Kotlin∇

A Shape Safe eDSL for Differentiable Functional Programming

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Overview

Differentiation

If we have a function, $P(x) : \mathbb{R} \to \mathbb{R}$, recall the derivative is defined as:

$$P'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} = \frac{\Delta y}{\Delta x} = \frac{dP}{dx} \tag{1}$$

For $P(x_0, x_1, \ldots, x_n) : \mathbb{R}^n \to \mathbb{R}$, the gradient is a vector of derivatives:

$$\nabla P = \left[\frac{\partial P}{\partial x_0}, \frac{\partial P}{\partial x_1}, \ldots, \frac{\partial P}{\partial x_n}\right] \text{ where } \frac{\partial P}{\partial x_i} = \frac{dP}{dx_i} \tag{2}$$

For $\mathbf{P}(\mathbf{x}) : \mathbb{R}^n \to \mathbb{R}^m$, the Jacobian is a vector of gradients:

$$\mathbf{J}_\mathbf{P} = [\nabla P_0, \nabla P_1, \ldots, \nabla P_n] \text{ or equivalently, } \mathbf{J}_{ij} = \frac{\partial P_i}{\partial x_j} \tag{3}$$

Type checking automatic differentiation

Suppose we have a scalar function $P_k : \mathbb{R} \to \mathbb{R}$ such that:

$$P_k(x) = \begin{cases} p_0(x) = x & \text{if } k = 0 \\ (p_k \circ P_{k-1})(x) & \text{if } k > 0 \end{cases}$$

From the chain rule of calculus, we know that:

$$\frac{dP}{dp_0} = \frac{dp_k}{dp_{k-1}} \frac{dp_{k-1}}{dp_{k-2}} \dots \frac{dp_1}{dp_0} = \prod_{i=1}^{k} \frac{dp_i}{dp_{i-1}}$$

For a vector function $\mathbf{P}_k(\mathbf{x}) : \mathbb{R}^n \to \mathbb{R}^m$, the chain rule still applies:

$$\mathbf{J_P} = \prod_{i=1}^{k} \mathbf{J}_{p_i} = \underbrace{\left(\left((\mathbf{J}_{p_k} \mathbf{J}_{p_{k-1}}) \dots \mathbf{J}_{p_2}\right) \mathbf{J}_{p_1}\right)}_{\textit{“Reverse accumulation”}} = \underbrace{\left(\mathbf{J}_{p_k} \left(\mathbf{J}_{p_{k-1}} \dots (\mathbf{J}_{p_2} \mathbf{J}_{p_1})\right)\right)}_{\textit{“Forward accumulation”}}$$

Parameter learning and gradient descent

For parametric models, let us rewrite $\mathbf{P}_k(\mathbf{x})$ as:

$$\hat{\mathbf{P}}_k(\mathbf{x}; \mathbf{\Theta} = [\boldsymbol{\theta}_0, \ldots, \boldsymbol{\theta}_k]) = \begin{cases} \mathbf{p}_0(\mathbf{x}; \boldsymbol{\theta}_0) & \text{if } k = 0 \\ \left(\mathbf{p}_k(\boldsymbol{\theta}_k) \circ \hat{\mathbf{P}}_{k-1}(\mathbf{\Theta})\right)(\mathbf{x}) & \text{if } k > 0 \end{cases}$$

Where $\mathbf{\Theta} \in \mathbb{R}^{\max(n,m) \times k}$ are free parameters and $\mathbf{x} \in \mathbb{R}^n$ is a single input. Assume we are given $\mathbf{Y} = [\mathbf{P}(\mathbf{x}^{(1)}), \ldots, \mathbf{P}(\mathbf{x}^{(z)})]$ from an oracle. In order to approximate $\mathbf{Y}$, repeat the following procedure until $\mathbf{\Theta}$ converges:

$$\mathbf{\Theta} \leftarrow \mathbf{\Theta} - \frac{1}{z} \nabla_{\mathbf{\Theta}} \sum_{i=0}^{z} \mathcal{L}\left(\hat{\mathbf{P}}_k(\mathbf{x}^{(i)}), \mathbf{P}(\mathbf{x}^{(i)})\right)$$

If $\hat{\mathbf{P}}_k$ were a program, what would the type signature of $\mathbf{p}_{0<i<k}$ be?

$$\mathbf{p}_i : \mathcal{T}_{out}(\mathbf{p}_{i-1}) \rightarrow \mathcal{T}_{in}(\mathbf{p}_{i+1})$$

Shape checking and inference

- Scalar functions implicitly represent shape as arity $f(1,2) : \mathbb{R}^2 \rightarrow \mathbb{R}$
- To check array programs, we need a type-level encoding of shape
- Arbitrary operations (e.g. convolution) may require dependent types
- But parametric polymorphism will suffice for most tensor functions
- For most algebraic operations, we just need to check for equality...

