

A functional tour of automatic differentiation with Racket

Oliver Strickson

2020-02-14

Kraków



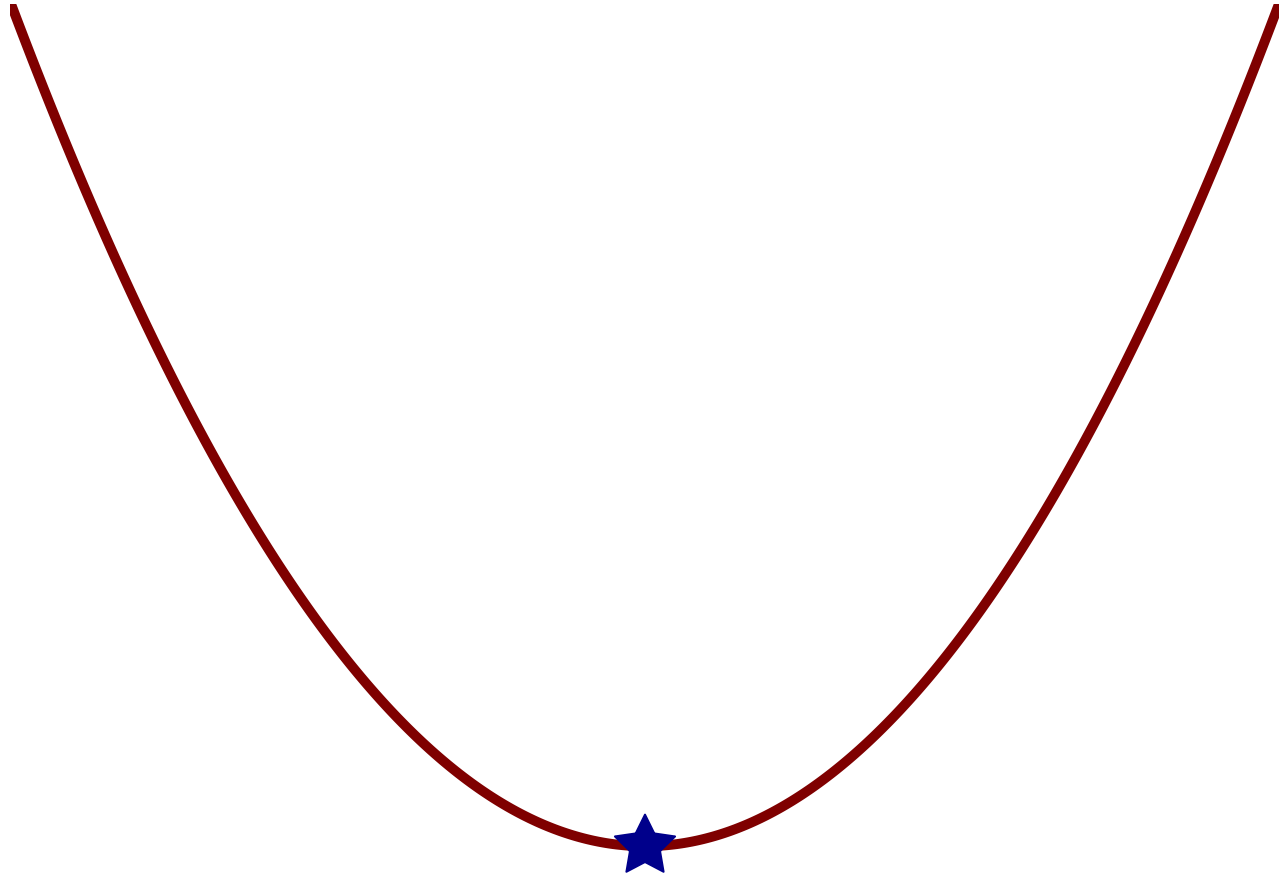
lambda
D A λ S

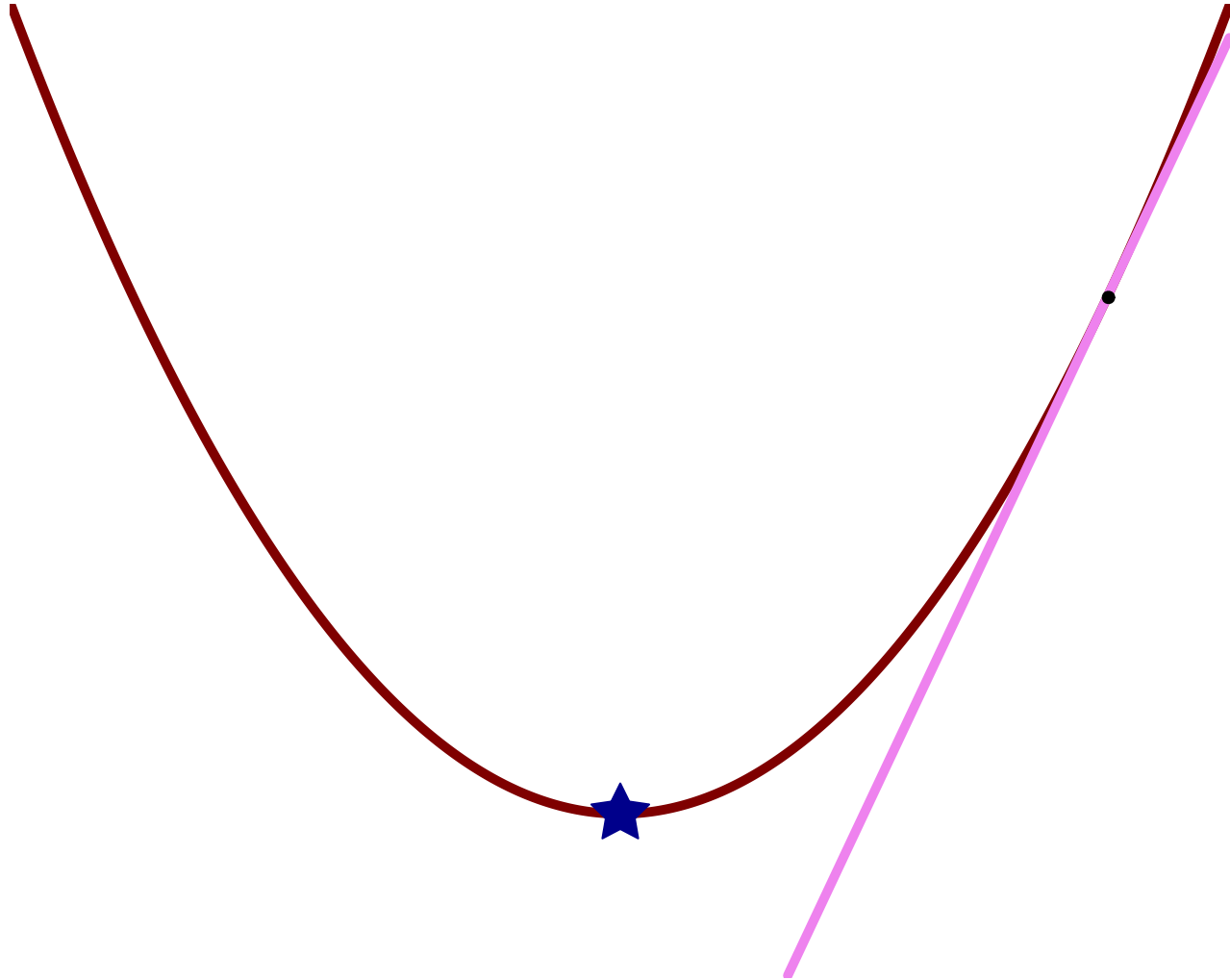
Oliver Strickson
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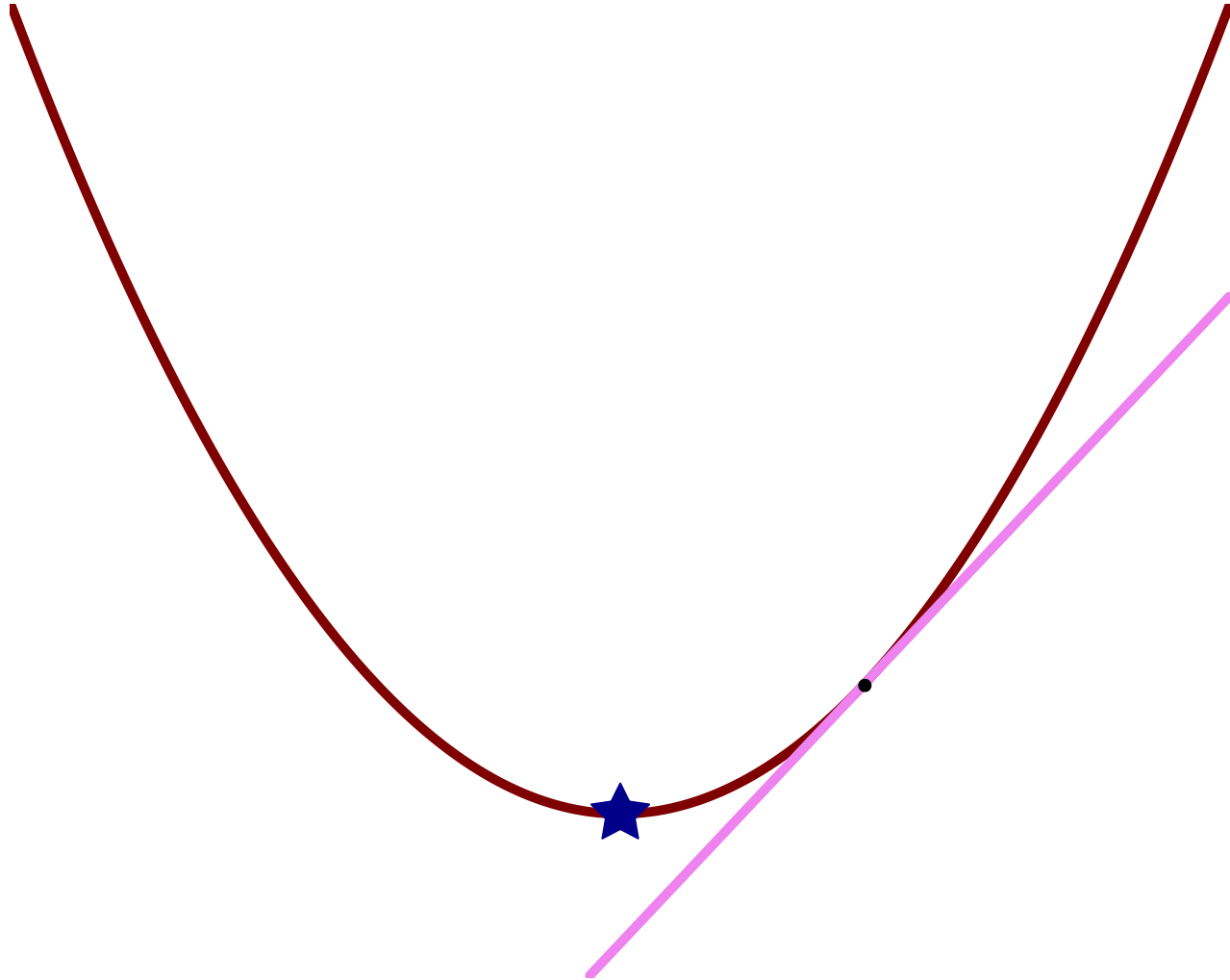
The Alan Turing Institute

