Overview of Automatic Differentiation

James Yang

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What is Automatic Differentiation (AD)?

- Addresses the question: *How do we write a framework (e.g. Tensorflow, PyTorch) where users can differentiate a wide class of functions automatically?*
- Users **should not** manually write derivatives.
- Solves issues with other forms of differentiation methods.
- Seppo Linnainmaa (1970) master thesis.

Why should we care about computing derivatives?

- Many optimization/statistical methods require the use of gradients.
- Optimizers: gradient descent and all its variants.
- Neural network + back propagation: differentiate loss w.r.t. all parameters.
- Bayesian Hamiltonian Monte Carlo Samplers (HMC, Langevin, NUTS, etc.): differentiate joint-log-pdf of hierarchical model.
- ODE/PDE solvers: differentiate a known function H, which is used to specify the dynamics of another variable.
- MLE computation: gradient descent on the (negative) log-likelihood.

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- Your homework: I know you used Wolfram at some point in your life O_O!

Finite Difference (FD)

- Given f and x, compute

$$\frac{f(x+h) - f(x)}{h}$$

for small h and declare it to be $f'(x)$.

Finite Difference (FD)

- Pros:
  - Very easy to implement.
  - Works for *any* programmable functions.
- Cons:
  - Suffers from numerical precision issues (dividing two small numbers leads to wild results) (example code: `fd_prec`).
  - Cannot take advantage of analytical forms even if they exist.
  - Must run p times if there are p input variables.

Symbolic Differentiation (SD)

- E.g. Wolfram, Mathematica.
- Given a formula or mathematical expression of the function of interest f, generate a new expression for the derivative.

Symbolic Differentiation (SD)

- Pros:
  - if f is composed of elementary functions, SD produces the analytical form for f' (no approximations).
  - Convenient output for mathematicians who need the functional form.
- Cons:
  - Difficult to represent programmatic expressions.
    - How do we differentiate an if-else statement?
    - How do we differentiate a for-loop?

Automatic Differentiation (AD)

- Combines (most of) the Pros and solves the Cons of SD and FD.
- Computes analytical derivatives for *any* (including programmatic) expressions.
- Does not suffer from numerical precision issues as in FD.
- Does not output an expression like SD, but rather the derivative at a given x like FD.
  - Allows for optimization in implementation if it doesn't need to return the full expression for gradient.

Introduction

Forward-Mode Automatic Differentiation

Reverse-Mode Automatic Differentiation

Tips

Applications

Benchmarks

Example Function and Expression Graph

$$(x(t), y(t)) = (\cos(\omega t), \sin(\omega t))$$

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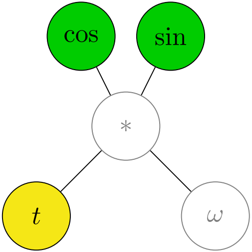


Forward AD

- Each node is represented by a *dual number*, $(w, \frac{dw}{dx})$.
- Extend elementary functions to dual numbers.
- Unary f:

$$f((w, \frac{dw}{dx})) := \left(f(w), \frac{df}{dw}\frac{dw}{dx} \right)$$

- Binary f:

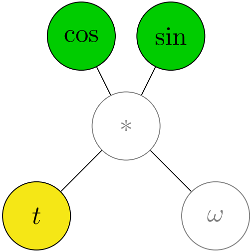
$$f\left((w_1, \frac{dw_1}{dx}), (w_2, \frac{dw_2}{dx}) \right) := \left(f(w_1, w_2), \frac{df}{dw_1}\frac{dw_1}{dx} + \frac{df}{dw_2}\frac{dw_1}{dx} \right)$$

Forward AD

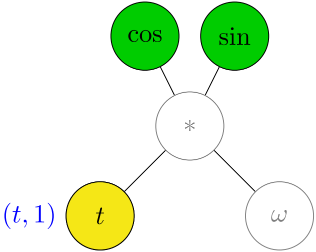
- Example:

$$\sin((w, \frac{dw}{dx})) = (\sin(w), \cos(w)\frac{dw}{dx})$$
$$(w_1, \frac{dw_1}{dx}) \cdot (w_2, \frac{dw_2}{dx}) = (w_1 w_2, \frac{dw_1}{dx} w_2 + w_1 \frac{dw_2}{dx})$$