Math	Derivative	Code	Type Signature
$a(b)$	$\mathbf{J}_a\mathbf{J}_b$	`a(b)`	$(\mathtt{a} : \mathbb{R}^\tau \rightarrow \mathbb{R}^\pi, \mathtt{b} : \mathbb{R}^\lambda \rightarrow \mathbb{R}^\tau) \rightarrow (\mathbb{R}^\lambda \rightarrow \mathbb{R}^\pi)$

$a+b$	$\mathbf{J}_a + \mathbf{J}_b$	`a + b`
		`a.plus(b)`
		`plus(a, b)`
			$(\mathtt{a} : \mathbb{R}^\tau \rightarrow \mathbb{R}^\pi, \mathtt{b} : \mathbb{R}^\lambda \rightarrow \mathbb{R}^\pi) \rightarrow (\mathbb{R}^? \rightarrow \mathbb{R}^\pi)$

ab	$\mathbf{J}_a b + \mathbf{J}_b a$	`a * b`
		`a.times(b)`
		`times(a, b)`
			$(\mathtt{a} : \mathbb{R}^\tau \rightarrow \mathbb{R}^{m\times n}, \mathtt{b} : \mathbb{R}^\lambda \rightarrow \mathbb{R}^{n\times p}) \rightarrow (\mathbb{R}^? \rightarrow \mathbb{R}^{m\times p})$

a^b	$a^b(a'\frac{b}{a} + b'\ln a)$	`a.pow(b)` `pow(a, b)`	$(\mathtt{a} : \mathbb{R}^\tau \rightarrow \mathbb{R}, \mathtt{b} : \mathbb{R}^\lambda \rightarrow \mathbb{R}) \rightarrow (\mathbb{R}^? \rightarrow \mathbb{R})$

Numerical tower

- Abstract algebra can be useful when generalizing to new structures
- Helps us to easily translate between mathematics and source code
- Fields are a useful concept when computing over real numbers
  - A field is a set $\mathbb{F}$ with two operations $+$ and $\times$, with the properties:
    - Associativity: $\forall a, b, c \in \mathbb{F}, a + (b + c) = (a + b) + c$
    - Commutivity: $\forall a, b \in \mathbb{F}, a + b = b + a$ and $a \times b = b \times a$
    - Distributivity: $\forall a, b, c \in \mathbb{F}, a \times (b \times c) = (a \times b) \times c$
    - Identity: $\forall a \in \mathbb{F}, \exists 0, 1 \in F$ s.t. $a + 0 = a$ and $a \times 1 = a$
    - $+$ inverse: $\forall a \in \mathbb{F}, \exists(-a)$ s.t. $a + (-a) = 0$
    - $\times$ inverse: $\forall a \neq 0 \in \mathbb{F}, \exists(a^{-1})$ s.t. $a \times a^{-1} = 1$
- Extensible to other number systems (e.g. complex, dual numbers)
- What is a program, but a series of arithmetic operations?

Why Kotlin?

- Goal: To implement automatic differentiation in Kotlin
- Kotlin is a language with strong static typing and null safety
- Supports first-class functions, higher order functions and lambdas
- Has support for algebraic data types, via tuples sealed classes
- Extension functions, operator overloading other syntax sugar
- Offers features for embedding domain specific languages (DSLs)
- Access to all libraries and frameworks in the JVM ecosystem
- Multi-platform and cross-platform (JVM, Android, iOS, JS, native)

