Lazy Multivariate Higher-Order Forward-Mode AD

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Wengert (1964)

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$$\mathcal{D}^{[i_1,\ldots,i_n]}\, f\, [c_1, \ldots, c_n] \quad \triangleq \quad \left.\frac{\partial^{i_1+\cdots+i_n} f(x_1, \ldots, x_n)}{\partial {x_1}^{i_1} \cdots \partial {x_n}^{i_n}}\right|_{x_1=c_1,\ldots,x_n=c_n}$$

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The Essence of Forward-Mode AD

Taylor expansion:

$$f(c+\varepsilon) = \frac{f(c)}{0!} + \frac{f'(c)}{1!}\varepsilon + \frac{f''(c)}{2!}\varepsilon^2 + \cdots + \frac{f^{(i)}(c)}{i!}\varepsilon^i + \cdots$$

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(Analogous to complex numbers $a + bi$ represented as $\langle a, b\rangle$.)

Arithmetic on Truncated Power Series (i.e. Dual Numbers)

$$(x_0 + x_1\varepsilon + \mathcal{O}(\varepsilon^2)) + (y_0 + y_1\varepsilon + \mathcal{O}(\varepsilon^2)) = (x_0 + y_0) + (x_1 + y_1)\varepsilon + \mathcal{O}(\varepsilon^2)$$

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$$\begin{aligned}(x_0 + x_1\varepsilon + \mathcal{O}(\varepsilon^2)) \times (y_0 + y_1\varepsilon + \mathcal{O}(\varepsilon^2))\\ = (x_0 \times y_0) + (x_0 \times y_1 + x_1 \times y_0)\varepsilon + \mathcal{O}(\varepsilon^2)\end{aligned}$$

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$$u\ (x_0 + x_1\varepsilon + \mathcal{O}(\varepsilon^2)) = (u\ x_0) + (x_1 \times (u'\ x_0))\varepsilon + \mathcal{O}(\varepsilon^2)$$

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\end{aligned}$$

Non-truncated is harder: Cannot ignore $\mathcal{O}(\varepsilon^2)$s.

Higher-Order Derivatives via Iteration

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Need mechanism to support arbitrary nesting of power series.

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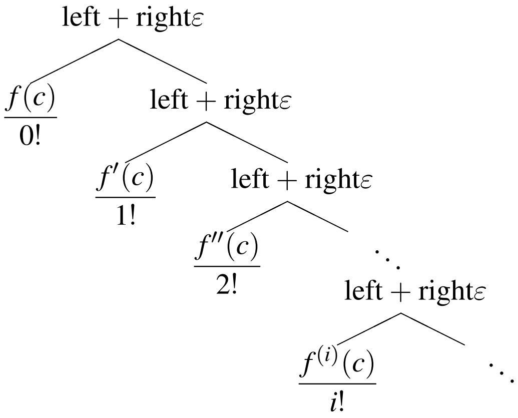
Can do a *nonstandard interpretation* of f over power series.

Bad news: The power series may be **infinite**.

Solution: Represent Power Series as Lazy Streams



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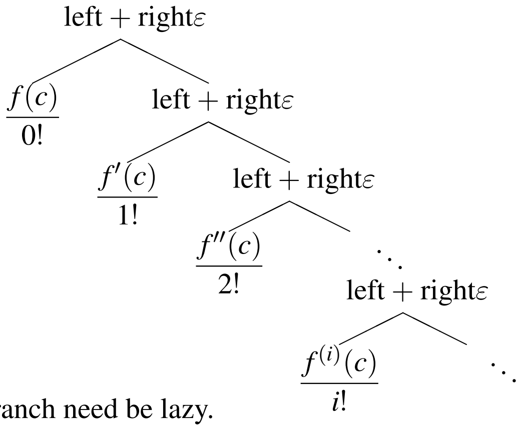

Only the right branch need be lazy.