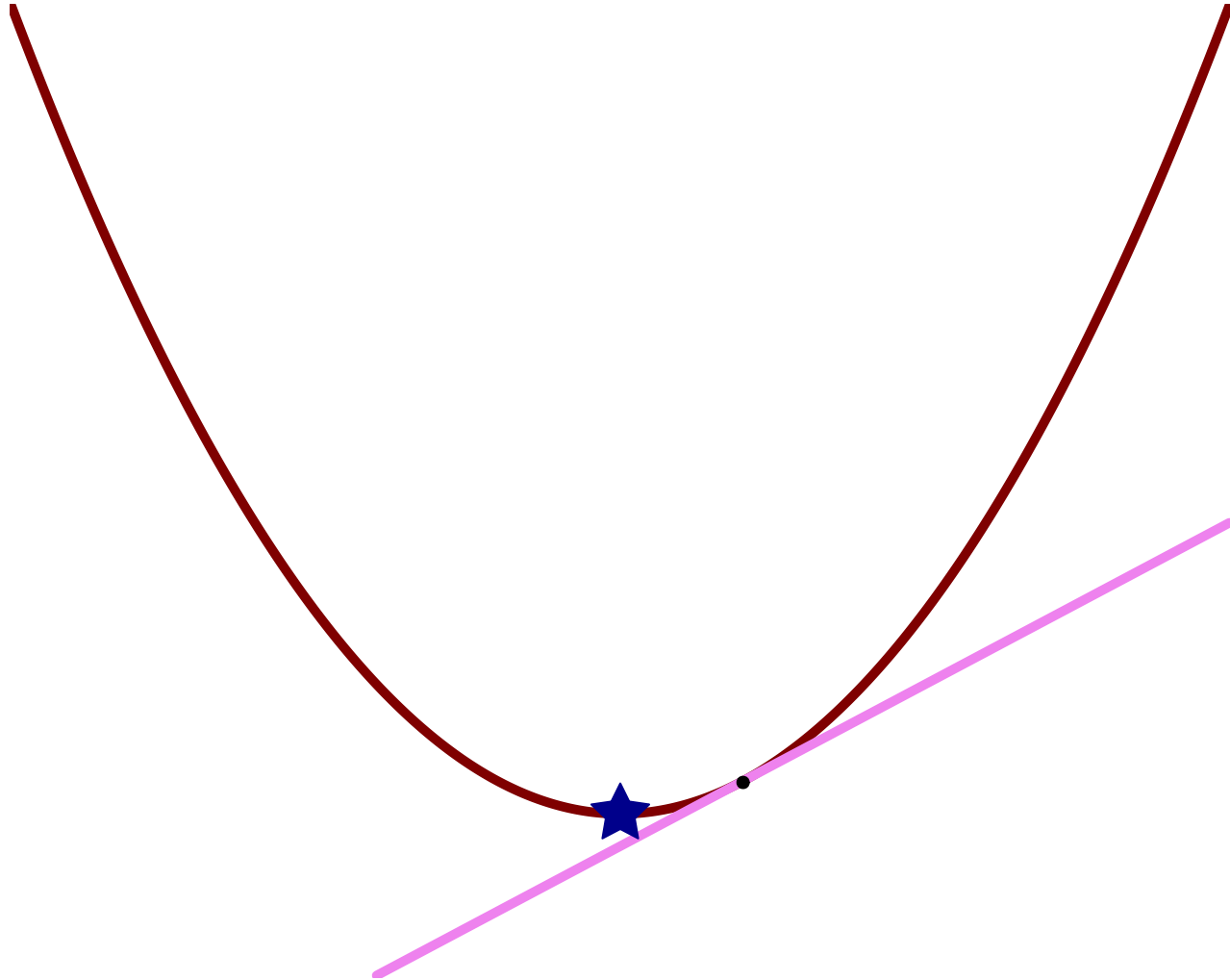


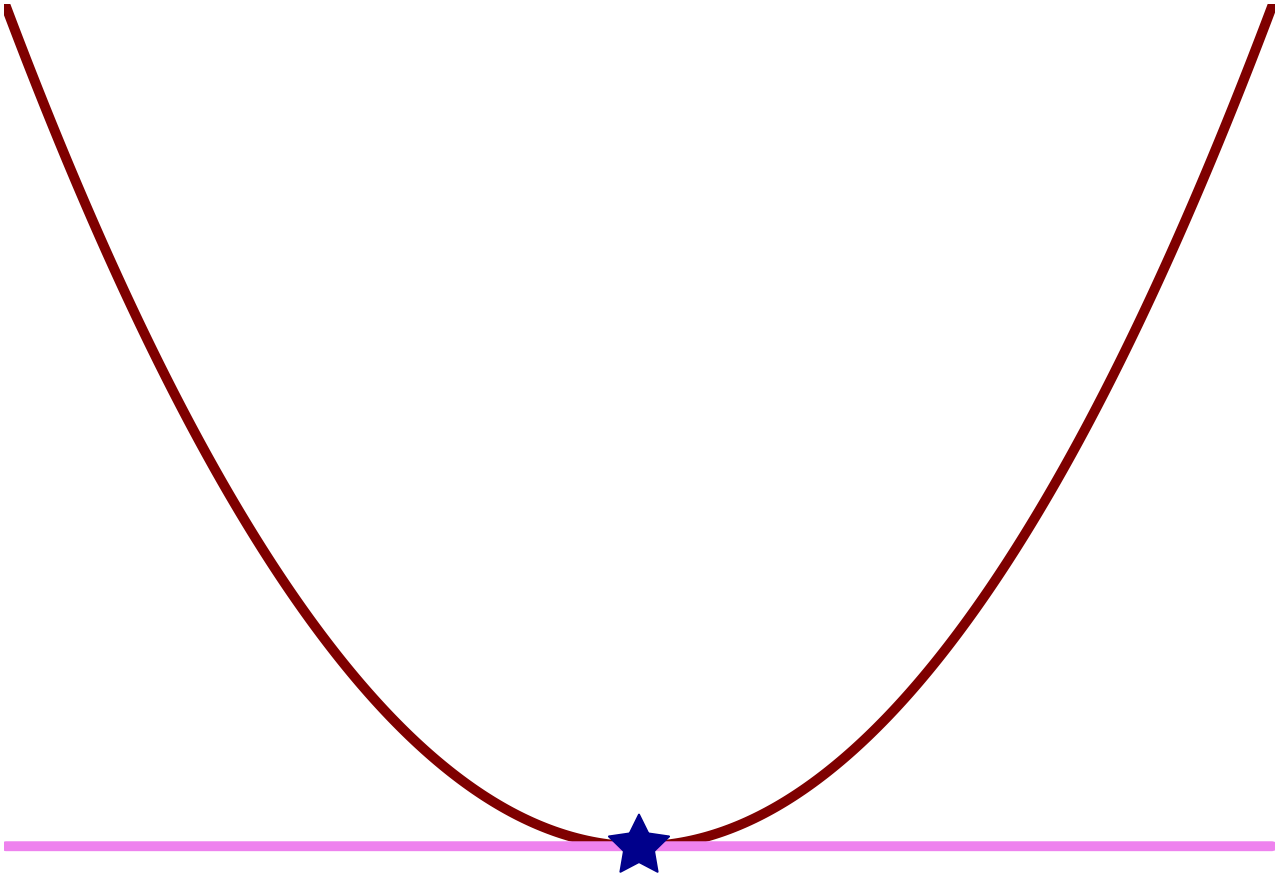
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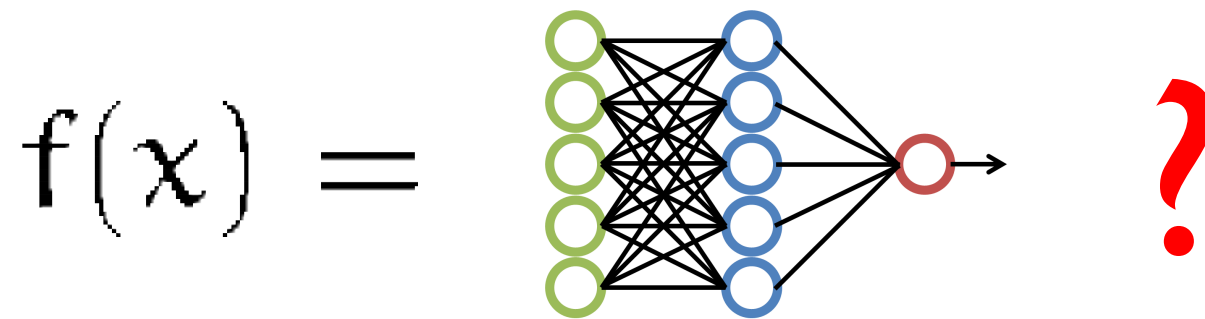
minimize f

minimize f Df

$$f(x) = x^2$$

$$f(\boldsymbol{x}) = \boldsymbol{x}^2$$
$$Df(\boldsymbol{x}) = ??$$

$$f(x) = x^2$$
$$Df(x) = 2x$$



$f(x) =$

```
import ..Layer, ..Request
using ..URIs
using ..Messages
using ..Pairs: setkv
import ..Header
import ..@debug, ..DEBUG_LEVEL

"""
request(RedirectLayer, method, ::URI, headers, body) -> HTTP.Response
Redirections the request in the case of 3xx response status.
"""
abstract type RedirectLayer{Next <: Layer} <: Layer end
export RedirectLayer
function request{::Type{RedirectLayer}(next),
                method::String, url::URI, headers, body,
                redirect_limit::Integer, forward_headers::Pair{String, String}...}
    count = 0
    true
end
```



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

Symbolic?

Automatic

Overview

- Some syntax
- Differentiation
- Automatic differentiation algorithm(s)
- Implementation

`(cons 'a 'b)` \Rightarrow `(a . b)`

`(cons 'a 'b) => (a . b)`

`(cons 'a (cons 'b 'c)) => (a b . c)`

`(cons 'a (cons 'b null)) => (a b)`

`(cons 'a 'b) => (a . b)`

`(cons 'a (cons 'b 'c)) => (a b . c)`

`(cons 'a (cons 'b null)) => (a b)`

`(list 'a 'b) => (a b)`

`(cons 'a 'b) => (a . b)`

`(cons 'a (cons 'b 'c)) => (a b . c)`

`(cons 'a (cons 'b null)) => (a b)`

`(list 'a 'b) => (a b)`

`(3 1 ((4 1)) (5 . 9) 3)`

`(cons 'a 'b)` \Rightarrow `(a . b)`

`(car '(a . b))` \Rightarrow `a`

`(cdr '(a . b))` \Rightarrow `b`

`(car '(a b c)) => a`

`(cdr '(a b c)) => (b c)`


```
(define (multiply x y) (* x y))
```

```
(define ((multiply x) y) (* x y))
```

```
(define (sum . xs) (apply + xs))
```

Differentiation

Differentiation

The best linear approximation to a function about a point (if it exists)

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The best linear approximation to a function about a point (if it exists)

Function f or \mathbf{f}

Derivative Df or $(D \mathbf{f})$

Differentiation

function $f(x)$

find a with

$$f(x) - f(x_0) \approx a(x - x_0)$$

Differentiation

function $f(x)$

find a with

$$f(x) - f(x_0) \approx a(x - x_0)$$

$$f(x) - f(x_0) = a(x - x_0) + \mathbf{O}((x - x_0)^2)$$

Differentiation

function $f(\mathbf{x})$

find \mathbf{a} with

$$f(\mathbf{x}) - f(\mathbf{x}_0) \approx \mathbf{a} (\mathbf{x} - \mathbf{x}_0)$$

$$f(\mathbf{x}) - f(\mathbf{x}_0) = \mathbf{a} (\mathbf{x} - \mathbf{x}_0) + \mathbf{O}((\mathbf{x} - \mathbf{x}_0)^2)$$

$$f(\mathbf{x}) - f(\mathbf{x}_0) = \mathbf{D}f(\mathbf{x}_0) (\mathbf{x} - \mathbf{x}_0) + \mathbf{O}((\mathbf{x} - \mathbf{x}_0)^2)$$

Differentiation

function $f(x, y)$

find a, b with

$$f(x, y) - f(x_0, y_0) \approx a(x - x_0) + b(y - y_0)$$

Differentiation

function $f(x, y)$

find a, b with

$$f(x, y) - f(x_0, y_0) \approx a(x - x_0) + b(y - y_0)$$

$$f(x, y) - f(x_0, y_0) \approx D_0 f(x_0, y_0)(x - x_0) + D_1 f(x_0, y_0)(y - y_0)$$

Differentiation

function $f(x, y)$

find a, b with

$$f(x, y) - f(x_0, y_0) \approx a(x - x_0) + b(y - y_0)$$

$$f(x, y) - f(x_0, y_0) \approx D_0 f(x_0, y_0)(x - x_0) + D_1 f(x_0, y_0)(y - y_0)$$

Partial derivative $D_i f$ or **(partial i f)**

Differentiation

function $f(x, y)$

find a, b with

$$f(x, y) - f(x_0, y_0) \approx a(x - x_0) + b(y - y_0)$$

$$f(x, y) - f(x_0, y_0) \approx D_0 f(x_0, y_0)(x - x_0) + D_1 f(x_0, y_0)(y - y_0)$$

Partial derivative $D_i f$ or **(partial i f)**

$$Df(x, y) = (D_0 f(x, y), D_1 f(x, y))$$

BOOK

Structure and Interpretation of Classical Mechanics (2nd ed.)

