# Fazang: A Reverse-mode Automatic differentiation tool in Fortran

User's Guide (Version 0.1.0)

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February 16, 2022

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## Introduction

Fazang is a reverse-mode automatic differentiation (AD) tool. The project is heavily influenced by Stan/Math [1], a project the author is also involved in. Fazang is intended to support general scientific computing in Fortran beyond Bayesian inference and Markov Chain Monte Carlo that Stan/Math is designed for.

User should be aware that the project is at early stage and still under development. For any questions, suggestions, and contributions, please visit the project at https://github.com/yizhang-yiz/fazang.

## **Quick Start**

Currently Fazang has been tested on Linux and MacOS platform, with Fortran compiler Intel Fortran 19.0.1+ and GNU Fortran 11.2.0+.

After downloading Fazang, user can use meson to build the library.

```
git clone git@github.com:yizhang-yiz/fazang.git
cd fazang && mkdir build && cd build
meson compile
```

This generates a shared library at build/src/. User needs to link this library when building an application. This can be done in meson by setting

```
executable('app_name', files('path/to/app_file.F90'), dependencies : fazang_dep)
```

Fazang provides a user-facing derived type var. This is the type for the dependent and independent variables of which the adjoint (derivative) will be calculated.

For example, consider the log of the Gaussian distribution density with mean  $\mu$  and standard deviation  $\sigma$ 

$$f(\mu, \sigma) = \log \left( \frac{1}{\sigma \sqrt{2\pi}} \exp \left( -\frac{1}{2} \left( \frac{y - \mu}{\sigma} \right)^2 \right) \right)$$
 (2.1)

The following programe calculates  $\frac{df}{d\mu}$  and  $\frac{df}{d\sigma}$  at  $y=1.3, \, \mu=0.5, \, \text{and} \, \sigma=1.2.$ 

```
program log_demo
    use fazang ! load Fazang library

implicit none

real(rk) :: y
    type(var) :: f, sigma, mu

! data
    y = 1.3d0

! independent variables
    mu = var(0.5d0)
    sigma = var(1.2d0)

! dependent
    f = var(-0.5d0 * log(2 * pi))
```

```
f = f - log(sigma)
f = f - 0.5d0 * ((y - mu) / sigma) ** 2.d0;

! use grad() to calculate df/d(mu) and df/d(sigma). Each var's
! derivative (also called adjoint) can be access through var%adj().

call f%grad()
write(*, *) "df/d(mu): ", mu%adj()
write(*, *) "df/d(sigma): ", sigma%adj()
end program log_demo
```

## Use Fazang

Fazang uses var type to record numerical and gradient operations. The type supports three functions

- var%val(): returns value
- var%adj(): returns derivative, henceforth referred as adjoint.
- var%grad(): takes gradient operation with respect to the current var variable.

#### 1. Constructors

var can be constructed using overloaded var interface.

## 2. Assignment

var can be assigned from consistent var and real(real64).

### 3. Gradient

Consider a variable z calculated by the composition of a series of operations

$$z = f_1(z_1), \quad z_1 = f_2(z_2), \quad \dots, \quad z_{n-1} = f_n(z_n).$$

For  $z_i, i = 1, ..., n$  we refer  $dz/dz_i$  as the adjoint of  $z_i$ , denoted by  $z_i^{\text{adj}}$ . The chain rule says the adjoints can be calculated recursively [2],

$$z^{\mathrm{adj}} = 1$$
,  $z_1^{\mathrm{adj}} = z^{\mathrm{adj}} \frac{df_1}{dz_1}$ , ...,  $z_i^{\mathrm{adj}} = z_{i-1}^{\mathrm{adj}} \frac{df_i}{dz_i}$ .

We often refer each  $(f_i, z_i)$  pair as a *node*, and  $z_i$  the *operand* of operation  $f_i$ . The above recursion through the nodes requires a way to store and visit the *callstack* of nodes. It is embodied in Fazang by the var%grad() function. When z%grad() is called, z's adjoint is

set to 1, and every other var variable is transversed with its adjoint updated. In order to calculate the adjoint with respect to another variable, user must call set\_zero\_all\_adj() first to reset all adjoints to zero.