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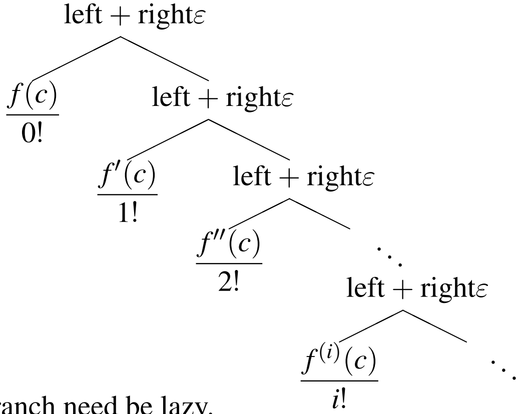

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API: $(\mathcal{Q}\ \varepsilon\ p)$ computes *quotient* of $\frac{p}{\varepsilon}$, analogous to forcing `cdr`.

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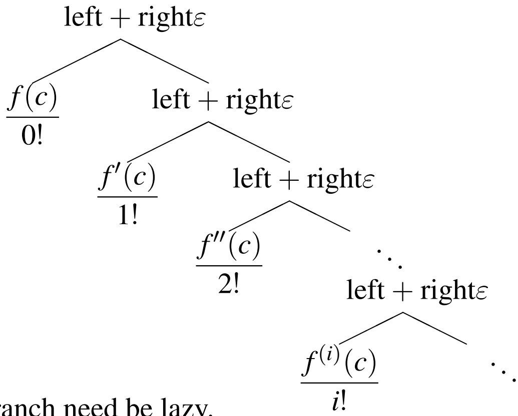

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API: $(\mathcal{Q}\ \varepsilon\ p)$ computes *quotient* of $\frac{p}{\varepsilon}$, analogous to forcing `cdr`.

$(\mathcal{R}\ \varepsilon\ p)$ computes *remainder* of $\frac{p}{\varepsilon}$, analogous to `car`.

Higher-Order Multivariate Derivatives

Multivariate Taylor expansion:

$$f((c_1+\varepsilon_1),\ldots,(c_n+\varepsilon_n)) =$$

$$\sum_{i_1=0}^{\infty}\cdots\sum_{i_n=0}^{\infty}\frac{1}{i_1!\cdots i_n!}\left.\frac{\partial^{i_1+\cdots+i_n}f(x_1,\ldots,x_n)}{\partial {x_1}^{i_1}\cdots\partial {x_n}^{i_n}}\right|_{x_1=c_1,\ldots,x_n=c_n}{\varepsilon_1}^{i_1}\cdots{\varepsilon_n}^{i_n}$$

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To compute $\mathcal{D}^{[i_1,\ldots,i_n]}\, f\ [c_1, \ldots, c_n]$:

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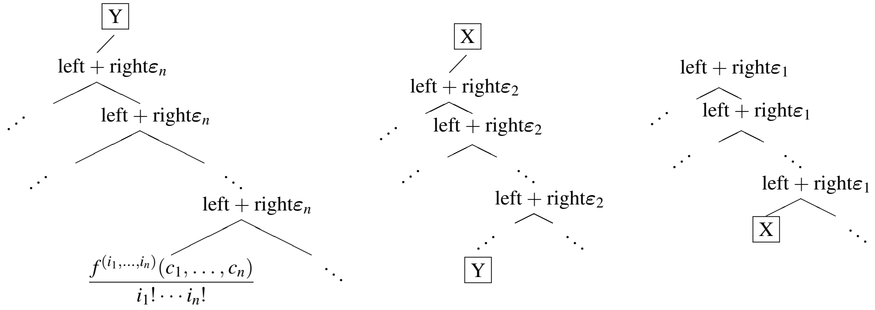
(and for each nested invocation of $\mathcal{D}$, **even in the univariate case**).