Forward AD Evaluation



Forward AD Evaluation



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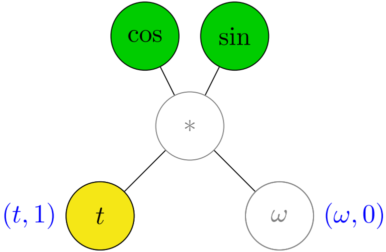

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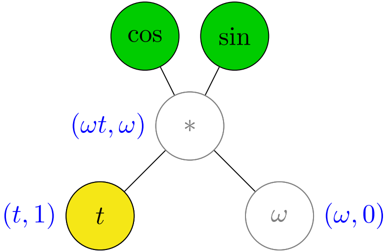

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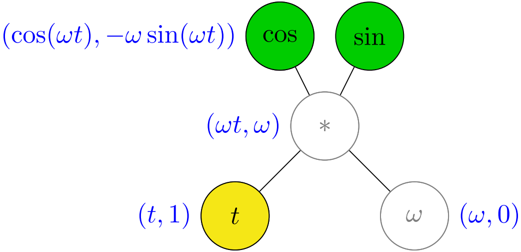

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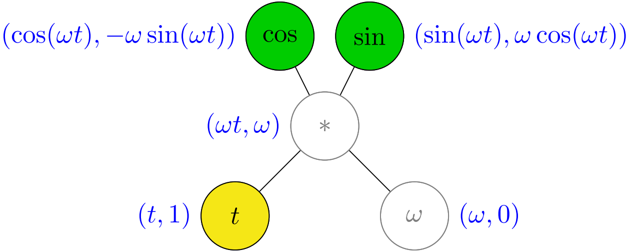

Forward AD

- Easy to implement.
- Fast for $f : \mathbb{R}^n \to \mathbb{R}^m$ where $m \gg n$ ($O(n)$ sweeps of computation graph).
- Useful in physics applications when differentiating w.r.t. time.
- Example code (`fwd_ad`).

Example Function and Expression Graph

$$f(x_1, x_2, x_3) = \sin(x_1) + \cos(x_2) \cdot x_3 - \log(x_3)$$

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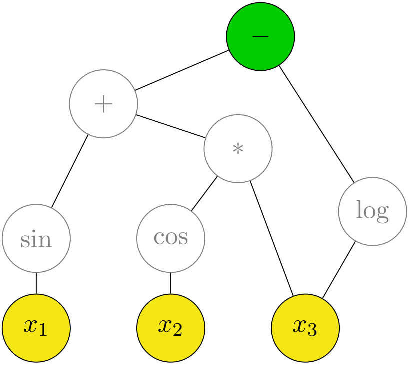
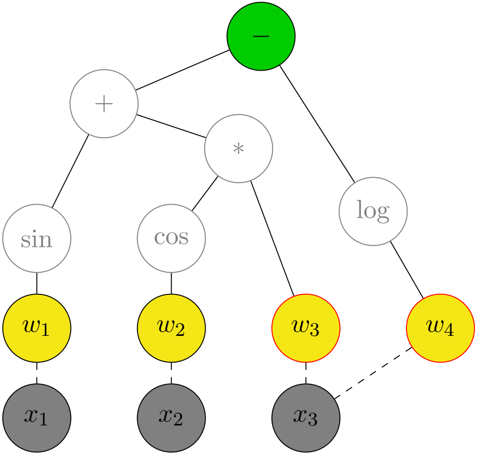