[https://mitpress.mit.edu/sites/default/files/
titles/content/sicm_edition_2/book.html](https://mitpress.mit.edu/sites/default/files/titles/content/sicm_edition_2/book.html)

Gerald Jay Sussman & Jack Wisdom (2015)



Composition

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

$$Df(\mathbf{x}) = Dg(h(\mathbf{x})) \cdot Dh(\mathbf{x})$$

Composition

$$f(x, y) = g(u(x, y), v(x, y))$$

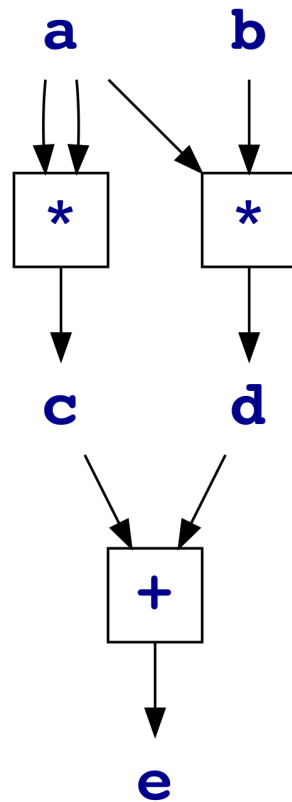
$$\begin{aligned} Df(x, y) &= D_0g(u(x, y), v(x, y)) \cdot Du(x, y) \\ &\quad + D_1g(u(x, y), v(x, y)) \cdot Dv(x, y) \end{aligned}$$

Arithmetic expressions

$(+ (* a a) (* a b))$

Arithmetic expressions

$(+ (* a a) (* a b))$



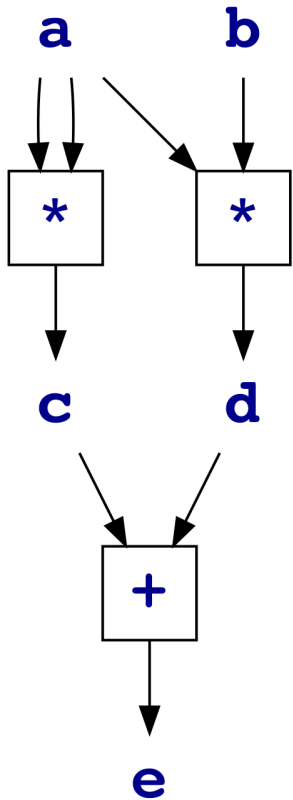
$c \leftarrow (* a a)$

$d \leftarrow (* a b)$

$e \leftarrow (+ c d)$

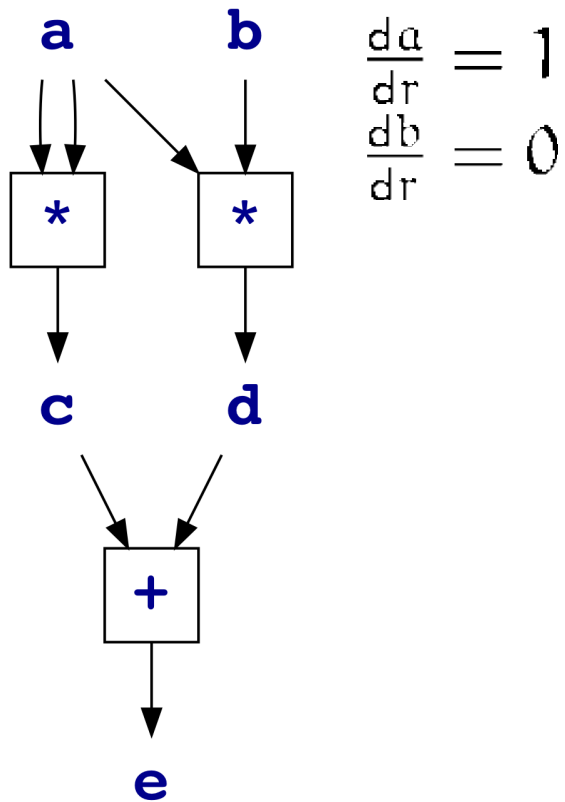
Automatic differentiation

Compute $Df(a, b)$



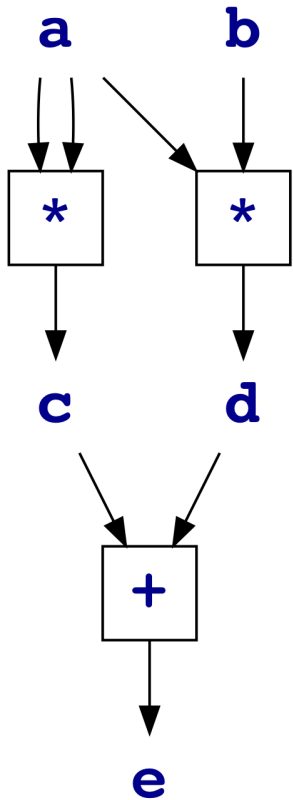
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Automatic differentiation

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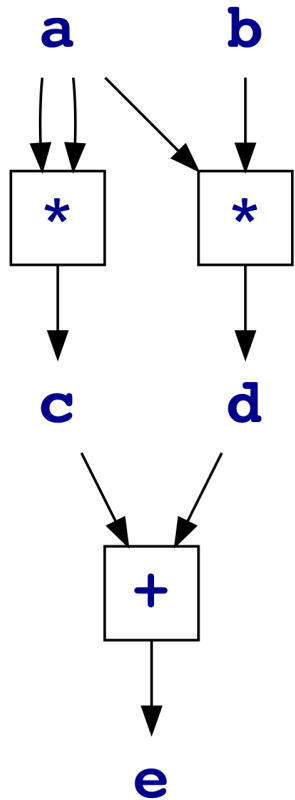
$$\frac{da}{dr} = 1$$

$$\frac{db}{dr} = 0$$

$$\frac{de}{dr} = D_0(*) (a, a) \frac{da}{dr} + D_1(*) (a, a) \frac{da}{dr}$$

Automatic differentiation

Compute $Df(a, b)$



$$\frac{da}{dr} = 1$$

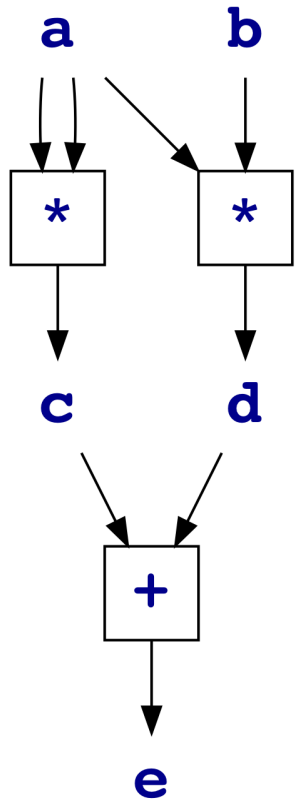
$$\frac{db}{dr} = 0$$

$$\frac{dc}{dr} = D_0(*) (a, a) \frac{da}{dr} + D_1(*) (a, a) \frac{da}{dr}$$

$$\frac{dd}{dr} = D_0(*) (a, b) \frac{da}{dr} + D_1(*) (a, b) \frac{db}{dr}$$

Automatic differentiation

Compute $Df(a, b)$



$$\frac{da}{dr} = 1$$

$$\frac{db}{dr} = 0$$

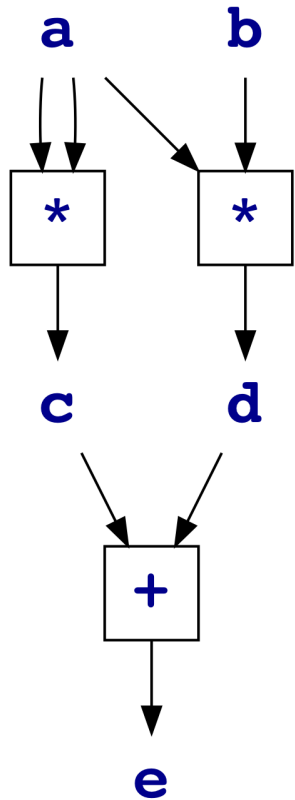
$$\frac{dc}{dr} = D_0(*) (a, a) \frac{da}{dr} + D_1(*) (a, a) \frac{da}{dr}$$

$$\frac{dd}{dr} = D_0(*) (a, b) \frac{da}{dr} + D_1(*) (a, b) \frac{db}{dr}$$

$$\frac{de}{dr} = D_0(+) (c, d) \frac{dc}{dr} + D_1(+) (c, d) \frac{dd}{dr}$$

Automatic differentiation

Compute $Df(a, b)$



$$\frac{da}{dr} = 1$$

$$\frac{db}{dr} = 0$$

$$\frac{dc}{dr} = D_0(*) (a, a) \frac{da}{dr} + D_1(*) (a, a) \frac{da}{dr}$$

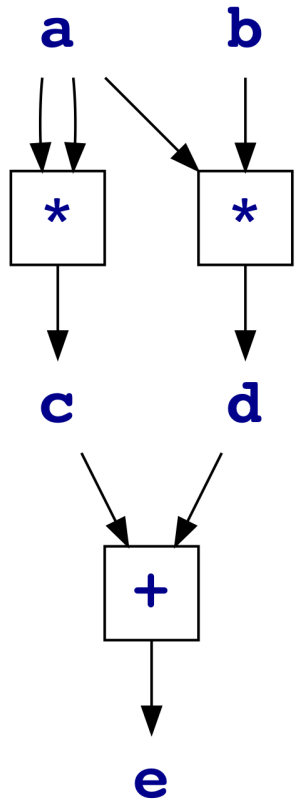
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$$\frac{de}{dr} = D_0(+) (c, d) \frac{dc}{dr} + D_1(+) (c, d) \frac{dd}{dr}$$

$$D_0 f(a, b) = \frac{de}{dr}$$

Automatic differentiation

Compute $Df(a, b)$



$$\begin{array}{l} \frac{da}{dr} = 1 \\ \frac{db}{dr} = 0 \end{array}$$

$$\frac{dc}{dr} = D_0(*) (a, a) \frac{da}{dr} + D_1(*) (a, a) \frac{da}{dr}$$

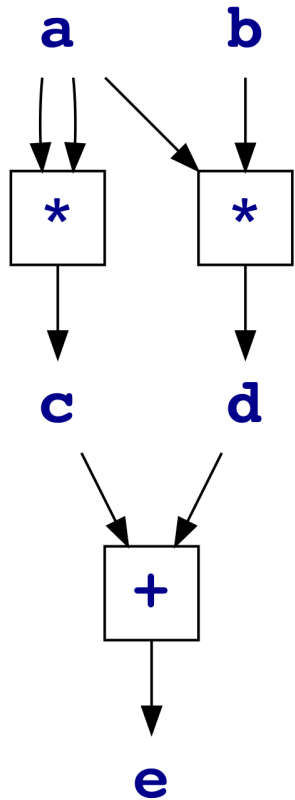
$$\frac{dd}{dr} = D_0(*) (a, b) \frac{da}{dr} + D_1(*) (a, b) \frac{db}{dr}$$

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$$D_0 f(a, b) = \frac{de}{dr}$$