Multivariate Power Series as Nested Univariate Power Series



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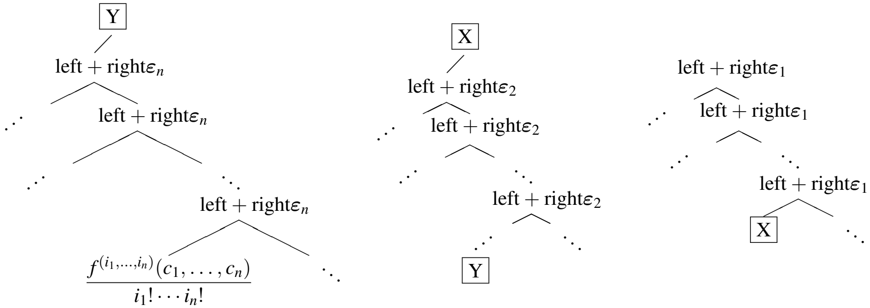

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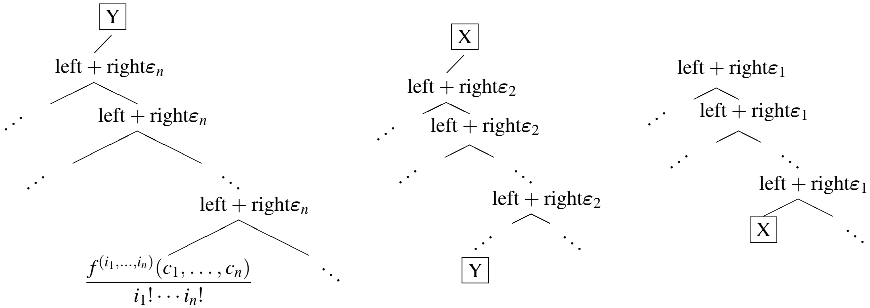

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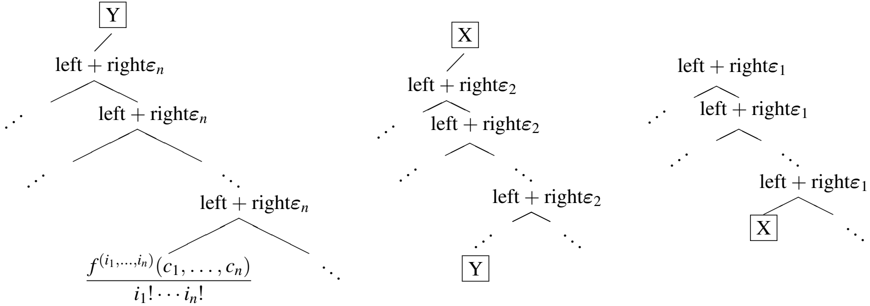

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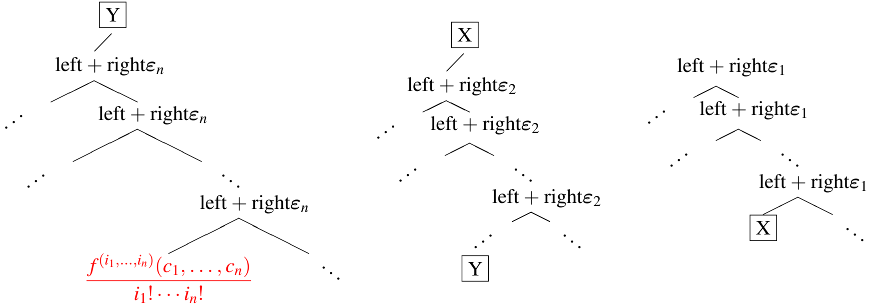

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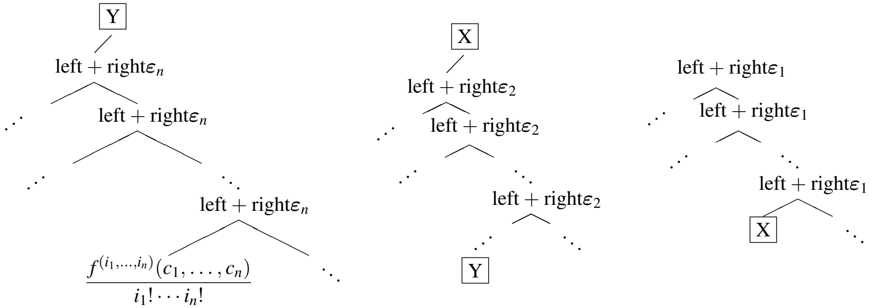

