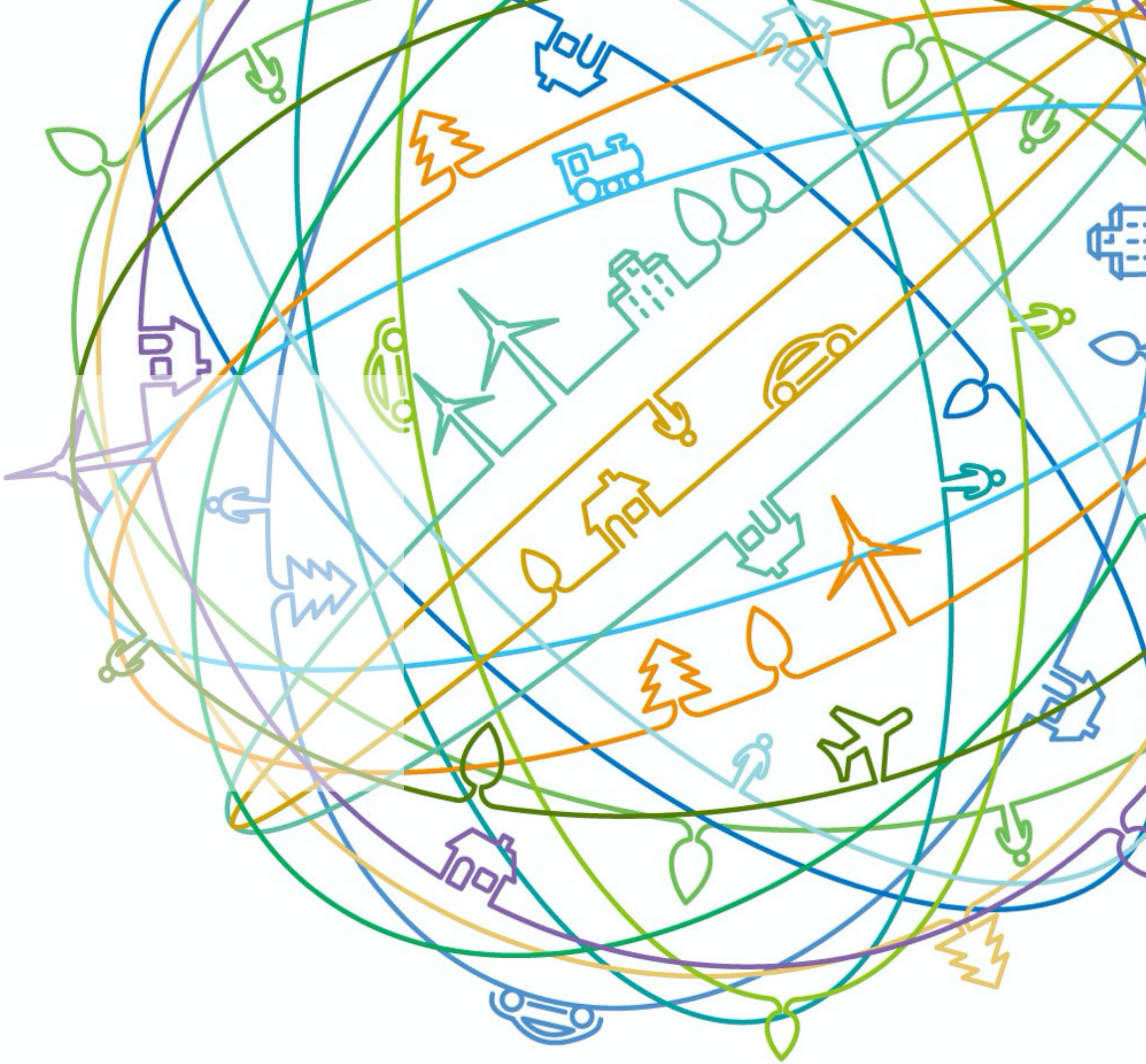
自动微分实现方式

ZOMI 酱



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关于本课程

1. 课程背景

- AI框架中自动微分的重要性

2. 课程内容

- 微分基本概念：数值微分 - 符号微分 - 自动微分
- 自动微分模式：前向微分 – 后向微分 – 雅克比原理
- 具体实现方式：表达式或图 – 操作符重载OO – 源码转换 AST
- MindSpore实现：基于图表示的源码转换Graph Base AST
- 自动微分的未来
- 自动微分的挑战

AD Implication Method

基本表达式法

LIB

- 封装基本的表达式及其微分表达式作为库函数
- 运行时记录基本表达式和相应的组合关系
- 链式法则对基本表达式的微分结果进行组合

操作符重载法

OO

- 利用语言多态特性，使用操作符重载基本运算表达式
- 运行时记录基本表达式和相应的组合关系
- 链式法则对基本表达式的微分结果进行组合

源码转换法

AST

- 语言预处理器、编译器或解释器的扩展
- 对程序表达进行分析得到基本表达式的组合关系
- 链式法则对基本表达式的微分结果进行组合

AD Implication Method

《Automatic Differentiation in Machine Learning: a Survey》

Table 5: Survey of AD implementations. Tools developed primarily for machine learning are highlighted in bold.