Automatic differentiation

Compute $Df(a, b)$



$$\begin{array}{l} \frac{da}{dr} = 0 \\ \frac{db}{dr} = 1 \end{array}$$

$$\frac{dc}{dr} = D_0(*) (a, a) \frac{da}{dr} + D_1(*) (a, a) \frac{da}{dr}$$

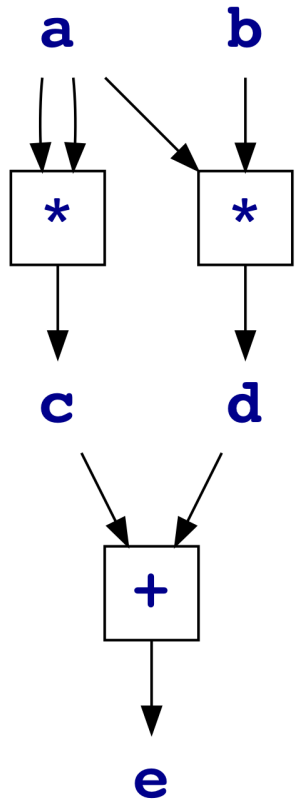
$$\frac{dd}{dr} = D_0(*) (a, b) \frac{da}{dr} + D_1(*) (a, b) \frac{db}{dr}$$

$$\frac{de}{dr} = D_0(+) (c, d) \frac{dc}{dr} + D_1(+) (c, d) \frac{dd}{dr}$$

$$D_1 f(a, b) = \frac{de}{dr}$$

Automatic differentiation

Compute $Df(a, b)$



$$\frac{da}{dr} = 0$$

$$\frac{db}{dr} = 1$$

$$\frac{dc}{dr} = D_0(*) (a, a) \frac{da}{dr} + D_1(*) (a, a) \frac{da}{dr}$$

$$\frac{dd}{dr} = D_0(*) (a, b) \frac{da}{dr} + D_1(*) (a, b) \frac{db}{dr}$$

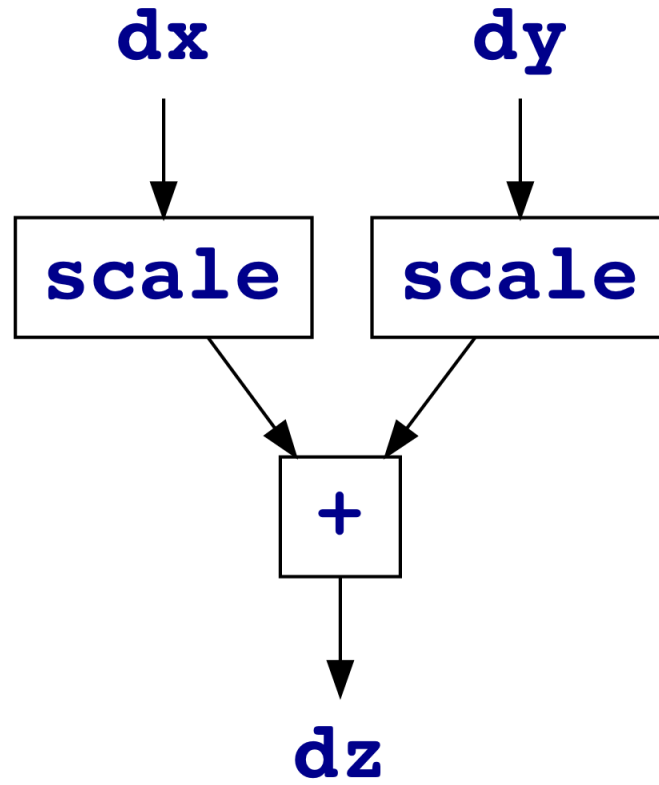
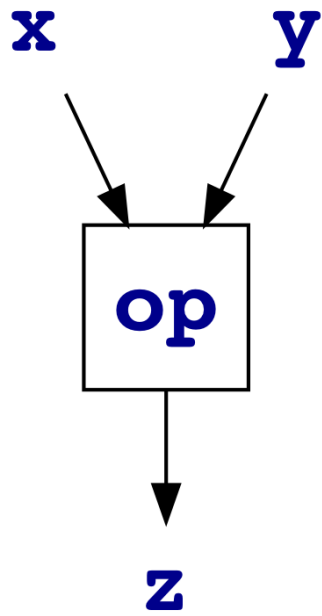
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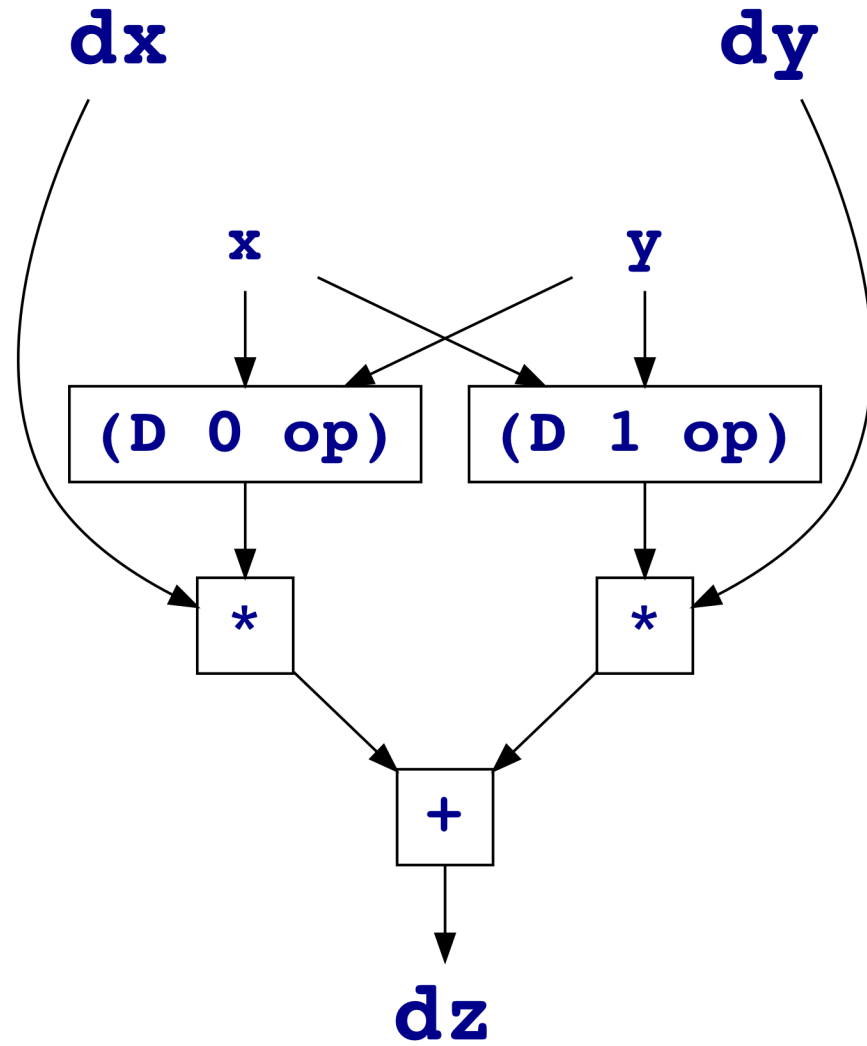
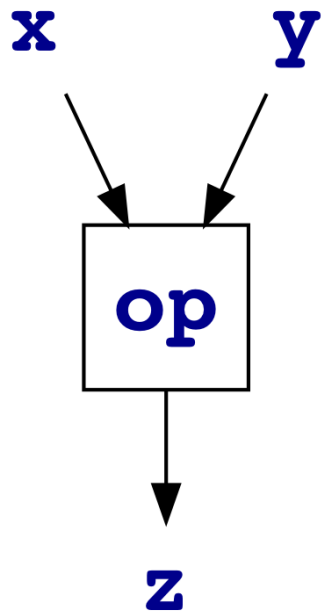
$$D_1 f(a, b) = \frac{de}{dr}$$