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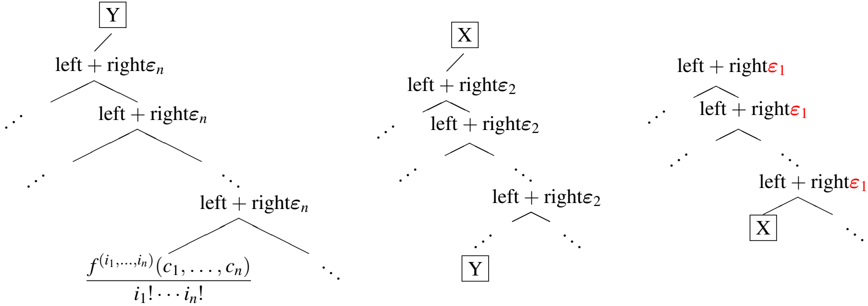

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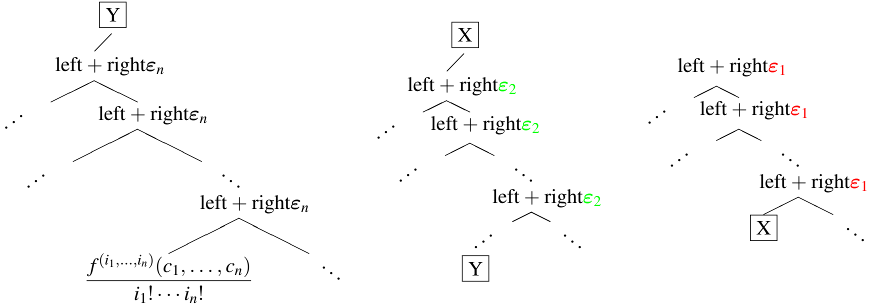

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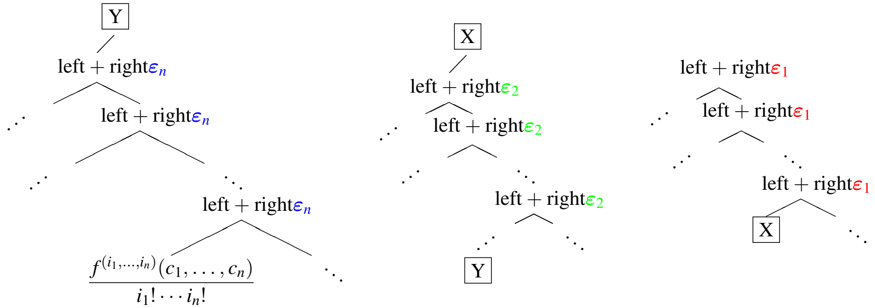

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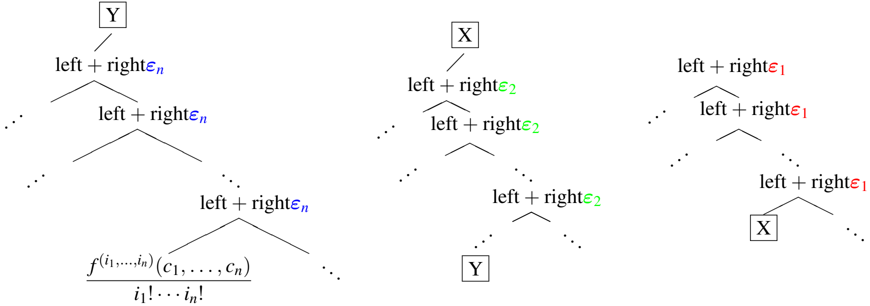