Expression Tree Conversion

- x_i can be referenced by multiple nodes.
  - e.g. x_3 is referenced by the `*` and `log` nodes.
- Convert expression graph into an expression tree.
  - Replace all nodes with multiple parents as separate nodes that reference back to the actual variables.
- Mathematically,

$$
\begin{aligned}
f(x_1, x_2, x_3) &= \tilde{f}(g(x_1, x_2, x_3)) \\
\tilde{f}(w_1, w_2, w_3, w_4) &= \sin(w_1) + \cos(w_2) \cdot w_3 - \log(w_4) \\
g(x_1, x_2, x_3) &= (x_1, x_2, x_3, x_3)
\end{aligned}
\tag{1}
$$

Expression Tree Conversion



Expression Tree Conversion

- Why do we need this conversion?
  - All nodes except x_i have exactly one parent.
  - Leads to cleaner implementation.
  - Better to treat x_i as *containers* for initial values and their **adjoints**, $\frac{\partial f}{\partial x_i}$, instead of nodes of the graph.

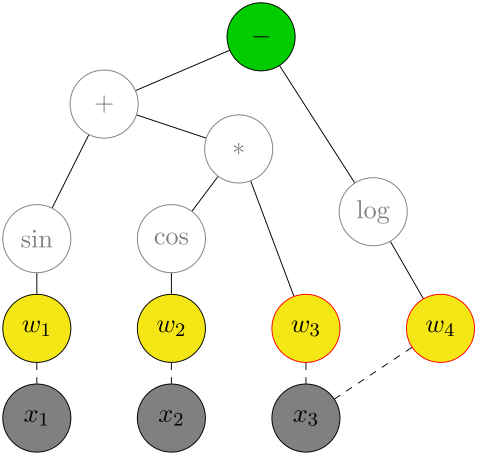
Reverse-Mode AD Algorithm

- Assume for the moment that $f : \mathbb{R}^n \to \mathbb{R}$.
- Reverse-mode algorithm consists of two passes of the expression tree:
  - *forward*-evaluation (not to be confused with forward-mode AD)
  - *backward*-evaluation

Forward-Evaluation

- Compute expression in the usual fashion.
  - Start at the root.
  - Recursively forward-evaluate left to right all its children.
  - Compute current node operation using children results.
    - e.g. for `sin` node, $x_1 \to w_1 \to \sin(w_1)$

Forward-Evaluation



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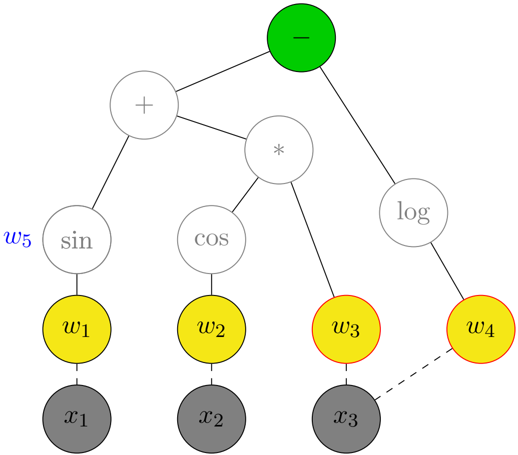

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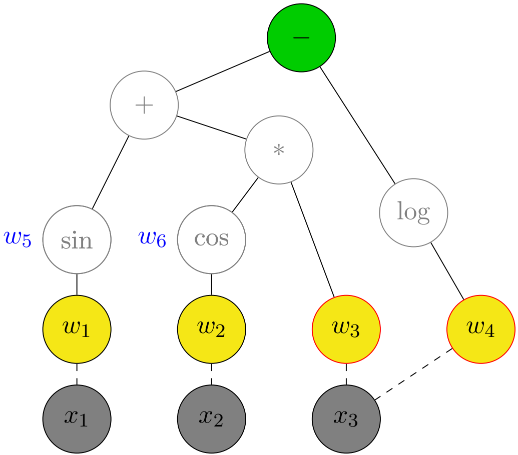