An alternative to invoke gradient calculation is to define the dependent as a function and feed it to Fazang's gradient function. Take Eq.(2.1) for example, we can first define the function for  $f(\mu, \sigma)$ .

```
module func
  use fazang ! load Fazang library
  implicit none

real(rk), parameter :: y = 1.3d0

contains
  type(var) function f(x)
    type(var), intent(in) :: x(:)
    type(var) :: mu, sigma
    mu = x(1)
    sigma = x(2)
    f = -0.5d0 * log(2 * pi) - log(sigma) - 0.5d0 * ((y - mu) / sigma) ** 2.d0;
  end function f

end module func
```

Then we can supply function f as a procedure argument.

```
program log_demo2
    use iso_c_binding
    use fazang
    use func

implicit none

real(real64) :: fx(3), x(2)
    x = [0.5d0, 1.2d0]

fx = gradient(f, x)
    write(*, *) "f(x): ", fx(1)
    write(*, *) "df/d(x(1)): ", fx(2)
    write(*, *) "df/d(x(2)): ", fx(3)
    end program log_demo2
```

The output of gradient(f, x) is an array of size 1 + size(x), with first component being the function value, and the rest the partial derivatives.

Note that the above approach of using gradient function does not involve explicitly setting up var variables. Fazang achieves this by using a *nested* AD envionment.

#### 4. Nested AD envionment

Let us take a look of the internals of Fazang's gradient function. The dependent\_function interface requires f to follow the above example's signature, and x is the real64 array of

5. JACOBIAN

independent variables. We then create the var version of x and introduct it to f. The evaluation result is saved in f\_var variable. The adjoints are obtained by calling f\_var%grad(). Unlike what we have seen, the above process happens within a pairing begin\_nested() and end nested() calls.

```
function gradient(f, x) result (f_df)
  procedure(dependent_function) :: f
  real(real64), intent(in) :: x(:)
  real(real64) :: f_df(1 + size(x))
  type(var) :: x_var(size(x)), f_var

  call begin_nested()

  x_var = var(x)
  f_var = f(x_var)
  f_df(1) = f_var%val()
  call f_var%grad()
  f_df(2:(1+size(x))) = x_var%adj()

  call end_nested()
  end function gradient
```

When we use these two functions, all the var variables created in between are "temporary", in the sense that the values and adjoints of these variables are no longer available after call end\_nested(). User can use this function pair to construct a local gradient evaluation procedure.

## 5. Jacobian

Similar to gradient, using the same nested technique Fazang provides a jacobian function that calculates the Jacobian matrix of f, a multivariate function  $f: \mathbb{R}^m \to \mathbb{R}^n$  for an input array x of dimension m.

```
function jacobian(f, n, x) result (f_df)
```

The input function must follow the interface

```
abstract interface
  function jac_dependent_function (x, n) result (fx)
   import :: var
   integer, intent(in) :: n
   type(var), intent(in) :: x(:)
   type(var) :: fx(n)
  end function jac_dependent_function
end interface
```

where n is the output dimension. Like gradient, the output  $f_{df}$  has dimension  $n \times (m+1)$ , with the first column being the function results and the rest columns the adjoints.

#### 6. Functions

Numeric functions supported by Fazang are listed in Appendix A. All unary and binary functions are elemental. The binary functions allow mixed argument types, namely, either argument can be real64 type while the other the var type.

Probability distributions supported by Fazang are list in Appendix B.

## 7. Ordinary differential equations

Fazang supports ODE solutions through CVODES from SUNDIALS library [3]. One can solve ODE like this.

```
! user defined ODE
module ode_mod
 use fazang
 use, intrinsic :: iso_c_binding
 implicit none
 real(rk), parameter :: params(2) = [0.2d0, 0.1d0]
contains
 ! user defined right-hand-side
 subroutine eval_rhs(t, y, fy)
   real(c_double), intent(in) :: t, y(:)
   real(c_double), intent(inout) :: fy(size(y))
   fy(1) = y(2)
   fy(2) = t * y(1) * sum(params%val())
 end subroutine eval_rhs
end module ode_mod
program cvodes_solve_data
                               ! import ODE
 use ode mod
                               ! import Fazang
 use fazang
 implicit none
 real(rk) :: yt(2, 3) ! output array
 real(rk) :: y0(2)
                              ! initial condition
 type(cvodes_tol) :: tol
                              ! basic solver control
 ! use BDF method with given relative tolerance, absolute tolerance,
 ! and max number of steps between outputs
 tol = cvodes_tol(CV_BDF, 1.d-10, 1.d-10, 1000_8)
 ! initial condition
 y0 = [1.2d0, 1.8d0]
 ! solve the ODE with initial time O.dO and
 ! output time 1.d0, 2.d0, 3.d0
 yt = cvodes_sol(0.d0, y0, [1.d0, 2.d0, 3.d0], eval_rhs, tol)
end program cvodes_solve_data
```

