Implicit Differentiation

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Differentiating numerical procedures

Consider a program that numerically converge to solutions:

```
function f(x)
    while abs(error) > tol
        y += # Make some step in the right direction
        error = # update error
    end
    return y
end
```

▶ **How can we differentiate with respect to `x` ? Forward, reverse, something else ?**

Square root example

To illustrate consider this Jax example rewriting $x^2 = a$ into $2x^2 = x^2 + a$ or $x = (x + a/x)/2$

```
fixed_point (generic function with 1 method)
```

```
function fixed_point(f, x)
    fx = f(x)
    while abs(x - fx) > 1e-6
        x = fx
        fx = f(x)
    end
    return x
end
```

```
my_sqrt (generic function with 1 method)
```

```
my_sqrt(a) = fixed_point(x -> (x + a / x) / 2, a)
```

```
1.4142135623746899
```

```
my_sqrt(2)
```

AD through fixed point

```
0.3535533906116973
```

```
FiniteDifferences.central_fdm(5, 1)(my_sqrt, 2.0)
```

```
0.35355339061171626
```

```julia
ForwardDiff.derivative(my_sqrt, 2.0)
```

```
0.35355339061171626
```

```julia
DI.derivative(my_sqrt, DI.AutoMooncake(), 2.0)
```

▶ **Can't we do something simpler using the solution of the fixed point and the fixed point equation ?**

Implicit function theorem

> *In a sense, the implicit function theorem can be thought as the mother theorem, as it can be used to prove envelope theorems, the adjoint state method and the inverse function theorem.* Section 11.6 of The Elements of Differentiable Programming book

Inverse function theorem

Assume

- $f : \mathcal{W} \to \mathcal{W}$ is C^2
- $\partial f(w_0)$ is **invertible**

Then

- f is bijective from a neighborhood of w_0 to a neighborhood of $f(w_0)$
- For ω in a neighborhood of $f(w_0)$, f^{-1} is C^2 and $\partial f^{-1}(\omega) = (\partial f(f^{-1}(\omega)))^{-1}$

▶ **Proof sketch**

Implicit function theorem (univariate case)

Assume

- $F : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$
- (w_0, λ_0) such that $F(w_0, \lambda_0) = 0$ and $\partial_1 F(w_0, \lambda_0) \neq 0$
- $F(w, \lambda)$ is C^2 in a neighborhood $\mathcal{U}$ of (w_0, λ_0)

Then there exists a neighborhood $\mathcal{V} \subseteq \mathcal{U}$ where exists $w^\star(\lambda)$ such that

$$\begin{aligned} w^\star(\lambda_0) &= w_0 \\ F(w^\star(\lambda), \lambda) &= 0, \qquad\qquad\qquad \forall (w^\star(\lambda), \lambda) \in \mathcal{V} \\ \partial w^\star(\lambda) &= -\frac{\partial_2 F(w^\star(\lambda), \lambda)}{\partial_1 F(w^\star(\lambda), \lambda)} \end{aligned}$$

Example

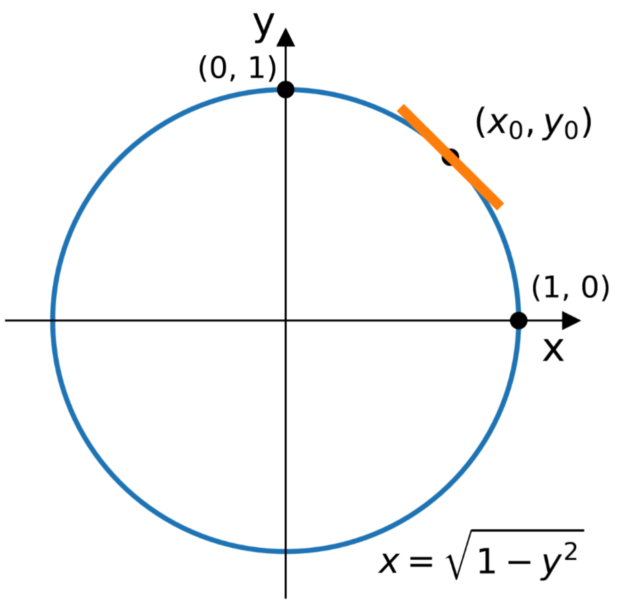
Implicit relation between x and y:

$$x^2 + y^2 = 1$$

Two possible explicit functions:

$$y^+(x) = \sqrt{1 - x^2}$$
$$y^-(x) = -\sqrt{1 - x^2}$$

▶ **Does that contradict the Implicit Function Theorem (IFT) ?**



Implicit function theorem (multivariate case)