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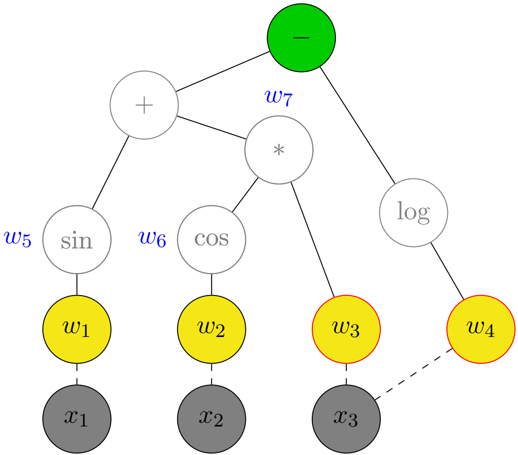

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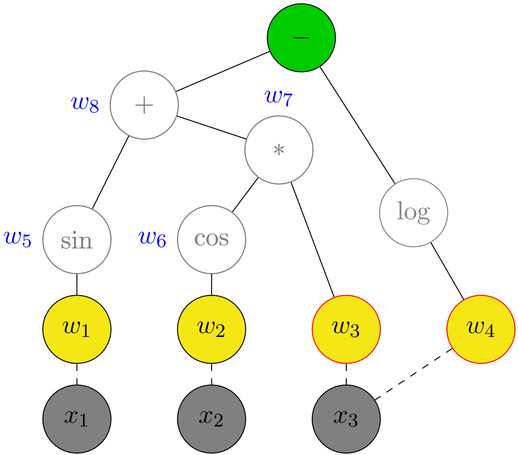

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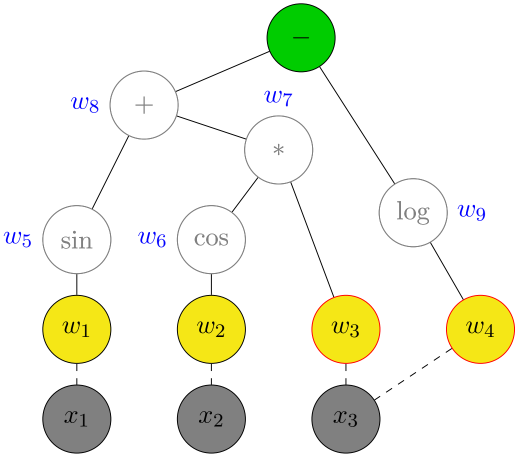

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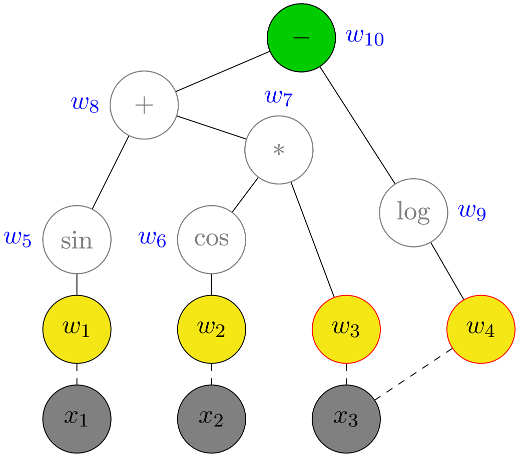


Backward-Evaluation

- Current node receives its adjoint from its parent.
- This adjoint is also referred to as *seed*.
- Hence, root will receive seed $= 1$ from the caller.
- Current node computes seeds for all its children and recursively backward-evaluates from *right-to-left*.

Backward-Evaluation: Computing Next Seed

- Next seed is computed by a simple chain-rule.
- Let the current node be $w \in \mathbb{R}^{p \times q}$ and $v \in \mathbb{R}^{m \times n}$ one of its children.
- The seed for v is given by

$$\frac{\partial f}{\partial v_{ij}} = \sum_{k=1}^{p} \sum_{l=1}^{q} \frac{\partial f}{\partial w_{kl}} \frac{\partial w_{kl}}{\partial v_{ij}} \tag{2}$$

- Since we are working with an expression tree, f only depends on v through w, hence this is the full adjoint.

