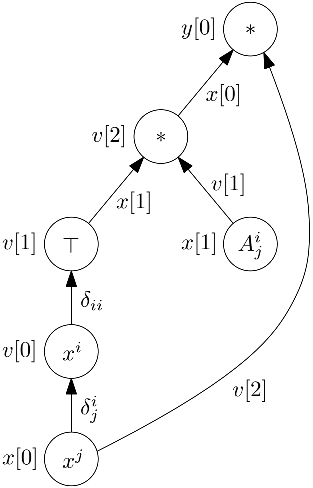

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&= (Ax)^\top + x^\top A
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- $x = x^i \quad x^\top = x_i$
- often, this precision / distinction is not needed

Matrix Calculus – Einstein Notation

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- does not distinguish between upper and lower indices
- $T = T[i, j, \ldots]$
- allows for compression of derivatives

Matrix calculus – Einstein notation

Let A, B and C be tensors. Any tensor/matrix multiplication can be written as:

$$C[s_3] = \sum_{(s_1 \cap s_2) \setminus s_3} A[s_1] \cdot B[s_2],$$

where s_1, s_2 and s_3 are index sets.

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multiplication symbol

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`einsum` in NumPy

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forward mode autodiff:

$$\dot{C} = A *_{(s_1, s_2 s_4, s_3 s_4)} \dot{B}$$

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reverse mode autodiff:

$$\bar{B} = A *_{(s_1, s_5 s_3, s_5 s_2)} \bar{C}$$

where s_5 is the new index set of $\frac{df}{df}$ (f - output function).

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$$C[s3] = g(A[s1])$$

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- cross-country mode for highest efficiency

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symbolic vs. automatic differentiation

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MatrixCalculus.org

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