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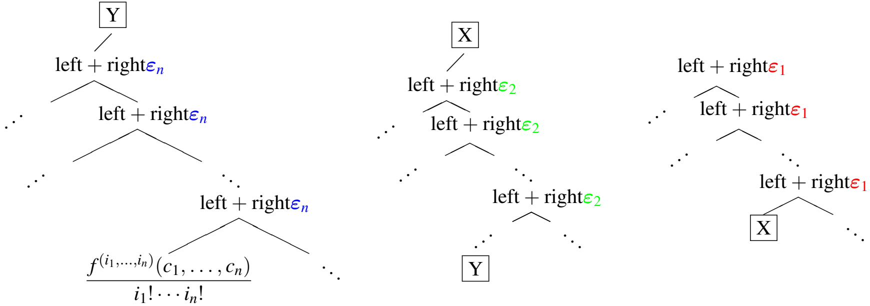

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Painfully ironic: Cannot *implement* $\mathcal{D}$ in a referentially transparent language even though $\mathcal{D}$ itself *is* referentially transparent!

Arithmetic on Non-Truncated Power Series

- Unary primitives:

$$u\ (x + x'\varepsilon) = (u\ x) + ((\mathcal{C}_{\varepsilon^0}\ (u'\ (x + x'\varepsilon)[\varepsilon \mapsto \xi]))[\xi \mapsto \varepsilon] \times x')\varepsilon$$

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- Read the paper for the details.

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- Many important numeric concepts are higher-order functions.
- For functional programming to interest numerical computing, it should provide useful numeric constructs.
- For instance: *exact efficient derivatives!*
- We have shown how to implement an unrestricted multivariate higher-order derivative operator using forward-mode AD.

Contingency Slides

Forward AD of Non-Scalar Functions

Discussed scalar functions for expository simplicity

- Can generalize higher-order scalar derivative

$$\mathcal{D} : \mathbb{N} \times (\mathbb{R} \to \mathbb{R}) \to (\mathbb{R} \to \mathbb{R})$$

  to higher-order vector directional derivative

$$\mathcal{J} : \mathbb{N} \times (\mathbb{R}^n \to \mathbb{R}^m) \to (\mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^m)$$

- using same mechanisms: find directional i-th derivative $\mathcal{J}\ i\ f\ \mathbf{c}\ \mathbf{c}'$ of $f : \mathbb{R}^n \to \mathbb{R}^m$ at $\mathbf{c} : \mathbb{R}^n$ in direction $\mathbf{c}' : \mathbb{R}^n$ by calculating

$$\mathbf{y} = f\ [c_1 + c_1'\varepsilon, \ldots, c_n + c_n'\varepsilon]$$

  and extracting

$$[y_1', \ldots, y_m'] = [\mathcal{C}_{\varepsilon^i}\ y_1, \ldots, \mathcal{C}_{\varepsilon^i}\ y_m]$$

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Two alternatives for representing

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- Tower of Derivatives (with factorials)

$$\begin{aligned}
&\langle x(0), \langle x'(0), \langle x''(0), \langle x'''(0), \ldots\rangle\rangle\rangle\rangle \\
&\quad = \langle 0! \times x_0, \langle 1! \times x_1, \langle 2! \times x_2, \langle 3! \times x_3, \ldots\rangle\rangle\rangle\rangle \\
&\quad\quad = \langle x_0, \langle x_1, \langle 2 \times x_2, \langle 6 \times x_3, \ldots\rangle\rangle\rangle\rangle
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- Identical in truncated case
- Fungible: trade off which "left shift" is fast,

$$\mathcal{Q}\ \varepsilon\ x(\varepsilon) = \frac{1}{\varepsilon}(x(\varepsilon) - x(0)) \qquad \text{or} \qquad \frac{\mathrm{d}}{\mathrm{d}\varepsilon}x(\varepsilon)$$

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(Oops)