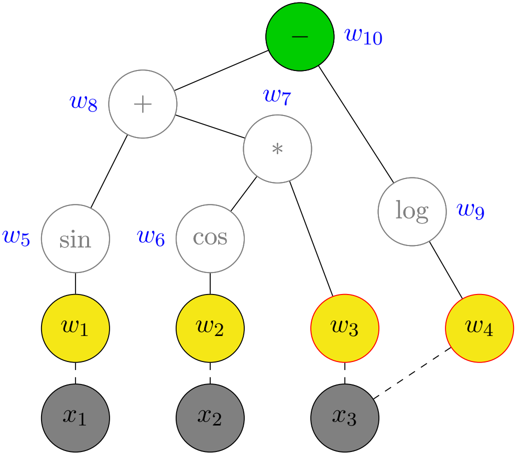
Backward-Evaluation: Computing Next Seed

- Nodes with reference to containers must increment the adjoints in the containers with their seed.
  - e.g. w_3 and w_4 increments the adjoint in x_3 with their seeds.
- Why? Chain-rule, once again.
- Let $w_1, \ldots, w_k$ denote all variables with a reference to x. For simplicity assume they are all scalars (easily generalizable). Then,

$$\frac{\partial f}{\partial x} = \sum_{i=1}^{k} \frac{\partial f}{\partial w_i} \frac{\partial w_i}{\partial x} = \sum_{i=1}^{k} \frac{\partial f}{\partial w_i}$$

- Accumulated adjoints for x_1, x_2, x_3 is the gradient of f.

Backward-Evaluation



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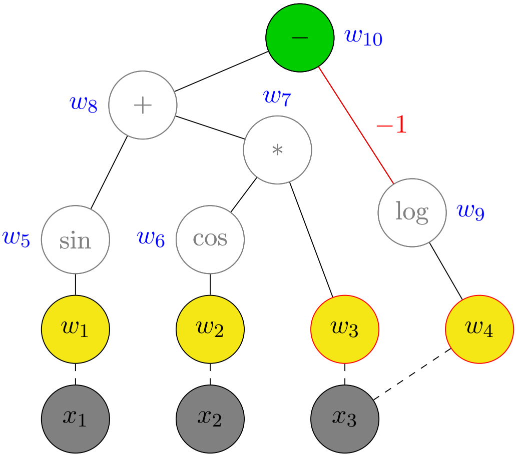

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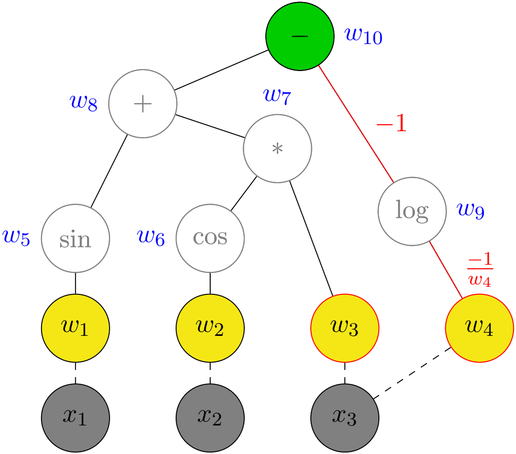

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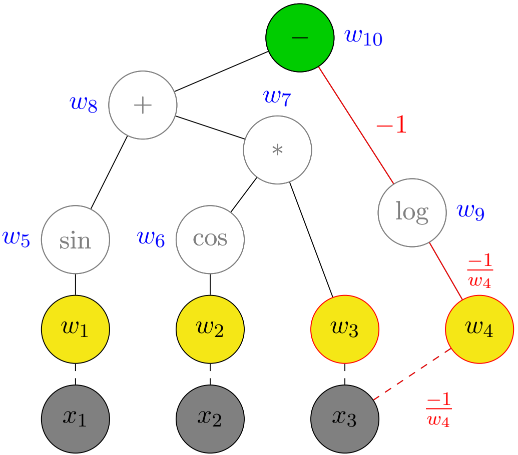