In the above example, we first define an ODE following Fazang's interface on the RHS. The defined RHS function eval\_rhs will be later used as an argument to cvodes\_sol. In addition to initial condition, one must also define an object for solver control. Such an object must be of a type that extend the cvodes\_options abstract type. Here we use Fazang's basic type cvodes\_tol, which gives: the integration scheme (CV\_BDF for BDF method or CV\_ADAMS for Adams-Moulton method), relative tolerance, absolution tolerance, and the maximum number of steps allowed between output.

Then to the solver interface cvodes\_sol we give the initial time, initial condition, array for output time, the RHS subroutine, and the solver control. It returns a 2D array with each column at a requested output time.

7.1. Forward sensitivity. Combining the sensitivity capability of CVODES and AD from Fazang, we can solve for ODE sensitivity with respect to given parameters without explicitly supplying Jacobian. For that the user-defined ODE must include an additional RHS definition with var parameters, following Fazang's RHS interface.

```
module ode mod
 use fazang
 use, intrinsic :: iso_c_binding
 implicit none
 real(rk), parameter :: omega = 0.5d0
 real(rk), parameter :: d1 = 1.0d0
 real(rk), parameter :: d2 = 1.0d0
contains
  ! right-hand-side for data input
 subroutine eval_rhs(t, y, fy)
    implicit none
   real(c_double), intent(in) :: t, y(:)
   real(c_double), intent(inout) :: fy(size(y))
   fy(1) = y(2)
   fy(2) = sin(omega * d1 * d2 * t)
  end subroutine eval_rhs
  ! right-hand-side for var input with parameters
  ! y, p, and output fy must all be of var type
 subroutine eval_rhs_pvar(t, y, fy, p)
    implicit none
   real(c_double), intent(in) :: t
    type(var), intent(in) :: y(:), p(:)
    type(var), intent(inout) :: fy(size(y))
   fy(1) = y(2)
   fy(2) = sin(p(1) * p(2) * p(3) * t)
 end subroutine eval_rhs_pvar
end module ode_mod
```

Now we can solve the defined ODE in a similar way.

```
program cvodes_demo
 use ode_mod
 use fazang
 implicit none
 type(var) :: yt(2, 3)
 type(cvodes_tol) :: tol
 real(rk), parameter :: ts(3) = [1.2d0, 2.4d0, 4.8d0]
 real(rk), parameter :: y00(2) = [0.2d0, 0.8d0]
 type(var) :: param(3)
 real(rk) :: y0(2), ga(2)
 integer :: i, j
 v_0 = v_0
                                ! init condition
 param = var([omega, d1, d2]) ! parameters
 tol = cvodes_tol(CV_BDF, 1.d-10, 1.d-10, 1000_8)
 yt = cvodes_sol(0.d0, y0, ts, param, eval_rhs,&
       & eval_rhs_pvar, tol)
end program cvodes_demo
```

Note that now the call to cvodes\_sol includes additional argument param as the sensitivity parameters, as well as the RHS function for var inputs. The sensitivities are obtained the same way by calling grad and adj functions.

```
call yt(1, 1) % grad()
write(*, *) "dy_1/ d_omega at time ts(1):", param(1)%adj()
```

#### 7.2. Functions.

(1) Data solution

(2) Sensitivity solution with respect to the initial condition

```
class(cvodes_options), intent(in) :: cvs_options ! solver control
type(var) :: yt(size(y), size(ts)) ! solution
```