Kotlin∇ Priorities

- Type system
  - Strong type system based on algebraic principles
  - Leverage the compiler for static analysis
  - No implicit broadcasting or shape coercion
  - Parameterized numerical types and arbitary-precision
- Design principles
  - Functional programming and lazy numerical evaluation
  - Eager algebraic simplification of expression trees
  - Operator overloading and tapeless reverse mode AD
- Usage desiderata
  - Generalized AD with functional array programming
  - Automatic differentiation with infix and Polish notation
  - Partials and higher order derivatives and gradients
- Testing and validation
  - Numerical gradient checking and property-based testing
  - Performance benchmarks and thorough regression testing

Feature Comparison Matrix

Framework	**Language**	SD	AD	FP	TS	SS	DP	MP
Kotlin∇	Kotlin	✓	✓	✓	✓	✓	✍	✍
DiffSharp	F#	✗	✓	✓	✓	✗	✓	✗
TensorFlow.FSharp	F#	✗	✓	✓	✓	✓	✓	✗
Myia	Python	✓	✓	✓	✓	✓	✓	✗
Deeplearning.scala	Scala	✗	✓	✓	✓	✗	✓	✗
Nexus	Scala	✗	✓	✓	✓	✓	✓	✗
Lantern	Scala	✗	✓	✓	✓	✗	✓	✗
Grenade	Haskell	✗	✓	✓	✓	✓	✗	✗
Eclipse DL4J	Java	✗	✓	✗	✓	✗	✗	✗
Halide	C++	✗	✓	✗	✓	✗	✓	✗
Stalin	Scheme	✗	✓	✓	✗	✗	✗	✗

SD: Symbolic Differentiation, AD: Automatic Differentiation, FP: Functional Program, TS: Type Safe, SS: Shape Safe, DP: Differentiable Programming, MP: Multiplatform

How do we define algebraic types in Kotlin∇?

```
// T: Group<T> is effectively a self type
interface Group<T: Group<T>> {
    operator fun plus(f: T): T
    operator fun unaryMinus(): X
    operator fun minus(f: X): X = this + -f
    operator fun times(f: T): T
}

interface Field<X: Group<X>> {
  val e: X
  val one: X
  val zero: X
  operator fun div(f: X): X = this * f.pow(-one)
  infix fun pow(f: X): X
  fun ln(): X
}
```

Algebraic Data Types

```
class Var<X: Fun<X>>(label: String): Fun<X>()
class Const<X: Fun<X>>(val num: Number): Fun<X>()
class Sum<X: Fun<X>>(val f1: X, val f2: X): Fun<X>()
class Prod<X: Fun<X>>(val f1: X, val f2: X): Fun<X>()

sealed class Fun<X: Fun<X>>: Field<Fun<X>>{
  open fun diff(): Fun<X> = when(this) {
    is Const -> Zero
    is Sum -> f1.diff() + f2.diff()
    is Prod -> f1.diff() * f2 + f1 * f2.diff()
    is Var -> One
  }

  operator fun plus(f: Fun<X>) = Sum(this, f)
  operator fun times(f: Fun<X>) = Prod(this, f)
}
```

Expression simplification

```
operator fun times(exp: Fun<X>): Fun<X> = when {
  this is Const && num == 0.0 -> Const(0.0)
  this is Const && num == 1.0 -> exp
  exp is Const && exp.num == 0.0 -> exp
  exp is Const && exp.num == 1.0 -> this
  this is Const && exp is Const -> Const(num*exp.num)
  else -> Prod(this, e)
}

// Sum(Prod(Const(2.0), Var()), Const(6.0))
val q = Const(2.0) * Sum(Var(), Const(3.0))
```

Extension functions and contexts

```kotlin
object DoublePrecision {
  operator fun Number.times(f: Fun<KDouble>) =
    Const(toDouble()) * f
}

class KDouble(num: Double): Const<KDouble>(num) {
  override val e by lazy { KDouble(Math.E) }
  override val one by lazy { KDouble(1.0) }
  override val zero by lazy { KDouble(0.0) }
  // Adapters for wrapping primitive Double...
}

// Uses `*` operator in DoubleContext
fun Fun<KDouble>.multiplyByTwo() =
  with(DoublePrecision) { 2 * this }
```