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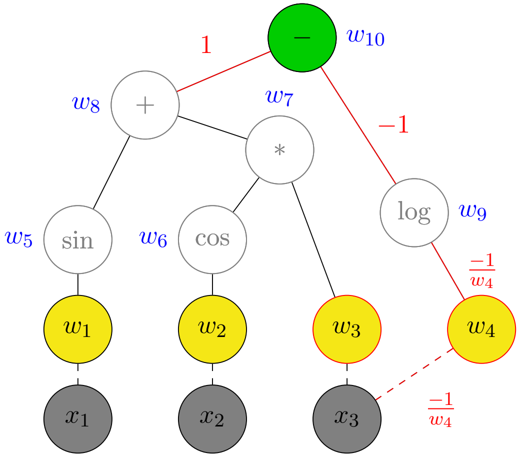

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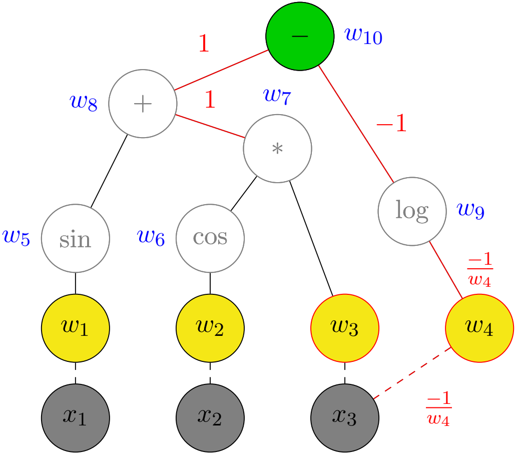

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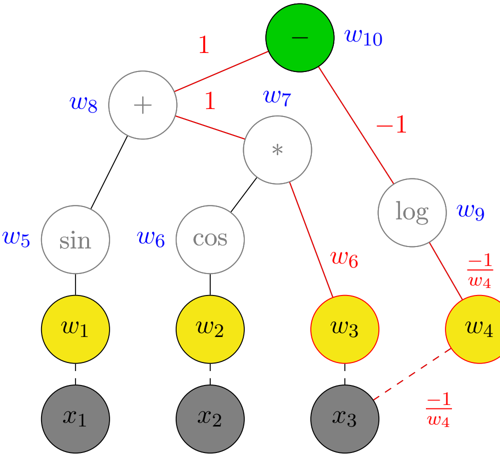

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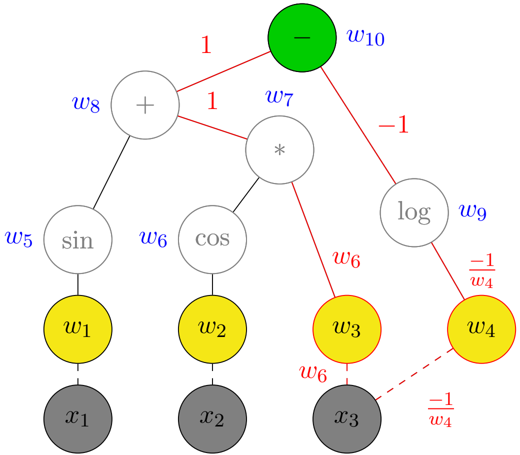

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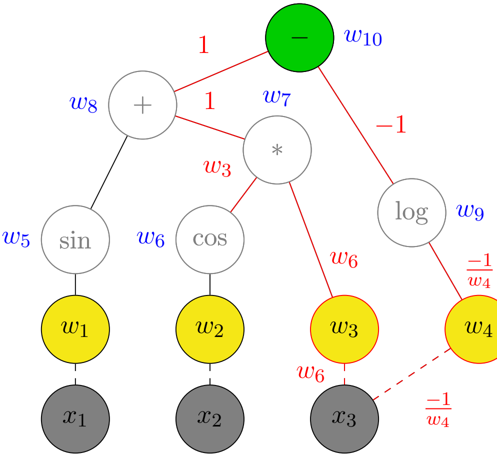