Language	Tool	Type	Mode	Institution / Project	Reference	URL
AMPL	AMPL	INT	F, R	Bell Laboratories	Fourer et al. (2002)	http://www.ampl.com/
C, C++	ADIC	ST	F, R	Argonne National Laboratory	Bischof et al. (1997)	http://www.mcs.anl.gov/research/projects/adic/
	ADOL-C	OO	F, R	Computational Infrastructure for Operations Research	Walther and Griewank (2012)	https://projects.coin-or.org/ADOL-C
C++	Ceres Solver	LIB	F	Google		http://ceres-solver.org/
	CppAD	OO	F, R	Computational Infrastructure for Operations Research	Bell and Burke (2008)	http://www.coin-or.org/CppAD/
	FADBAD++	OO	F, R	Technical University of Denmark	Bendtsen and Stauning (1996)	http://www.fadbad.com/fadbad.html
	Mxyzptlk	OO	F	Fermi National Accelerator Laboratory	Ostiguy and Michelotti (2007)	
C#	AutoDiff	LIB	R	George Mason Univ., Dept. of Computer Science	Shtof et al. (2013)	http://autodiff.codeplex.com/
F#, C#	**DiffSharp**	OO	F, R	Maynooth University, Microsoft Research Cambridge	Baydin et al. (2016a)	http://diffsharp.github.io
Fortran	ADIFOR	ST	F, R	Argonne National Laboratory	Bischof et al. (1996)	http://www.mcs.anl.gov/research/projects/adifor/
	NAGWare	COM	F, R	Numerical Algorithms Group	Naumann and Riehme (2005)	http://www.nag.co.uk/nagware/Research/ad_overview.asp
	TAMC	ST	R	Max Planck Institute for Meteorology	Giering and Kaminski (1998)	http://autodiff.com/tamc/
Fortran, C	COSY	INT	F	Michigan State Univ., Biomedical and Physical Sci.	Berz et al. (1996)	http://www.bt.pa.msu.edu/index_cosy.htm
	Tapenade	ST	F, R	INRIA Sophia-Antipolis	Hascoët and Pascual (2013)	http://www-sop.inria.fr/tropics/tapenade.html
Haskell	ad	OO	F, R	Haskell package		http://hackage.haskell.org/package/ad
Java	ADiJaC	ST	F, R	University Politehnica of Bucharest	Slusanschi and Dumitrel (2016)	http://adijac.cs.pub.ro
	Deriva	LIB	R	Java & Clojure library		https://github.com/lambder/Deriva
Julia	JuliaDiff	OO	F, R	Julia packages	Revels et al. (2016a)	http://www.juliadiff.org/
Lua	**torch-autograd**	OO	R	Twitter Cortex		https://github.com/twitter/torch-autograd
MATLAB	ADiMat	ST	F, R	Technical University of Darmstadt, Scientific Comp.	Willkomm and Vehreschild (2013)	http://adimat.sc.informatik.tu-darmstadt.de/
	INTLab	OO	F	Hamburg Univ. of Technology, Inst. for Reliable Comp.	Rump (1999)	http://www.ti3.tu-harburg.de/rump/intlab/
	TOMLAB/MAD	OO	F	Cranfield University & Tomlab Optimization Inc.	Forth (2006)	http://tomlab.biz/products/mad
Python	ad	OO	R	Python package		https://pypi.python.org/pypi/ad
	autograd	OO	F, R	Harvard Intelligent Probabilistic Systems Group	Maclaurin (2016)	https://github.com/HIPS/autograd
	Chainer	OO	R	Preferred Networks	Tokui et al. (2015)	https://chainer.org/
	PyTorch	OO	R	PyTorch core team	Paszke et al. (2017)	http://pytorch.org/
	Tangent	ST	F, R	Google Brain	van Merriënboer et al. (2017)	https://github.com/google/tangent
Scheme	R6RS-AD	OO	F, R	Purdue Univ., School of Electrical and Computer Eng.		https://github.com/qobi/R6RS-AD
	Scmutils	OO	F	MIT Computer Science and Artificial Intelligence Lab.	Sussman and Wisdom (2001)	http://groups.csail.mit.edu/mac/users/gjs/6946/refman.txt
	Stalingrad	COM	F, R	Purdue Univ., School of Electrical and Computer Eng.	Pearlmutter and Siskind (2008)	http://www.bcl.hamilton.ie/~qobi/stalingrad/