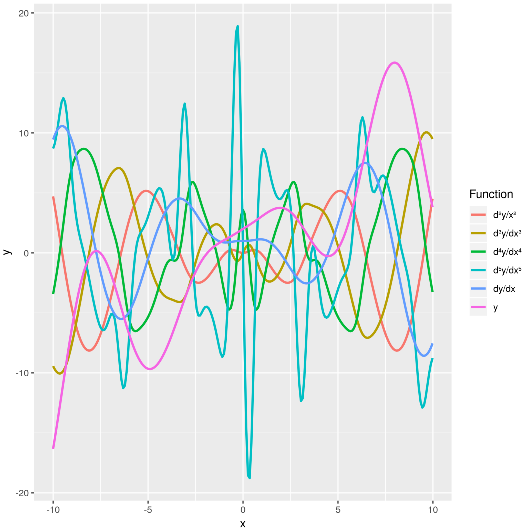
Automatic test case generation

```
val x = Var("x")
val y = Var("y")

val z = y * (sin(x * y) - x) // Function under test
val dz_dx = d(z) / d(x)      // Automatic derivative
val manualDx = y * (cos(x * y) * y - 1)

"dz/dx should be y * (cos(x * y) * y - 1)" {
  assertAll(DoubleGenerator) { cx, cy ->
    // Evaluate the results at a given seed
    val autoEval = dz_dx(x to cx, y to cy)
    val symbEval = manualDx(x to cx, y to cy)
    // Should pass if |adEval - manualEval| < eps
    autoEval shouldBeApproximately symbEval
  }
}
```

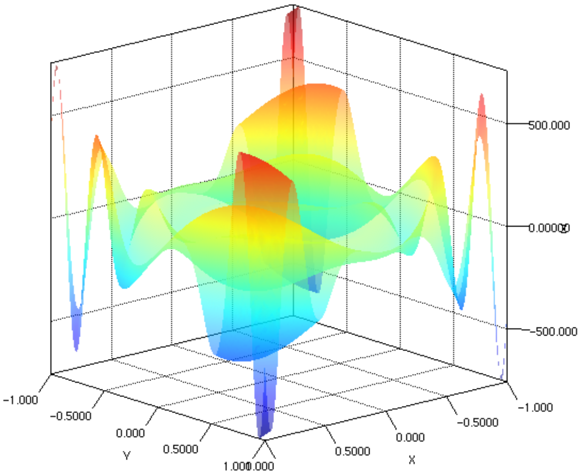
Usage: plotting higher derivatives of nested functions

```
with(DoublePrecision) {// Use double-precision
 val x = variable()  // Declare an immutable variable
 val y = sin(sin(sin(x)))/x + sin(x) * x + cos(x) + x

 // Lazily compute reverse-mode automatic derivatives
 val dy_dx = d(y) / d(x)
 val d2y_dx = d(dy_dx) / d(x)
 val d3y_dx = d(d2y_dx2) / d(x)
 val d4y_dx = d(d3y_dx3) / d(x)
 val d5y_dx = d(d4y_dx4) / d(x)

 plot(-10..10, dy_dx, dy2_dx, d3y_dx, d4y_dx, d5y_dx)
}
```

$$y = \frac{\sin\sin\sin x}{x} + x\sin x + \cos x + x,\ \frac{dy}{dx},\ \frac{d^2y}{dx^2},\ \frac{d^3y}{dx^3},\ \frac{d^4y}{dx^4},\ \frac{d^5y}{dx^5}$$



$z = \sin(10(x^2 + y^2))/10, \ \frac{\partial^3 z}{\partial^2 y \partial x}$



Further directions to explore

- Theory Directions
  - Generalization of types to higher order functions, vector spaces
  - Dependent types via code generation to type-check convolution
  - General programming operators and data structures
  - Imperative define-by-run array programming syntax
  - Program induction and synthesis, cf.
    - The Derivative of a Regular Type is its Type of One-Hole Contexts
    - The Differential Lambda Calculus (2003)
  - Asynchronous gradient descent (cf. HogWild, YellowFin, et al.)
- Implementation Details
  - Closer integration with Kotlin/Java standard library
  - Encode additional structure, i.e. function arity into type system
  - Vectorized optimizations for matrices with certain properties
  - Configurable forward and backward AD modes based on dimension
  - Automatic expression refactoring for numerical stability
  - Primitive type specialization, i.e. `FloatVector <: Vector<T>`?

Learn more at:

http://kg.ndan.co

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