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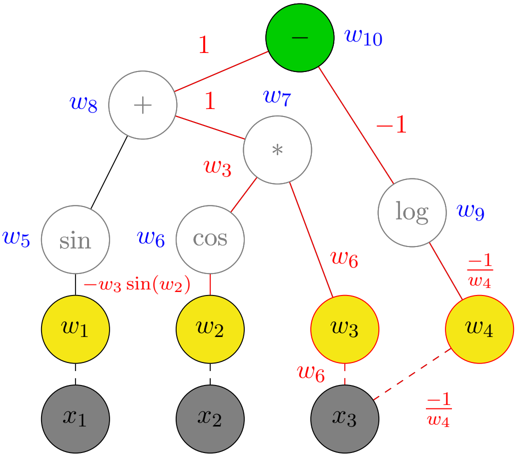

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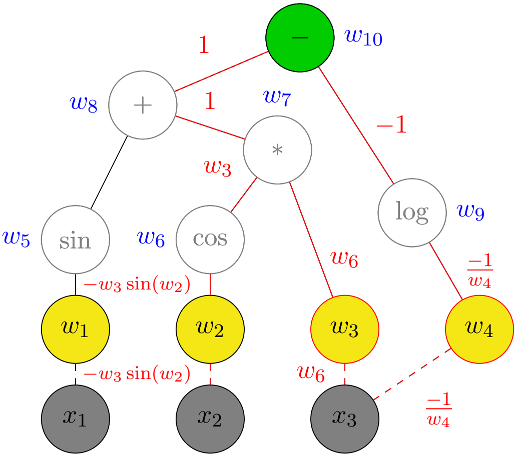

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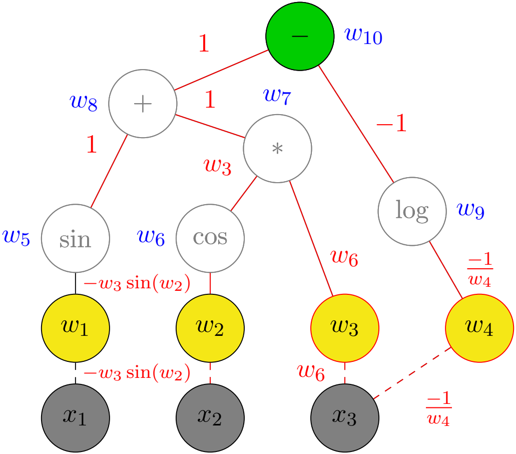

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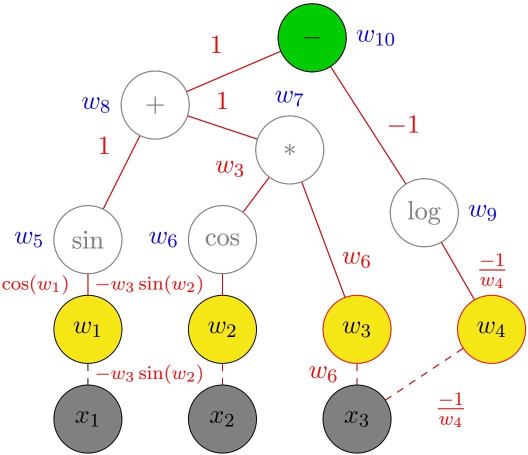

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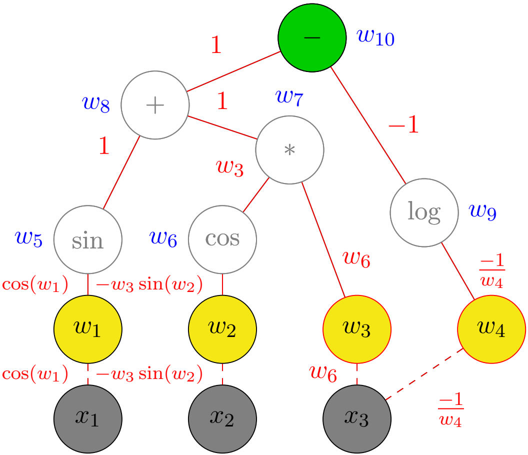