(3) Sensitivity solution with respect to the parameters

(4) Interfaces for different solvers

```
abstract interface
  subroutine cvs_rhs_func(t, y, fy)
    import c_double
    real(c_double), intent(in) :: t, y(:)
    real(c_double), intent(inout) :: fy(size(y))
  end subroutine cvs_rhs_func
  subroutine cvs_rhs_func_yvar(t, y, f)
    import c_double, var
    real(c_double), intent(in) :: t
    type(var), intent(in) :: y(:)
    type(var), intent(inout) :: f(size(y))
  end subroutine cvs_rhs_func_yvar
  subroutine cvs_rhs_func_pvar(t, y, f, p)
    import c_double, var
    real(c double), intent(in) :: t
    type(var), intent(in) :: y(:), p(:)
    type(var), intent(inout) :: f(size(y))
  end subroutine cvs_rhs_func_pvar
end interface
```

(5) Solver controls The last argument of the solver call is a solver control object. User-defined type must be able to follow CVODES user guide to modify CVODES memory object, by extending the abstract type cvodes\_options.

```
type, abstract :: cvodes_options
   integer :: cv_method = -1
   contains
    procedure(set_cvodes), deferred :: set
end type cvodes_options

abstract interface
```

```
subroutine set_cvodes(this, mem)
  import c_ptr, cvodes_options
  class(cvodes_options), intent(in) :: this
  type(c_ptr), intent(inout) :: mem ! CVODES memory
  end subroutine set_cvodes
end interface
```

One can follow Fazang's tolerance control type as an example.

```
type, extends(cvodes_options) :: cvodes_tol
    real(c_double) :: rtol, atol
    integer(c_long) :: max_nstep
contains
    procedure :: set
end type cvodes_tol

contains

subroutine set(this, mem)
    class(cvodes_tol), intent(in) :: this
    type(c_ptr), intent(inout) :: mem ! CVODES memory
    integer :: ierr
! call cvodes functions
    ierr = FCVodeSStolerances(mem, this % rtol, this % atol)
    ierr = FCVodeSetMaxNumSteps(mem, this % max_nstep)
end subroutine set
```

## Design

The core of any reverse-mode automatic differentiation is the data structure to store and visit the callstack. Fazang achieves this through two derived types, tape and vari.

## 1. tape data structure

A tape is an int32 array emulating a stack, with an integer marker head pointing to the head to the current stack top.

```
type :: tape
     integer(ik) :: head = 1
     integer(ik), allocatable :: storage(:)
! . . .
```

Each time a new AD node is created, space in storage is allotted to store the node's

- value  $f_i(z_i)$ , adjoint  $z_{i-1}^{\text{adj}}$ ,
- number of var operands of  $f_i$ ,
- The var operands' index in the same tape array,
- number of real64 operands of  $f_i$ ,
- The real64 operands' value.

Since a node's value, adjoint, and data operands are real64, they are first converted to int32 using transfer function before stored in the tape array, so that each such a value occupies two storage entries. After each allotation, the head is moved to point to the next empty slot in the array after saving its current value to a vari type variable for future retrieval.

### 2. vari type

The vari type is simply a proxy of a node's storage location in the tape

```
type :: vari
 integer(ik) :: i = 0
 procedure(chain_op), pass, pointer :: chain
contains
   1....
```

where i is the index to the beginning of a node's storage, and the chain procedure encodes the node's operation  $f_i$ . chain follows an interface that describes the chain rule operation

3. VAR TYPE 15

```
abstract interface
   subroutine chain_op(this)
   import :: vari
   class(vari), intent(in) :: this
   end subroutine chain_op
end interface
```

An alternative to integer index is to a pointer to the according enry in the tape array. However, we will need to expand the storage when it is filled up, and Fazang does this by doubling the storage size and use move\_alloc to restore the original values. Since there is no guarantee that move\_alloc will keep the original memory, a pointer to the original address would be corrupted.

As a Fazang program steps forward, a series of vari variables are generated, with their values calculated and stored. This is called a *forward pass*. The generated vari variables in the forward pass are stored in array varis. Each entry in varis is a dependent (operation output) of one or more previous entries.