F: Forward, R: Reverse; COM: Compiler, INT: Interpreter, LIB: Library, OO: Operator overloading, ST: Source transformation

Library

实现以下表达式计算：

$$f(x,y,z) = (x+y)/z$$

手动将表达式函数分解为库函数中基本表达式组合：

$$a = x + y \qquad b = x/y$$

库函数中定义对应表达式的数学微分规则和链式法则：

$$da = dx + dy \qquad db = dx/y - dy * x/y^2$$

优点：

- 实现简单
- 任意编程语言

缺点：

- 使用库函数进行编程
- 无法使用原语言运算表达式

Library

```
def ADAdd(x, dx, y, dy, z, dz):
    z = x + y
    dz = dx + dy

def ADDiv(x, dx, y, dy, z, dz):
    z = x / y
    dz = dx / y + (x / (y * y)) * dy

>>> call ADAdd(x, dx, y, dy, a, da)
>>> call ADDiv(x, dx, y, dy, b, db)
```

$$a = x + y$$
$$da = dx + dy$$

$$\mathrm{b} = x/y$$
$$db = dx/y - dy * x/y^2$$

OO，Operator Overload

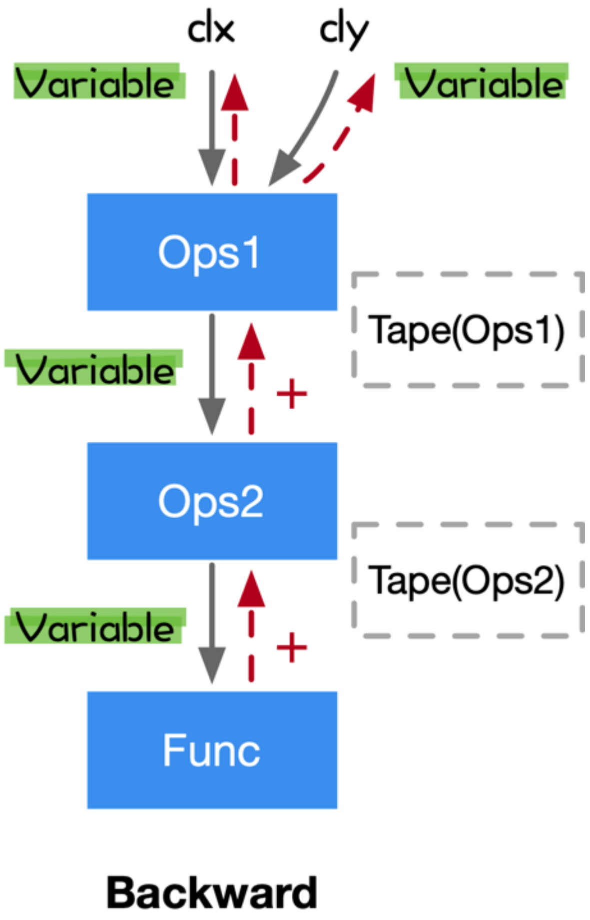
1. 利用语言的多态性，重载基本运算操作符
2. 将表达式操作类型和输入输出信息，记录到 Tape 中
3. 对 Tape 遍历，并对其中记录的基本运算操作进行微分
4. 把结果通过链式法则进行组合

优点：

- 实现简单
- 语言具备多态性
- 易用性高，贴合原生语言

缺点：

- 显式的构造 Tape 数据结构和对 Tape 进行读写
- 额外数据结构和操作的引入，不利于高阶微分
- if，while 等控制流表达式，通常难以通过操作符重载



OO , Operator Overload

①

```
class Variable:
    def __mul__(self, other):
        return ops_mul(self, other)
    def __add__(self, other):
        return ops_add(self, other)
```

②

```
def grad(l, results):
    for entry in reversed(gradient_tape):
        dl_doutputs = entry.outputs
        dl_dinputs = entry.propagate(dl_doutputs)
```

③

```
class Tape:
    inputs: List[str]
    outputs: List[str]
    propagate: d_inputs, d_ outputs
```

④

```
for input, dl_din in zip(entry.inputs, dl_dinputs):
    dl_d[input] += dl_ din
```

AST

1. 分析获得语言程序的 AST 表达形式（Parse）
2. 基于 AST 完成基本表达式的分解和微分操作（Infer）
3. 遍历 AST 得到基本表达式间的依赖关系
4. 应用链式法则组成完成自动微分