Assume

- $F : \mathcal{W} \times \Lambda \to \mathcal{W}$
- (w_0, λ_0) such that $F(w_0, \lambda_0) = 0$ and $\partial_1 F(w_0, \lambda_0)$ is invertible
- $F(w, \lambda)$ is C^2 in a neighborhood $\mathcal{U}$ of (w_0, λ_0)

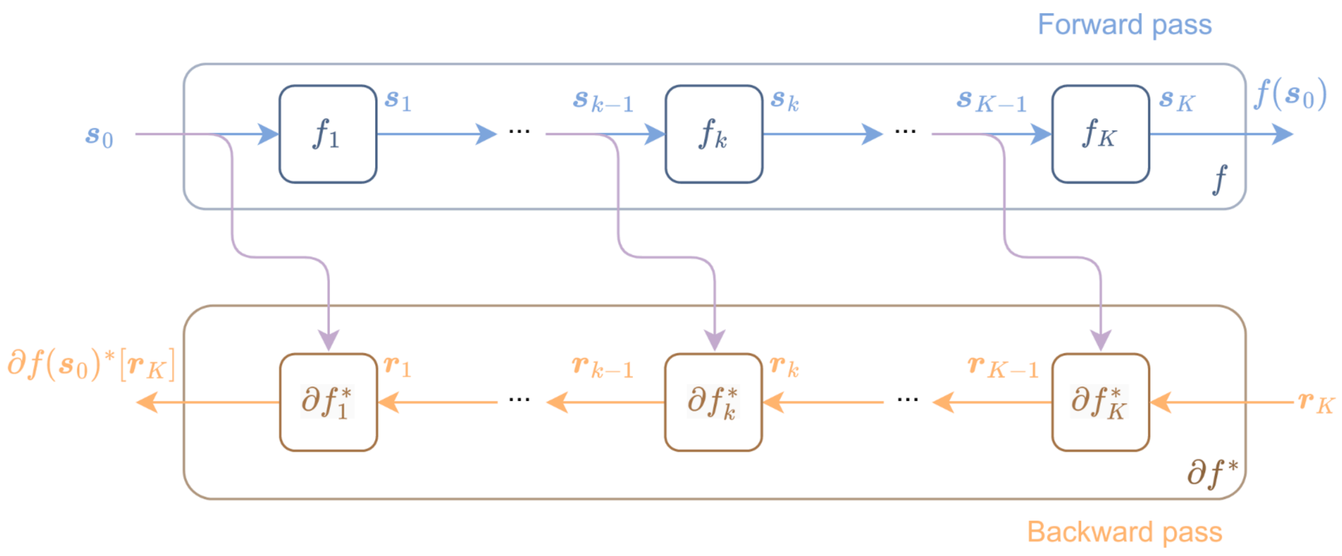
Then there exists a neighborhood $\mathcal{V} \subseteq \mathcal{U}$ where exists $w^\star(\lambda)$ such that

$$\begin{aligned} w^\star(\lambda_0) &= w_0 \\ F(w^\star(\lambda), \lambda) &= 0, \qquad\qquad \forall (w^\star(\lambda), \lambda) \in \mathcal{V} \\ \partial w^\star(\lambda) &= -\partial_1 F(w^\star(\lambda), \lambda)^{-1} \partial_2 F(w^\star(\lambda), \lambda) \end{aligned}$$

▶ **Proof**

Implicit VJP and JVP

How can we integrate implicit function in a chain of functions ? Say, $s_{k-1} = \lambda$ and $f_k(\lambda) = w^\star(\lambda)$ such that $F(w^\star(\lambda), \lambda) = 0$.



Pushforward operator (JVP)

Let $A = -\partial_1 F(w^\star(\lambda), \lambda)$ and $B = \partial_2 F(w^\star(\lambda), \lambda)$. Assuming the condition of the IFT holds, we have

$$A \partial w^\star(\lambda)/\partial s_0 = B \partial \lambda / \partial s_0$$

Given a forward tangent $t_{k-1} = \partial \lambda / \partial s_0$, the forward tangent $t_k = \partial w^\star(\lambda)/\partial s_0$ can be obtained by solving the linear system:

$$\begin{aligned} A t_k &= B t_{k-1} \\ t_k &= A^{-1} B t_{k-1} \end{aligned}$$

Interlude: Repeated linear system solve

We need to solve the system $At_k = Bt_{k-1}$ once by forward tangent, so once by entry of s_0 in case of forward-mode AD. We may also pre-compute $A^{-1}B$ by solving one linear system by column of B. In both case, we need to solve several linear system with the **same** A matrix.

```
A = 2×2 Matrix{Int64}:
     1  2
     3  4
```

```julia
A = [1 2; 3 4]
```

```
b = ▶[5, 6]
```

```julia
b = [5, 6]
```