Forward mode

Will write **dx** instead of $\frac{dx}{dr}$

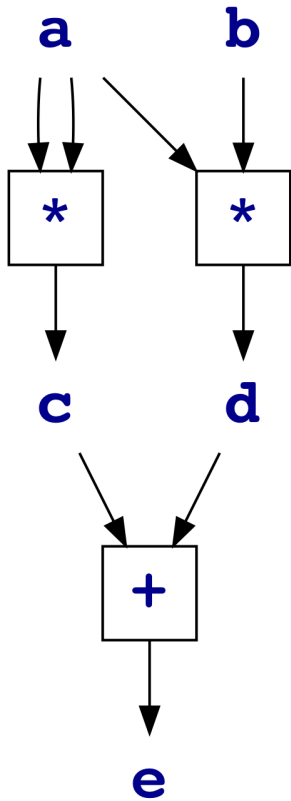
Known as *perturbation variables*





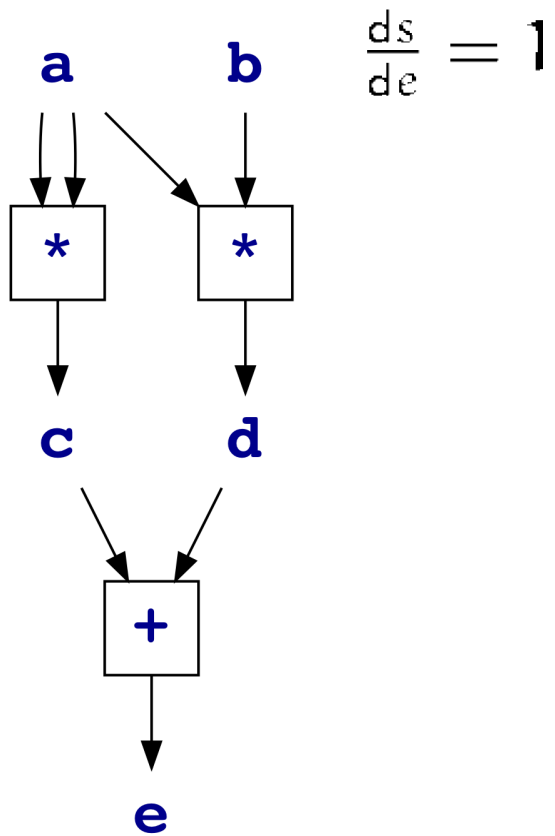
Automatic differentiation

Compute $Df(a, b)$



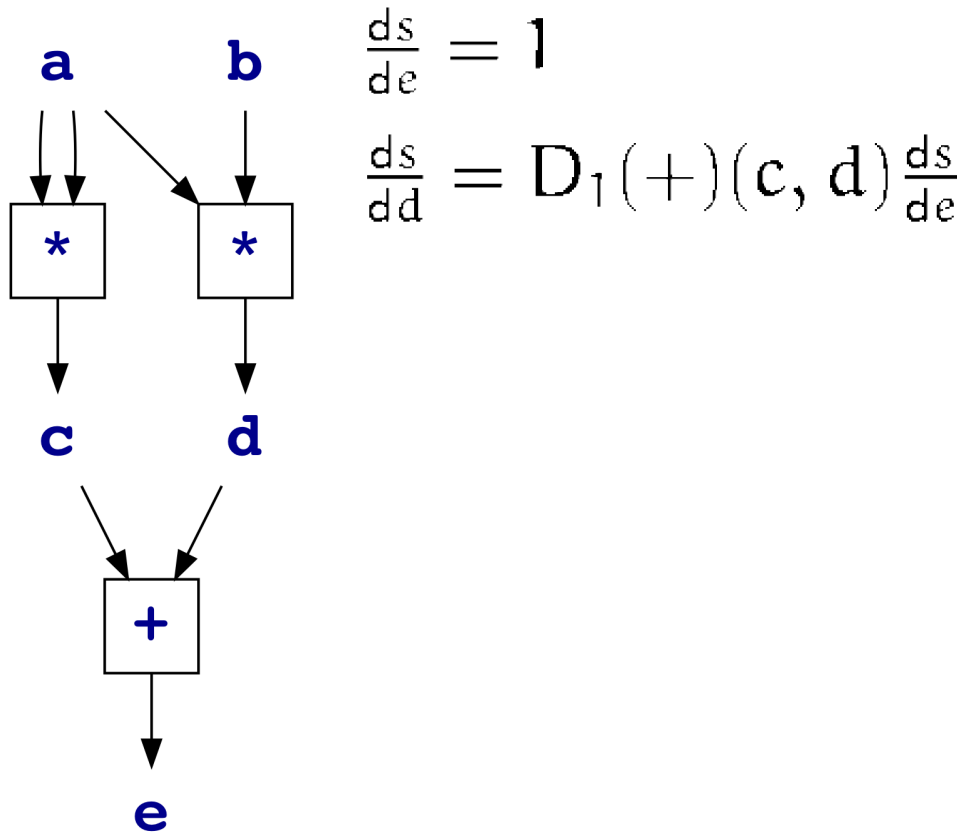
Automatic differentiation

Compute $Df(a, b)$



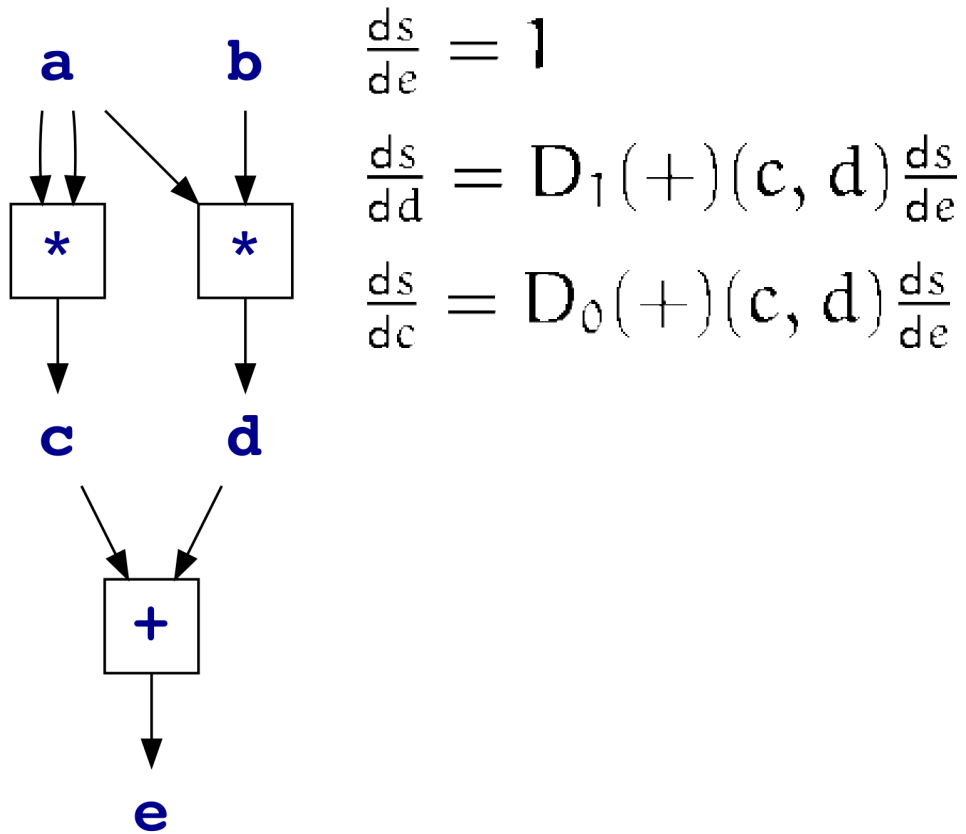
Automatic differentiation

Compute $Df(a, b)$



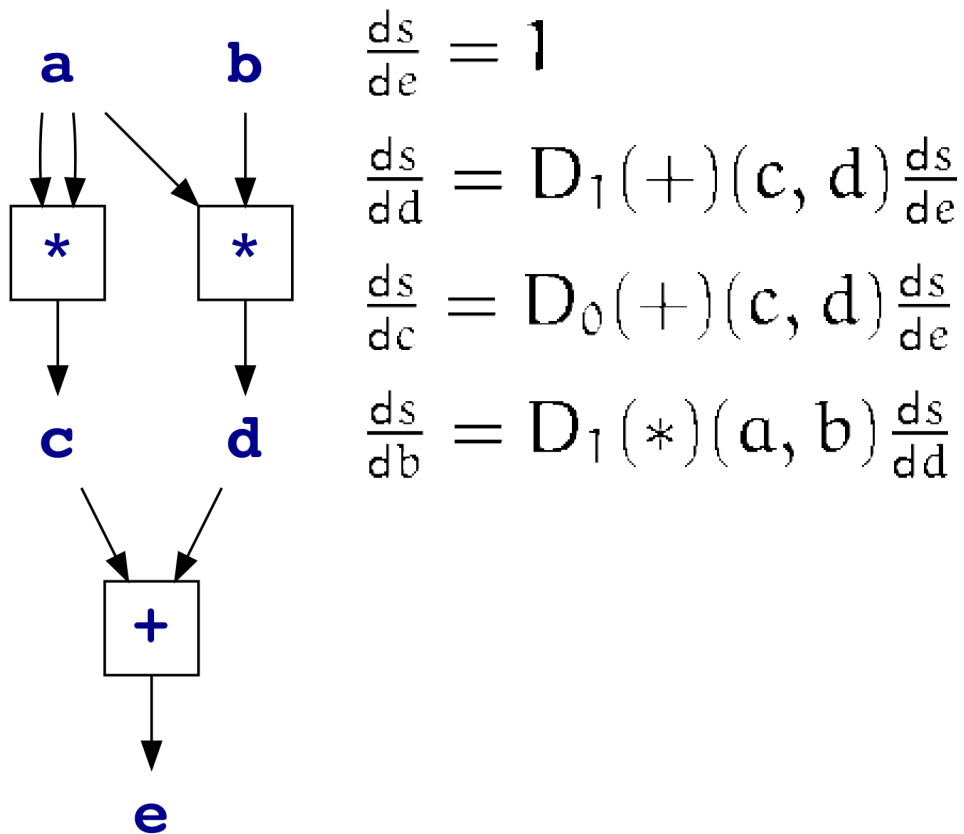
Automatic differentiation

Compute $Df(a, b)$



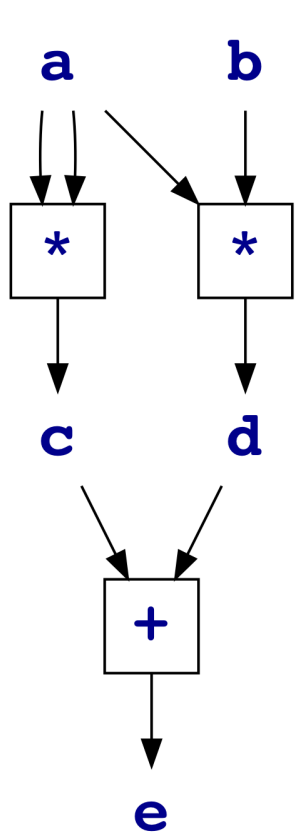
Automatic differentiation

Compute $Df(a, b)$



Automatic differentiation

Compute $Df(a, b)$



$$\frac{ds}{de} = 1$$

$$\frac{ds}{dd} = D_1(+)(c, d) \frac{ds}{de}$$

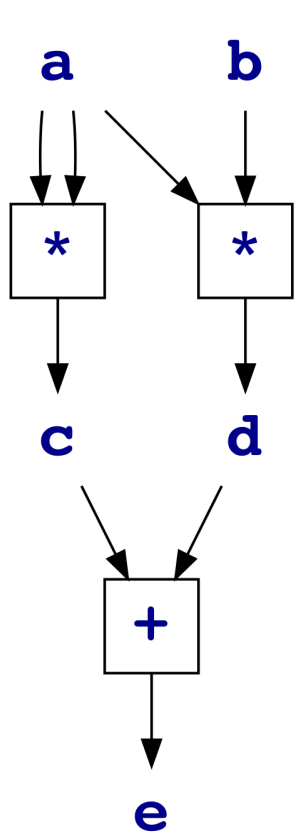
$$\frac{ds}{dc} = D_0(+)(c, d) \frac{ds}{de}$$

$$\frac{ds}{db} = D_1(*) (a, b) \frac{ds}{dd}$$

$$\begin{aligned} \frac{ds}{da} = & D_0(*) (a, a) \frac{ds}{dc} + D_1(*) (a, a) \frac{ds}{dc} \\ & + D_0(*) (a, b) \frac{ds}{dd} \end{aligned}$$

Automatic differentiation

Compute $Df(a, b)$



$$\frac{ds}{de} = 1$$

$$\frac{ds}{dd} = D_1(+)(c, d) \frac{ds}{de}$$

$$\frac{ds}{dc} = D_0(+)(c, d) \frac{ds}{de}$$

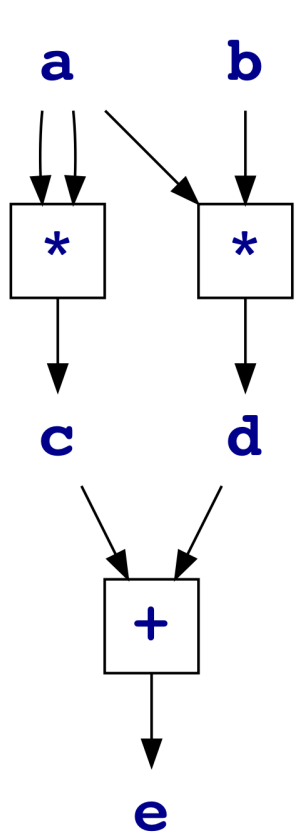
$$\frac{ds}{db} = D_1(*) (a, b) \frac{ds}{dd}$$

$$\begin{aligned} \frac{ds}{da} = & D_0(*) (a, a) \frac{ds}{dc} + D_1(*) (a, a) \frac{ds}{dc} \\ & + D_0(*) (a, b) \frac{ds}{dd} \end{aligned}$$

$$Df(a, b) = \left(\frac{ds}{da}, \frac{ds}{db} \right)$$

Automatic differentiation

Compute $Df(a, b)$



$$\frac{ds}{de} = 1$$

$$\frac{ds}{dd} = D_1(+)(c, d) \frac{ds}{de}$$

$$\frac{ds}{dc} = D_0(+)(c, d) \frac{ds}{de}$$

$$\frac{ds}{db} = D_1(*) (a, b) \frac{ds}{dd}$$

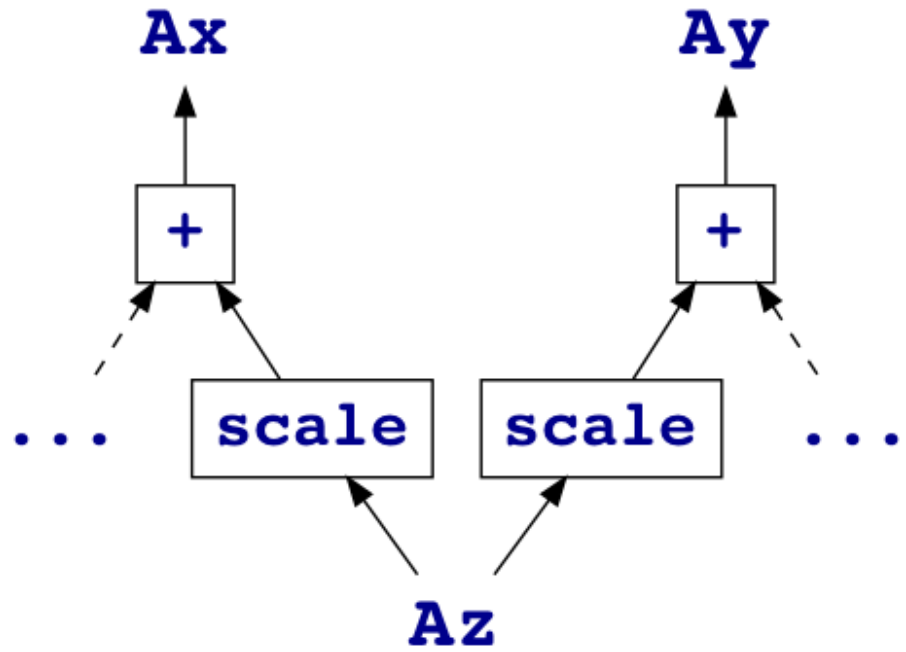
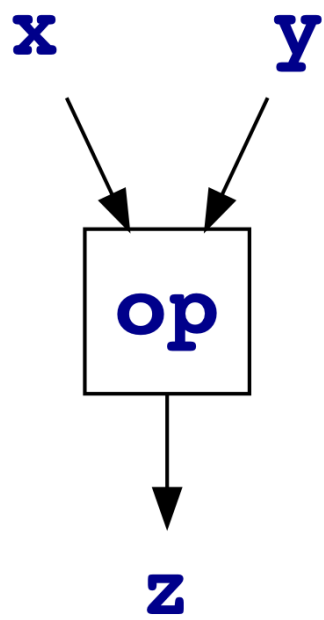
$$\begin{aligned} \frac{ds}{da} = & D_0(*) (a, a) \frac{ds}{dc} + D_1(*) (a, a) \frac{ds}{dc} \\ & + D_0(*) (a, b) \frac{ds}{dd} \end{aligned}$$