优点：

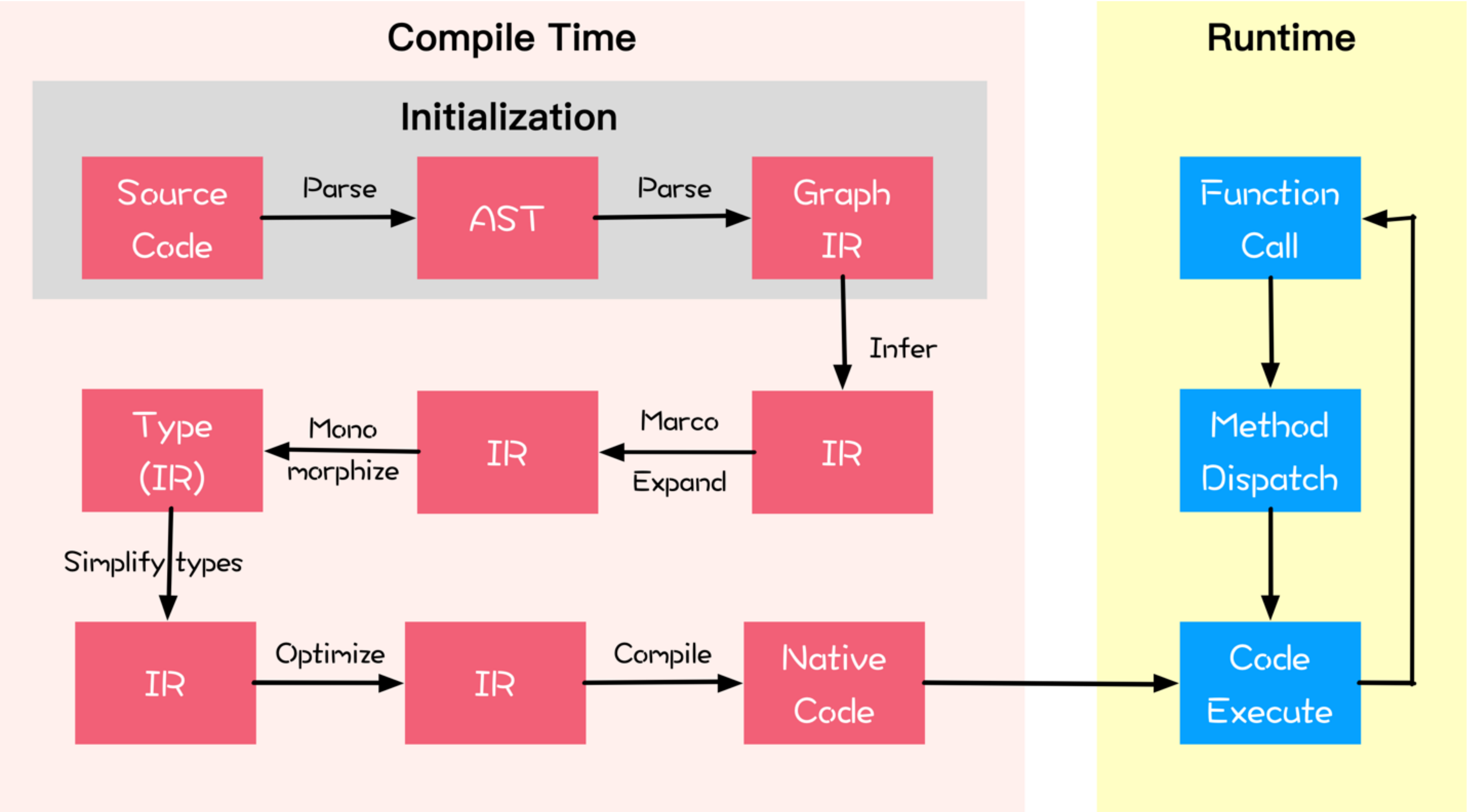
- 丰富数据类型和与语言原生操作
- 无额外Tape等数据结构，易于实现高阶微分
- 微分结果以代码的形式存在，方便分布式系统计算

缺点：

- 代码理解难，涉及更多计算机底层编译等原理
- 实现复杂度高，需要扩展语言的预处理器、编译器或解释器
- 容易写出不支持的代码导致错误，需要更强的检查告警系统

AST

- Parse
- Infer
- Monomorphism
- Optimize
- Compile
- Execute
- Function Call



Conclusion

1. 自动微分的实现方式可以分为三种：表达式或图、操作符重载和源码转换
2. 基于表达式实现主要依赖构建基础微分表达库，手动调用库
3. 基于操作符重载依赖于语言的多态性来记录实现
4. 基于源码转换核心在于AST完成基本表达式的分解和微分操作

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THANK YOU