## 3. var type

The user-facing var type serves as proxy to vari. Each var stores the index of a vari in the varis array.

```
type :: var
   integer(int32) :: vi
contains
   procedure :: val
   procedure :: adj
   procedure :: grad
   procedure :: set_chain
end type var
```

After the forward pass, when adjoints are desired, we call grad or gradient procedure. This initiates a *backward pass*, in which the varis array is traversed backward so that each vari's chain procedure is called to update the operand adjoints.

```
subroutine grad(this)
  class(var), intent(in) :: this
  integer i
  call callstack % varis (this%vi) % init_dependent()
  do i = callstack % head - 1, 1, -1
      call callstack % varis(i) % chain()
  end do
end subroutine grad
```

Here callstack is the module variable that encapsulate tape and varis arrays.

## 4. Nested tape

Fazang use begin\_nested() and end\_nested() to record and terminate a nested tape. With call begin\_nested() Fazang records the current tape and varis array head. When end\_nested() is called, the storage between the recorded head and current head are wiped, and the head is moved back to the recorded location. Multiple levels of nested envionment are supported this way.

## Add operation functions

Adding an operation  $f_i$  involves creating functions for forward pass and backward pass. Let us first use log function as a simple example.

First, we create a log v function for the forward pass.

```
impure elemental function log_v(v) result(s)
  type(var), intent(in) :: v
  type(var) :: s
  s = var(log(v\%val()), [v])
  call s%set_chain(chain_log)
end function log_v
```

The function generates a new var variable s using a special constructor var(value, array of operands) which stores the value as well as the single operand v's index (in the tape storage array). It also points s's chain to a dedicated procedure chain log.

```
subroutine chain_log(this)
  class(vari), intent(in) :: this
 real(rk) :: adj(1), val(1)
 val = this%operand_val()
 adj(1) = this%adj() / val(1)
 call this%set_operand_adj(adj)
end subroutine chain log
```

To understand this function, recall the recursion in Section 3, assume the log operation is node i, then  $f_i = \log()$  and  $z_i$  is the operand v, and the new var s would be  $z_{i-1}$ . During the backward pass when the node is visited, chain\_log first retrieves current  $(z_i, z_i^{\mathrm{adj}})$  using operand\_val() and operand\_adj(), then updates  $z_i^{adj}$  with an additional

$$z_{i-1}^{\operatorname{adj}} \frac{df_i}{dz_i} = z_{i-1}^{\operatorname{adj}} \frac{d \log(z_i)}{dz_i} = \frac{z_{i-1}^{\operatorname{adj}}}{z_i}.$$

Adding a binary operation  $f_i(z_i^{(1)}, z_i^2)$  is slightly more complex, as we will need to address possibly different scenarios when  $z_i^{(1)}$  and  $z_i^{(2)}$  are either var or real64. Let us use overloaded division operator(/) as an example.

With

$$f_i(z_i^{(1)}, z_i^2) = z_i^{(1)}/z_i^{(2)}$$

we need to account for

- both  $z_i^{(1)}$  and  $z_i^2$  are var's  $z_i^{(1)}$  is var,  $z_i^2$  is real64,

•  $z_i^{(1)}$  is real64,  $z_i^2$  is var,

For the first scenario, we create

```
impure elemental function div_vv(v1, v2) result(s)
  type(var), intent(in) :: v1, v2
  type(var) :: s
  s = var(v1%val() / v2%val(), [v1, v2])
  call s%set_chain(chain_div_vv)
end function div_vv
```

Similar to the log example, we create a new s with both operands stored. In the corresponding chain procedure, we need update the adjoints of both v1 and v2.

```
subroutine chain_div_vv(this)
  class(vari), intent(in) :: this
  real(rk) :: adj(2), val(2)
  val = this%operand_val()
  adj(1) = this%adj()/val(2)
  adj(2) = - this%val() * this%adj()/val(2)
  call this%set_operand_adj(adj)
end subroutine chain_div_vv
```

For the second scenario, we create

```
impure elemental function div_vd(v, d) result(s)
  type(var), intent(in) :: v
  real(rk), intent(in) :: d
  type(var) :: s
  s = var(v%val() / d, [v], [d])
  call s%set_chain(chain_div_vd)
  end function div_vd
```