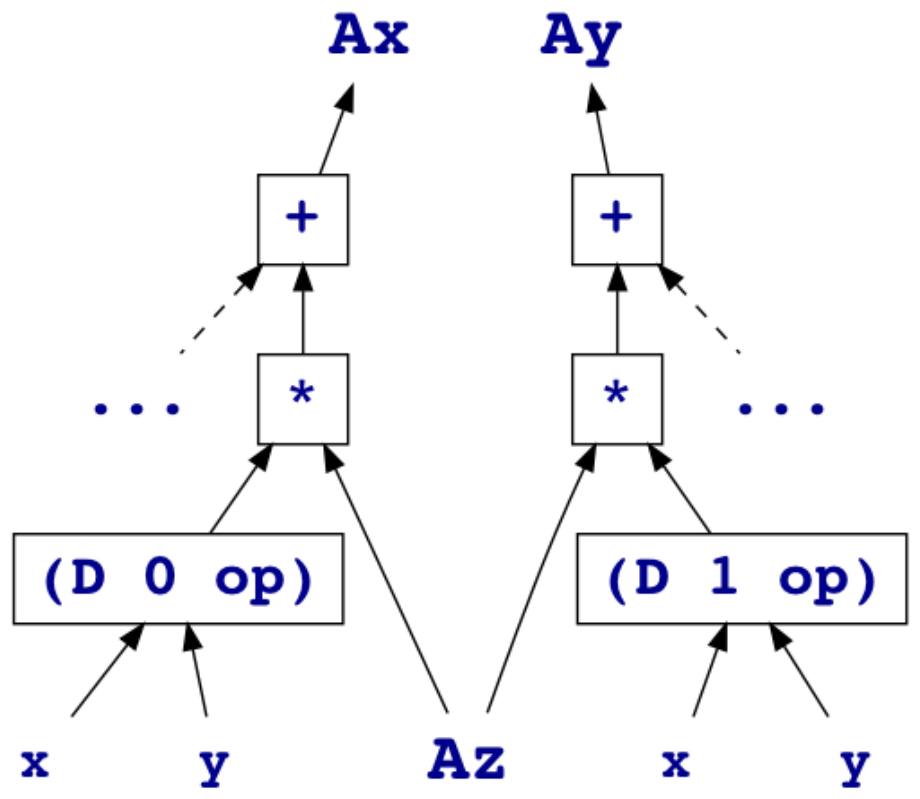
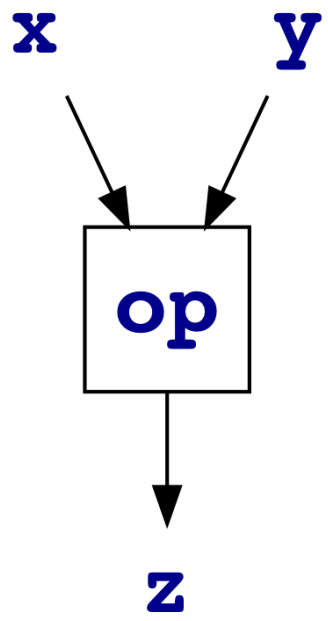
$$Df(a, b) = \left(\frac{ds}{da}, \frac{ds}{db} \right)$$

Reverse mode

Will write **λ** instead of $\frac{ds}{dx}$

Known as *sensitivity variables* or *adjoints*





We can now differentiate any *expression*
involving *primitive operations*

Idea: the return value of a function was determined from a particular (dynamic) call graph.

Differentiate *that*

Options:

- runtime trace
- static code transformation
- local transformations: dual numbers or continuations

Options:

- **runtime trace**
- static code transformation
- local transformations: dual numbers or continuations

Tracing program execution

We want a *flat* trace, which:
contains only *primitive operations*

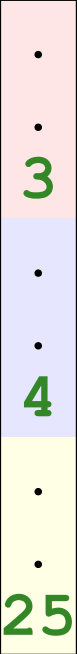
`(sum-squares x y)`

`=> (sum-squares 3 4)`

`=> 25`

(sum-squares x y)

=> (sum-squares  )

=> 

x

=> 3, as

t1		(constant 3)		3
----	--	--------------	--	---

y

=> 4, as

t2		(constant 4)		4
----	--	--------------	--	---

(sum-squares x y)

=> 25, as

t1		(constant 3)		3
t2		(constant 4)		4
t3		(app * t1 t1)		9
t4		(app * t2 t2)		16
t5		(app + t3 t4)		25

Let's make a little language that does this...

assignments

```
(struct assignment (id expr val))
```

assignments

```
(struct assignment (id expr val)
  #:guard (struct-guard/c symbol? expr? any/c))
```

assignments

```
(struct assignment (id expr val)
 #:guard (struct-guard/c symbol? expr? any/c))

(define (expr? e)
  (match e
    [(list 'constant _) #t]
    [(list 'app (? symbol? _) ..1) #t]
    [_ #f]))
```

trace

```
(struct trace (assignments))
```

trace

```
(struct trace (assignments))
```

```
(trace-add tr assgn)
```

```
(trace-append trs ...)
```

```
(trace-get tr id)
```

trace

```
(struct trace (assignments))
```

```
(trace-add tr assgn)
```

```
(trace-append trs ...)
```

```
(trace-get tr id)
```

top of a trace is the most recent assignment

```
(top tr)
```


trace

```
(struct trace (assignments))
```

```
(trace-add tr assgn)
```

```
(trace-append trs ...)
```

```
(trace-get tr id)
```

top of a trace is the most recent assignment

```
(top tr)
```

```
(top-val tr)
```

```
(top-id tr)
```

```
(top-expr tr)
```

trace-lang functions

```
(define (+& a b)
  (trace-add
    (trace-append a b)
    (make-assignment
      #:expr (list 'app '+ (top-id a) (top-id b))
      #:val (+ (top-val a) (top-val b))))))
```

trace-lang functions

```
(define (*& a b)
  (trace-add
   (trace-append a b)
   (make-assignment
    #:expr (list 'app '* (top-id a) (top-id b))
    #:val  (* (top-val a) (top-val b)))))
```

trace-lang functions

```
(define (exp& x)
  (trace-add
   x
   (make-assignment
    #:expr (list 'app 'exp (top-id x))
    #:val  (exp (top-val x)))))
```

```
(define (f a ...)  
  (trace-add  
    (trace-append a ...)  
    (make-assignment  
      #:expr (list 'app f-name (top-id a) ...)  
      #:val (let ([a (top-val a)] ...)   
              body ...))))
```

```
(define-syntax-rule
  (define-traced-primitive (f a ...) f-name
    body ...)
  (define (f a ...)
    (trace-add
     (trace-append a ...)
     (make-assignment
      #:expr (list 'app f-name (top-id a) ...)
      #:val (let ([a (top-val a)] ...)
              body ...))))))
```

```
(define-syntax-rule
  (define-traced-primitive (f a ...) f-name
    body ...)
  (define (f a ...)
    (trace-add
      (trace-append a ...)
      (make-assignment
        #:expr (list 'app f-name (top-id a) ...)
        #:val (let ([a (top-val a)] ...)
                 body ...))))))
```

trace-lang functions

```
(define-traced-primitive (+& a b) '+  
  (+ a b))  
(define-traced-primitive (*& a b) '*  
  (* a b))  
; ...  
(define-traced-primitive (<& a b) '<  
  (< a b))  
; ...  
(define-traced-primitive (cons& a b) 'cons  
  (cons a b))  
; ...
```



```
#lang racket
; ...
(provide (rename-out [+& +]
                    [*& *]
                    [exp& exp]
                    ...))
; ...
```

```
(define-syntax-rule (define& (f args ...)
                        body ...)
  (define (f args ...)
    (trace-append (let () body ...)
                  args ...)))
```

```
(define-syntax-rule (if& test-expr  
                    then-expr  
                    else-expr)  
  (if (top-val test-expr)  
      then-expr  
      else-expr))
```

```
#lang rackpropagator/trace  
; ...
```

(+ 1 2)

(+ 1 2)

```
; trace-items: contract violation  
; expected: trace?  
; given: 1
```

Interposition points

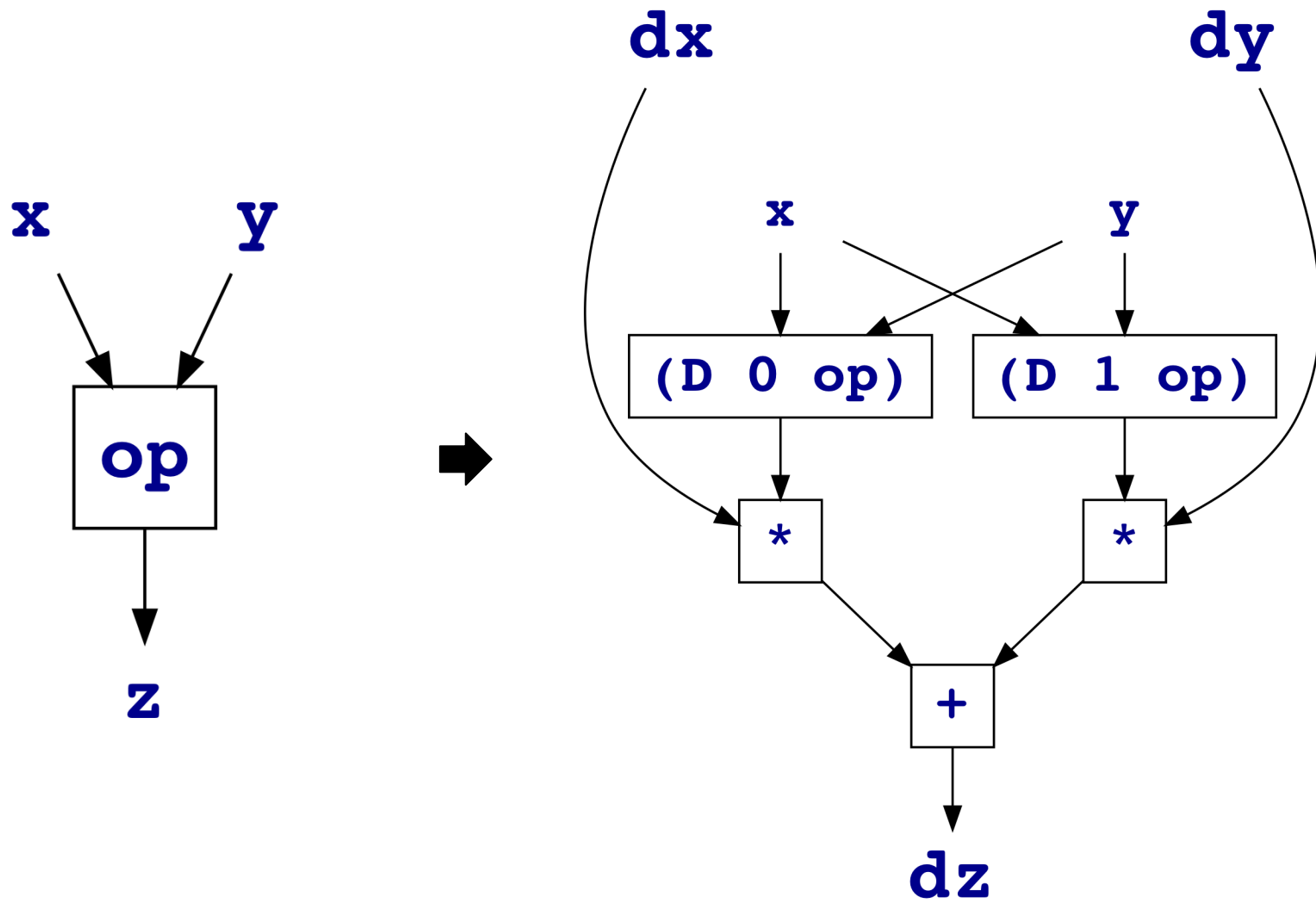
(+ 1 2)