Classical Gaussian elimination finds the solution for one vector only, even though the same row operations would be applied for different vectors.

```
2×3 Matrix{Float64}:
 1.0  0.0  -4.0
 0.0  1.0   4.5
```

```julia
rref([A b])
```

Solution: precompute the LU decomposition

LU decomposition remember the row operations to make U triangular in the L matrix.

```
F = LU{Float64, Matrix{Float64}, Vector{Int64}}
    L factor:
    2×2 Matrix{Float64}:
     1.0       0.0
     0.333333  1.0
    U factor:
    2×2 Matrix{Float64}:
     3.0  4.0
     0.0  0.666667
```

As L and U are triangular, solving the linear systems $LUx = b$ can now be done by solving two simple linear systems (and permutation in case of pivoting)

1. $Lc = b$
2. $Ux = c$

▶ **Can we also solve the linear system with only access to the matrix-vector product of the linear map $\partial_1 F(w^\star(\lambda), \lambda)$? (aka matrix-free inversion)**

Interlude: Adjoint of inverse

Consider a linear map $A : \mathcal{X} \to \mathcal{Y}$ between linear spaces of the same dimension. Assume A is invertible, what is the adjoint of A^{-1} ?

▶ **Is the adjoint A^* always invertible ?**

▶ **Is the adjoint of the inverse equal to the inverse of the adjoint ?**

Pullback operator (VJP)

The pullback operation is the adjoint of the pushforward operator:

$$\langle r, A^{-1}Bt\rangle = \langle (A^{-1})^* r, Bt\rangle = \langle (A^*)^{-1} r, Bt\rangle = \langle B^*(A^*)^{-1} r, t\rangle$$

So the pullback operator maps r to $B^*(A^*)^{-1}r$.

This means that it first solves the linear system $A^*v = r$ (possibly in a matrix-free way) and then returns B^*v.

Sensitivity of a linear program

Consider the primal-dual pair of programs

$$\begin{aligned} \min\ c^\top x \qquad & \max\ b^\top y \\ Ax = b \qquad & A^\top y \le c \\ x \ge 0 \qquad & \end{aligned}$$

The Lagrangian function is

$$\mathcal{L}(x, y) = c^\top x - y^\top (Ax - b) = y^\top b - (A^\top y - c)^\top x$$

The KKT condition give

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial y} = Ax - b = 0 \qquad & \Leftrightarrow \qquad Ax = b \\ (A^\top y - c) \perp x \ge 0 \qquad & \Leftrightarrow \qquad \operatorname{Diag}(x)(A^\top y - c) = 0 \end{aligned}$$

IFT for linear programs

The system of equation to consider for the IFT is therefore

$$F((x, y), (A, b, c)) = (Ax - b, \operatorname{Diag}(x)(A^\top y - c))$$

We have

$$\partial_1 F = \begin{bmatrix} A & 0 \\ \operatorname{Diag}(A^\top y - c) & \operatorname{Diag}(x) A^\top \end{bmatrix}$$

See OptNet: Differentiable optimization as a layer in neural networks for a generalization to quadratic objective.

Acknowledgements and further readings

- Example from : Implicit function differentiation of iterative implementations
- Chapter 11 of The Elements of Differentiable Programming book
- See DiffOpt.jl for implicit differentiation of JUMP optimization problems.

Utils

```julia
using PlutoUI, PlutoUI.ExperimentalLayout, HypertextLiteral; PlutoTeachingTools
```

```julia
import ForwardDiff, FiniteDifferences, Mooncake
```

```julia
import DifferentiationInterface as DI
```

```julia
using LinearAlgebra, RowEchelon
```

```
img (generic function with 3 methods)
```

```
qa (generic function with 2 methods)
```

```julia
begin
function qa(question, answer)
    return @htl("<details><summary>$question</summary>$answer</details>")
end
function _inline_html(m::Markdown.Paragraph)
    return sprint(Markdown.htmlinline, m.content)
end
function qa(question::Markdown.MD, answer)
    # `html(question)` will create `<p>` if `question.content[]` is `Markdown.Paragraph`
    # This will print the question on a new line and we don't want that:
    h = HTML(_inline_html(question.content[]))
    return qa(h, answer)
end
end
```