Again we create a new var s. But this time we use another constructor var(value, var operands, data operands) to store value, var operand v, and real64 operand d. In the corresponding backward pass chain procedure, not only we need retrieve var operand v but also data operand d, as the new adjoint of  $z_i^{(1)}$  is

$$z_i^{(1)\text{new adj}} = z_i^{(1)\text{old adj}} + z_{i-1}^{\text{adj}} \frac{df_i}{dz_i^{(1)}} = z_i^{(1)\text{old adj}} + z_{i-1}^{\text{adj}} \frac{1}{dz_i^{(2)}}$$

So with v as  $z_i^{(1)}$  and d as  $z_i^{(2)}$  we have

```
subroutine chain_div_vd(this)
  class(vari), intent(in) :: this
  real(rk) d(1), adj(1)
  d = this%data_operand()
  adj(1) = this%adj() / d(1)
  call this%set_operand_adj(adj)
  end subroutine chain_div_vd
```

The third scenario is treated similarly.

## APPENDIX A

# Fazang Functions

Function	Argument(s)	Operation
sin	scalar or array	same as intrinsic
cos	scalar or array	same as intrinsic
tan	scalar or array	same as intrinsic
asin	scalar or array	same as intrinsic
acos	scalar or array	same as intrinsic
atan	scalar or array	same as intrinsic
log	scalar or array	same as intrinsic
exp	scalar or array	same as intrinsic
sqrt	scalar or array	same as intrinsic
erf	scalar or array	same as intrinsic
erfc	scalar or array	same as intrinsic
abs	scalar or array	same as intrinsic
norm2	1D array	same as intrinsic
hypot	scalars or arrays	same as intrinsic
sinh	scalar of array	same as intrinsic
cosh	scalar of array	same as intrinsic
tanh	scalar of array	same as intrinsic
asinh	scalar of array	same as intrinsic
acosh	scalar of array	same as intrinsic
atanh	scalar of array	same as intrinsic
log_gamma	scalar or array	same as intrinsic
square	scalar or array	For input $x$ , calculate $x**2$
inv	scalar or array	For input $x$ , calculate $1/x$
inv_square	scalar or array	For input $x$ , calculate $1/x**2$
inv_sqrt	scalar or array	For input x, calculate 1/sqrt(x)
logit	scalar or array	For input $x$ , calculate $log(x/(1-x))$
inv_logit	scalar or array	For input $x$ , calculate $1/(1+exp(-x))$
operator (+)	scalars or arrays	same as intrinsic
operator (-)	scalars or arrays	same as intrinsic
operator (*)	scalars or arrays	same as intrinsic
operator (/)	scalars or arrays	same as intrinsic
operator (**)	scalars	same as intrinsic
sum	1D array	same as intrinsic
dot_product	1D arrays	same as intrinsic
log_sum_exp	1D array	For input x, calculate log(sum(exp((x))))
matmul	2D arrays	same as intrinsic

## APPENDIX B

## Fazang Probability distributions

#### 1. Normal distribution

Normal
$$(y, \mu, \sigma) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2}\left(\frac{y_i - \mu}{\sigma}\right)^2\right), \quad \forall y \in \mathbb{R}^n, \mu \in \mathbb{R}, \sigma \in \mathbb{R}^+.$$
 (B.1)

- normal lpdf(y, mu, sigma)
  - y: real64 array.
  - mu: real64 or var.
  - sigma: real64 or var.
  - Return: the log of Normal $(y, \mu, \sigma)$ .

## 2. LogNormal distribution

$$\operatorname{LogNormal}(y, \mu, \sigma) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} \frac{1}{y_i} \exp\left(-\frac{1}{2} \left(\frac{\log y_i - \mu}{\sigma}\right)^2\right), \quad \forall y \in (\mathbb{R}^+)^n, \mu \in \mathbb{R}, \sigma \in \mathbb{R}^+.$$
(B.2)

- lognormal\_lpdf(y, mu, sigma)
  - y: real64 array.
  - mu: real64 or var.
  - sigma: real64 or var.
  - Return: the log of LogNormal( $y, \mu, \sigma$ ).

### 3. **TODO** additional distributions

## **Bibliography**

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