=> (#%app + (#%datum . 1) (#%datum . 2))

```
(datum& . 1)
=> (make-trace (make-assignment #:val 1))

(provide (rename-out [datum& #%datum]))
```


Recap: Forward-mode AD



Forward-mode AD

```
(define ((partial/f i f) . xs)
  (let ([x      (top-id (list-ref xs i))]
        [indep-ids (map top-id xs)]
        [result  (apply f xs)])
    (define-values (Dresult _)
      (for/fold ([tr result]
                 [deriv-dict (hash)])
                ([z (reverse (trace-items result))])
                (let ([dz (d-prim-op z x indep-ids
                                     tr deriv-dict)])
                  {values
                    (trace-append dz tr)
                    (hash-set deriv-dict
                              (id z) (top-id dz))}))))))
```

Forward-mode AD

```
(define ((partial/f i f) . xs)
  (let ([x      (top-id (list-ref xs i))]
        [indep-ids (map top-id xs)]
        [result  (apply f xs)])
    (define-values (Dresult _)
      (for/fold ([tr result]
                 [deriv-dict (hash)])
                ([z (reverse (trace-items result))])
                (let ([dz (d-prim-op z x indep-ids
                                     tr deriv-dict)])
                  {values
                    (trace-append dz tr)
                    (hash-set deriv-dict
                              (id z) (top-id dz))}))))))
```

Forward-mode AD

```
(for/fold ([sum 0]
          [prod 1])
          ([x (range 1 6)])
          (values (+ x sum)
                  (* x prod)))
```

=>

15

120

Forward-mode AD

```
(define ((partial/f i f) . xs)
  (let ([x      (top-id (list-ref xs i))]
        [indep-ids (map top-id xs)]
        [result  (apply f xs)])
    (define-values (Dresult _)
      (for/fold ([tr result]
                 [deriv-dict (hash)])
                ([z (reverse (trace-items result))])
                (let ([dz (d-prim-op z x indep-ids
                                     tr deriv-dict)])
                  {values
                    (trace-append dz tr)
                    (hash-set deriv-dict
                              (id z) (top-id dz))}))))))
```

Forward-mode AD

```
(define ((partial/f i f) . xs)
  (let ([x      (top-id (list-ref xs i))]
        [indep-ids (map top-id xs)]
        [result  (apply f xs)])
    (define-values (Dresult _)
      (for/fold ([tr result]
                 [deriv-dict (hash)])
                ([z (reverse (trace-items result))])
                (let ([dz (d-prim-op z x indep-ids
                                     tr deriv-dict)])
                  {values
                    (trace-append dz tr)
                    (hash-set deriv-dict
                              (id z) (top-id dz))}))))))
```

Forward-mode AD

```
(define ((partial/f i f) . xs)
  (let ([x      (top-id (list-ref xs i))]
        [indep-ids (map top-id xs)]
        [result  (apply f xs)])
    (define-values (Dresult _)
      (for/fold ([tr result]
                 [deriv-dict (hash)])
                ([z (reverse (trace-items result))])
                (let ([dz (d-prim-op z x indep-ids
                                     tr deriv-dict)])
                  {values
                    (trace-append dz tr)
                    (hash-set deriv-dict
                              (id z) (top-id dz))}))))))
```

Forward-mode AD

```
(define ((partial/f i f) . xs)
  (let ([x      (top-id (list-ref xs i))]
        [indep-ids (map top-id xs)]
        [result  (apply f xs)])
    (define-values (Dresult _)
      (for/fold ([tr result]
                 [deriv-dict (hash)])
                ([z (reverse (trace-items result))])
                (let ([dz (d-prim-op z x indep-ids
                                     tr deriv-dict)])
                  {values
                    (trace-append dz tr)
                    (hash-set deriv-dict
                              (id z) (top-id dz))}))))))
```


Forward-mode AD

```
(define ((partial/f i f) . xs)
  (let ([x      (top-id (list-ref xs i))]
        [indep-ids (map top-id xs)]
        [result  (apply f xs)])
    (define-values (Dresult _)
      (for/fold ([tr result]
                 [deriv-dict (hash)])
                ([z (reverse (trace-items result))]
                 ([dz (d-prim-op z x indep-ids
                                tr deriv-dict))]
                 {values
                  (trace-append dz tr)
                  (hash-set deriv-dict
                            (id z) (top-id dz))}))))))
```

Forward-mode AD

```
(define ((partial/f i f) . xs)
  (let ([x      (top-id (list-ref xs i))]
        [indep-ids (map top-id xs)]
        [result  (apply f xs)])
    (define-values (Dresult _)
      (for/fold ([tr result]
                 [deriv-dict (hash)])
                ([z (reverse (trace-items result))])
                (let ([dz (d-prim-op z x indep-ids
                                     tr deriv-dict)])
                  {values
                    (trace-append dz tr)
                    (hash-set deriv-dict
                              (id z) (top-id dz))}))))))
```

Forward-mode AD

```
(define ((partial/f i f) . xs)
  (let ([x      (top-id (list-ref xs i))]
        [indep-ids (map top-id xs)]
        [result  (apply f xs)])
    (define-values (Dresult _)
      (for/fold ([tr result]
                 [deriv-dict (hash)])
                 ([z (reverse (trace-items result))])
                (let ([dz (d-prim-op z x indep-ids
                                     tr deriv-dict)])
                  {values
                    (trace-append dz tr)
                    (hash-set deriv-dict
                              (id z) (top-id dz))}))))))
```

Forward-mode AD

```
(define ((partial/f i f) . xs)
  (let ([x      (top-id (list-ref xs i))]
        [indep-ids (map top-id xs)]
        [result  (apply f xs)])
    (define-values (Dresult _)
      (for/fold ([tr result]
                 [deriv-dict (hash)])
                ([z (reverse (trace-items result))])
                (let ([dz (d-prim-op z x indep-ids
                                     tr deriv-dict)])
                  {values
                    (trace-append dz tr)
                    (hash-set deriv-dict
                              (id z) (top-id dz))}))))))
```

```
; d-prim-op: assignment? symbol? (Listof symbol?)
; trace? (HashTable symbol? symbol?) -> trace?
(define (d-prim-op z x-symb indep-ids
                tr deriv-dict)

; d : symbol? -> trace?
(define (d s)
  (trace-get tr (hash-ref deriv-dict s)))

(cond
  ; ...
  ))
```

```
; ...
(cond
  [(eq? (id z) x-symb) (datum& . 1.0)]
  [(memq (id z) indep-ids) (datum& . 0.0)]
  [else
   (match (expr z)
     ; ...
     )])])
```

```
; ...  
(match (expr z)  
  [(list 'constant null) (datum& . null)]  
  [(list 'constant c) (datum& . 0.0)]  
  ; ...  
)
```

```

; ...
(match (expr z)
  ; ...
  [(list 'app op xs ...)
   (let ([xs& (map (curry trace-get tr) xs)])
     (for/fold ([acc (datum& . 0.0)])
               ([x xs]
                [i (in-naturals)])
               (define D_i_op (apply (partial i op) xs&))
               (+& (*& D_i_op (d x)) acc))))])

```

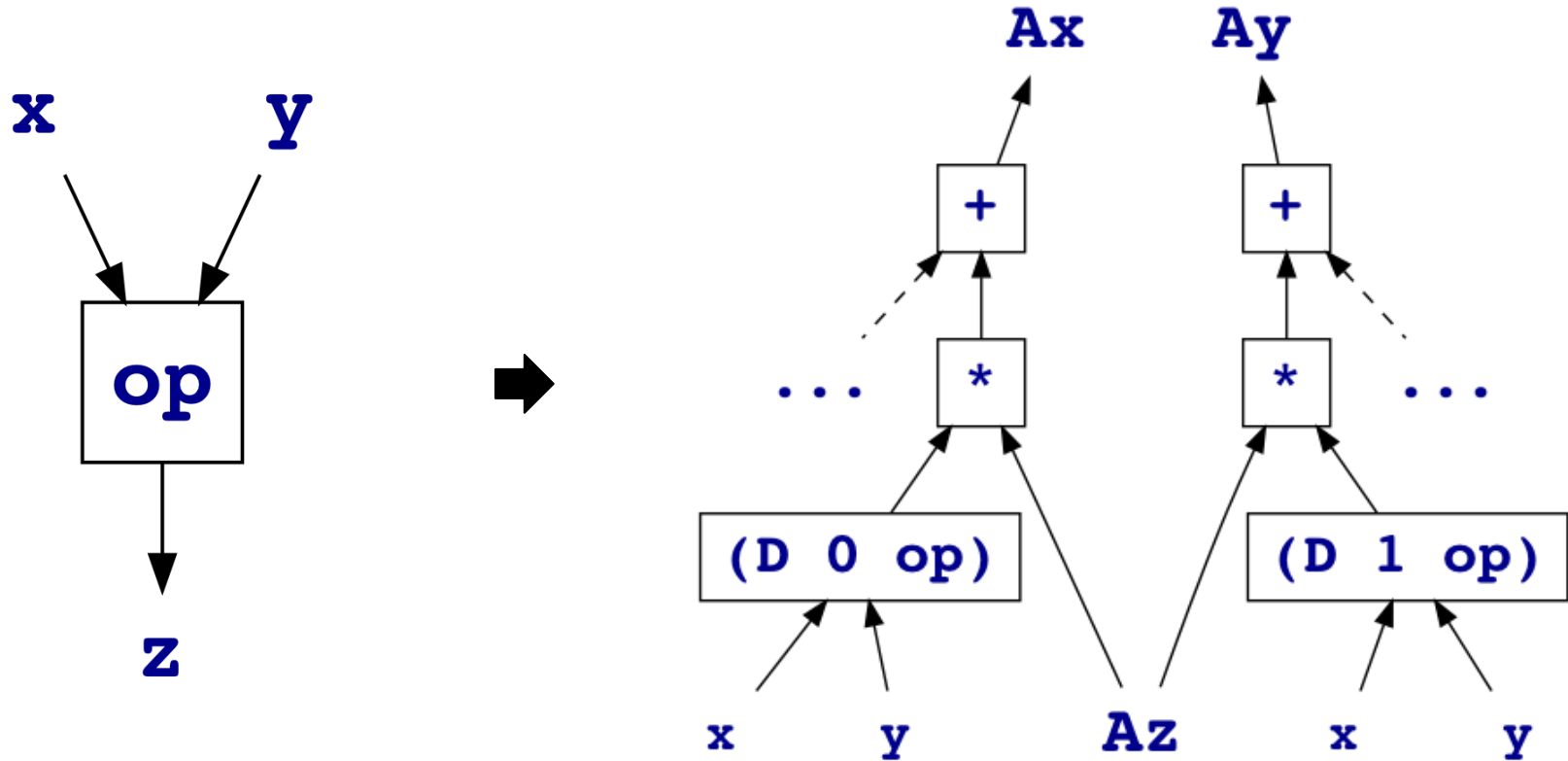

$$\begin{aligned} & ((D \text{ cons}) (f \ x) (g \ y)) \\ = & (\text{cons} ((D \ f) \ x) ((D \ g) \ y)) \end{aligned}$$

```
((D car) (cons (f x) (g y)))  
= ((D f) x)
```

```
((D cdr) (cons (f x) (g y)))  
= ((D g) y)
```

```
; ...
(match (expr z)
  ; ...
  [(list 'app 'cons x y) (cons& (d x) (d y))]
  [(list 'app 'car ls)   (car&   (d ls))]
  [(list 'app 'cdr ls)   (cdr&   (d ls))]
  ; ...
)
```

Recap: Reverse-mode AD



```

(define (A/r result-tr indep-ids s)
  (define seed-id (top-id result-tr))
  (define seed-tr (trace-append s result-tr))

  (define-values (tr _ adjoints)
    (for/fold ([tr seed-tr]
              [adjoint-terms
               (hash seed-id
                    (list (top-id seed-tr)))]
              [adjoints (hash)])
      ([w (trace-items result-tr)])

      ; ...
    ))
  ; ...
)