Backward-Evaluation

- Sanity check:

$$
\begin{aligned}
f(x_1, x_2, x_3) &= \sin(x_1) + \cos(x_2) \cdot x_3 - \log(x_3) \\
\nabla f &= \left(\cos(x_1), -x_3 \sin(x_2), \cos(x_2) - x_3^{-1}\right)
\end{aligned}
$$

Remarks

- Much harder to implement (memory management is tricky).
- Fast for $f : \mathbb{R}^n \to \mathbb{R}^m$ where $n \gg m$ ($O(m)$ sweeps of computation graph).
- Useful when we need to compute gradient (of a scalar function).
- Example code:
  - `rv_ad`
  - `for_each`
  - `if_else`

Reverse-Mode

- Extract common sub-expression into a placeholder variable, to avoid recomputation, e.g.

$$t = x + y$$
$$f(t) = \sin(t)\cos(t)$$

- Use package-provided functions mostly to take advantage of vectorization, e.g.

$$\text{for-loop sum over } x \quad ✗$$
$$\text{sum}(x) \quad ✓$$

Reverse-Mode

- Minimize number of nodes in computation graph, e.g. if $x \in \mathbb{R}^{10}$,

$$x[1] + \ldots + x[10] \implies 9 \text{ adjoints } ✗$$
$$\text{sum}(x) \implies 1 \text{ adjoint } ✓$$

- Minimize size of each node of computation graph, e.g. if $x, y \in \mathbb{R}^n$,

$$\text{sum}(x + y) \implies O(n) \text{ memory } ✗$$
$$\text{sum}(x) + \text{sum}(y) \implies O(1) \text{ memory } ✓$$

Taste of using AD

- MLE: Gaussian model.
- MLE: Gaussian mixture model.
- MAP: Ridge.

MLE: Gaussian model

- $X_i \overset{iid}{\sim} N(\mu, 1)$
- μ unknown.
- Negative log-pdf is given by

$$-\sum_{i=1}^{n} \log(p(x_i)) = \frac{1}{2}\sum_{i=1}^{n}(X_i - \mu)^2$$

- Example code (`mle`).

MLE: Gaussian mixture model

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- This is for you Kevin Senpai.

MLE: Gaussian mixture model

- This is for you Kevin Senpai.
- $X_i \overset{iid}{\sim} \pi N(\mu_1, \sigma_1^2) + (1-\pi)N(\mu_2, \sigma_2^2)$
- $(\pi, \mu_1, \mu_2, \sigma_1, \sigma_2)$ unknown.
- Negative log-pdf is given by

$$-\sum_{i=1}^{n} \log(p(x_i)) = -\sum_{i=1}^{n} \log\left(\pi p_{\mu_1,\sigma_1}(X_i) + (1-\pi)p_{\mu_2,\sigma_2}(X_i)\right)$$

- Example code (`kevin_senpai_mle`).

MAP: Ridge

- MLE is really just MAP of likelihood + non-informative prior.
- In general, can apply any (differentiable) prior.
- Ridge regression (fixed X):

$$\begin{aligned} y|\beta &\sim \mathcal{N}\left(X\beta, I\right) \\ \beta &\sim \mathcal{N}\left(0, \lambda^{-1}\right) \end{aligned}$$

- MAP is posterior mean:

$$\mathbb{E}\left(\beta|y\right) = (X^\top X + \lambda I)^{-1} X^\top y$$

- Example code (`map`).

Introduction

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Reverse-Mode Automatic Differentiation

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Comparison with Finite Difference and Manual

- Example function: $x \in \mathbb{R}^p$, $M \in \mathbb{R}^{n \times p}$

$$f(x) = \mathsf{sum}(Mx) - 2\log(\sum_{i=1}^{p} \exp(x_i))$$

Config	FD	AD	Manual (df only)	Manual (f + df)
n=10, p=100	2.2e-3	5.78e-5	3.66e-5	4.31e-5
n=10, p=10000	NA	4.3e-3	3.4e-3	4.1e-3
n=100, p=10	1.1e-4	4.2-5	9.09e-6	1.61e-5
n=10000, p=10	8.56e-3	2.64e-3	3e-4	1e-3