```

```

(define (A/r result-tr indep-ids s)
  (define seed-id (top-id result-tr))
  (define seed-tr (trace-append s result-tr))

  (define-values (tr _ adjoints)
    (for/fold ([tr seed-tr]
               [adjoint-terms
                (hash seed-id
                     (list (top-id seed-tr)))]
               [adjoints (hash)])
              ([w (trace-items result-tr)]
               ; ...
               ))
    ; ...
    )

```

```

(define (A/r result-tr indep-ids s)
  (define seed-id (top-id result-tr))
  (define seed-tr (trace-append s result-tr))

  (define-values (tr _ adjoints)
    (for/fold ([tr seed-tr]
              [adjoint-terms
               (hash seed-id
                    (list (top-id seed-tr)))]
              [adjoints (hash)])
      ([w (trace-items result-tr)])

      ; ...
    ))

  ; ...
)

```



```

(for/fold (...)
  ([w (trace-items result-tr)])
  (define Aw-terms
    (map (curry trace-get tr)
         (hash-ref adjoint-terms (id w))))
  (define Aw
    (trace-append
     (foldl cons-add (car Aw-terms) (cdr Aw-terms))
     tr))
  (define-values (tr* adjoint-terms*)
    (A-prim-op w Aw adjoint-terms))
  {values tr*
     adjoint-terms*
     (hash-set adjoints (id w) (top-id Aw))})

```

```

(for/fold (...)
  ([w (trace-items result-tr)])
  (define Aw-terms
    (map (curry trace-get tr)
      (hash-ref adjoint-terms (id w))))
  (define Aw
    (trace-append
      (foldl cons-add (car Aw-terms) (cdr Aw-terms))
      tr))
  (define-values (tr* adjoint-terms*)
    (A-prim-op w Aw adjoint-terms))
  {values tr*
    adjoint-terms*
    (hash-set adjoints (id w) (top-id Aw))})

```

```

(for/fold (...)
  ([w (trace-items result-tr)])
  (define Aw-terms
    (map (curry trace-get tr)
         (hash-ref adjoint-terms (id w))))
  (define Aw
    (trace-append
      (foldl cons-add (car Aw-terms) (cdr Aw-terms)
        tr))
    (define-values (tr* adjoint-terms*)
      (A-prim-op w Aw adjoint-terms))
    {values tr*
      adjoint-terms*
      (hash-set adjoints (id w) (top-id Aw))})

```

```
(cons-add '(1 2 (3) . 4)
          '(0 1 (2) . 3))
=> '(1 3 (5) . 7)
```

```
(cons-zero '(1 () (2) . 4))
=> '(0 () (0) . 0)
```

```

(for/fold (...)
  ([w (trace-items result-tr)])
  (define Aw-terms
    (map (curry trace-get tr)
         (hash-ref adjoint-terms (id w))))
  (define Aw
    (trace-append
     (foldl cons-add (car Aw-terms) (cdr Aw-terms))
     tr))
  (define-values (tr* adjoint-terms*)
   (A-prim-op w Aw adjoint-terms))
  {values tr*
    adjoint-terms*
    (hash-set adjoints (id w) (top-id Aw))})

```

```

(for/fold (...)
  ([w (trace-items result-tr)])
  (define Aw-terms
    (map (curry trace-get tr)
         (hash-ref adjoint-terms (id w))))
  (define Aw
    (trace-append
     (foldl cons-add (car Aw-terms) (cdr Aw-terms))
     tr))
  (define-values (tr* adjoint-terms*)
    (A-prim-op w Aw adjoint-terms))
  {values tr*
     adjoint-terms*
     (hash-set adjoints (id w) (top-id Aw))})

```

```

; ...
(let* ([tr* (trace-add
            tr
            (make-assignment #:val 0.0))]
       [zero-id (top-id tr*)])
  (trace-prune
   (apply
    list&
    (for/list ([x indep-ids])
      (trace-get
       tr*
       (hash-ref adjoints x zero-id))))))

```

w ← (cons **x** **y**)

⇒

Ax ← (car **Aw**)

Ay ← (cdr **Aw**)

=>

w ← **(car xs)**

(car Axs) ← **Aw**

$w \leftarrow (\text{cdr } xs)$

\Rightarrow

$(\text{cdr } Axs) \leftarrow Aw$

w ← (car **xs**)

⇒

Axs ← (cons **Aw** (cons-zero (cdr **xs**)))

`w ← (cdr xs)`

`=>`

`Axs ← (cons (cons-zero (car xs)) Aw)`

```

(define (A-prim-op w Aw adjoint-terms)

  (match (expr w)
    ; ...
    [(list 'app 'cons x y)
     (let ([Ax (car& Aw)]
           [Ay (cdr& Aw)])
       {values (trace-append Ay Ax Aw)
            (upd-adj adjoint-terms
                     x Ax
                     y Ay) })])
    ; ...
  ))

```

```

(define (A-prim-op w Aw adjoint-terms)

  (match (expr w)
    ; ...
    [(list 'app 'car xs)
     (let ([xs& (trace-get Aw xs)]
           [tr (cons& Aw (cons-zero (cdr& xs&)))]])
       {values (trace-append tr Aw)
          (upd-adj adjoint-terms xs tr)}})]
    ; ...
  ))

```

<http://github.com/ots22/rackpropagator>

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From automatic differentiation to message passing

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Matthew Butterick

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titles/content/sicm_edition_2/book.html](https://mitpress.mit.edu/sites/default/files/titles/content/sicm_edition_2/book.html)

Gerald Jay Sussman & Jack Wisdom (2015)

Program transformation

Can apply the previous work to straight-line code, at compile time

define instead of **assignment**

Program transformation

```
#lang rackpropagator/straightline
(define (f x y)
  (define a (+ x y))
  (define b (+ a a))
  (define c (* a y))
  (define d 1.0)
  (+ c d))

(define (Df x y)
  (define a (+ x y))
  (define t2 1.0)
  (define t3 1.0)
  (define t4 (* t2 t3))
  (define t7 (* t4 y))
  (define t8 (* t4 a))
  (define t9 1.0)
  (define t10 (* t7 t9))
  (define t11 1.0)
  (define t12 (* t7 t11))
  (define t17 (+ t8 t12))
  (define t19 '())
  (define t20 (cons t17 t19))
  (cons t10 t20))
```

Program transformation

```
(define-syntax (define/d stx)
  (syntax-case stx ()
    [ (_ (f args ...) body ...)
      (with-syntax
        ([ (body* ...)
           (handle-assignments #' (args ...)
                                #' (body ...)) ]])
        #' (define (f args ...)
              body* ...)) ]))
```


Program transformation

```
(define-syntax (define/d stx)
  (syntax-case stx ()
    [ (_ (f args ...) body ...)
      (with-syntax
        ([ (body* ...)
           (handle-assignments #' (args ...)
                                #' (body ...)) ])]
        #' (define (f args ...)
              body* ...))]))

(provide (rename-out [define/d define]))
```

Dual numbers

Dual numbers

sum-of-squares:

Given **a** and **b**

$$c \leftarrow (* \ a \ a)$$

$$d \leftarrow (* \ b \ b)$$

$$e \leftarrow (+ \ c \ d)$$

Dual numbers

sum-of-squares:

Given **a** and **b**

$$c \leftarrow (* \ a \ a)$$

$$d \leftarrow (* \ b \ b)$$

$$e \leftarrow (+ \ c \ d)$$

The "forward-mode" transformation:

$$dc \leftarrow (+ \ (* \ a \ da) \ (* \ da \ a))$$

$$dd \leftarrow (+ \ (* \ b \ db) \ (* \ db \ b))$$

$$de \leftarrow (+ \ dc \ dd)$$

Dual numbers

sum-of-squares:

Can interleave the operations computing x and dx

$$c \leftarrow (* a a)$$

$$dc \leftarrow (+ (* a da) (* da a))$$

$$d \leftarrow (* b b)$$

$$dd \leftarrow (+ (* b db) (* db b))$$

$$e \leftarrow (+ c d)$$

$$de \leftarrow (+ dc dd)$$

- dx depends on dy if and only if x depends on y
- dx depends on y only if x depends on y

Dual numbers

Idea: treat the pair of x and dx as a single entity. Define combined operations.

Dual numbers

```
(struct dual-number (p d))
```

Dual numbers

```
          (struct dual-number (p d))

(define (primal x)
  (cond
    [(dual-number? x) (dual-number-p x)]
    [(number? x) x]
    [else (raise-argument-error
            'primal "number? or dual-number?" x)]))
```


Dual numbers

```
          (struct dual-number (p d))  
  
(define (dual x)  
  (cond  
    [(dual-number? x) (dual-number-d x)]  
    [(number? x) (zero x)]  
    [else (raise-argument-error  
           'dual "number? or dual-number?" x)]))
```

Dual numbers

```
(define (dual-+ x y)
  (if (or (dual-number? x) (dual-number? y))
      (dual-number (+ (primal x) (primal y))
                    (+ (dual x) (dual y)))
      (+ x y)))
```

Dual numbers

```
(define (dual-+ x y)
  (if (or (dual-number? x) (dual-number? y))
      (dual-number (+ (primal x) (primal y))
                   (+ (dual x) (dual y)))
      (+ x y)))
```

Dual numbers

```
(define (dual-* x y)
  (if (or (dual-number? x) (dual-number? y))
      (dual-number (* (primal x) (primal y))
                    (+ (* (dual x) (primal y))
                       (* (primal x) (dual y))))
      (* x y)))
```

Dual numbers

```
(define (dual-* x y)
  (if (or (dual-number? x) (dual-number? y))
      (dual-number (* (primal x) (primal y))
                   (+ (* (dual x) (primal y))
                      (* (primal x) (dual y))))
      (* x y)))
```

Dual numbers

```
; ...  
(define (dual-log x)  
  (if (dual-number? x)  
      (dual-number (log (primal x))  
                    (/ (dual x) (primal x)))  
      (log x)))  
; ...
```

Dual numbers

- **only** need to define the primitive numerical functions
- Can be implemented with operator overloading
- A **local** program transformation

Dual numbers: Differentiation

```
(define ((D n f) . args)
  (let ([args* (for/list [(i (in-naturals))
                          (a args)]
                        (if (= i n)
                            (dual-number a 1)
                            (dual-number a 0)))])
    (get-dual-part (apply f args*))))
```


Dual numbers: Differentiation

```
(define ((D n f) . args)
  (let ([args* (for/list [(i (in-naturals))
                          (a args)]
                        (if (= i n)
                            (dual-number a 1)
                            (dual-number a 0)))])
    (get-dual-part (apply f args*))))
```

Dual numbers: Differentiation

```
(define ((D n f) . args)
  (let ([args* (for/list [(i (in-naturals))
                          (a args)]
                        (if (= i n)
                            (dual-number a 1)
                            (dual-number a 0)))])
    (get-dual-part (apply f args*))))
```

Dual numbers: Differentiation

```
(define ((D n f) . args)
  (let ([args* (for/list [(i (in-naturals))
                          (a args)]
                        (if (= i n)
                            (dual-number a 1)
                            (dual-number a 0)))])
    (get-dual-part (apply f args*))))
```

Dual numbers: Differentiation

```
(define ((D n f) . args)
  (let ([args* (for/list [(i (in-naturals))
                          (a args)]
                       (if (= i n)
                            (dual-number a 1)
                            (dual-number a 0)))])
    (get-dual-part (apply f args*)))))
```

Dual numbers: Differentiation

```
(define ((D n f) . args)
  (let ([args* (for/list [(i (in-naturals))
                          (a args)]
                       (if (= i n)
                           (dual-number a 1)
                           (dual-number a 0)))])
    (get-dual-part (apply f args*)))))
```

Helper function:

```
(get-dual-part
 (list (dual-number 0.0 1.0)
       2.0
       (cons (dual-number 3.0 0.0)
              (dual-number 4.0 5.0))))
=> (1.0 0.0 (0.0 . 5.0))
```