Efficient Automatic Differentiation of Implicit Functions

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Abstract. Derivative-based algorithms are ubiquitous in statistics, machine learning, and applied mathematics. Automatic differentiation offers an algorithmic way to efficiently evaluate these derivatives from computer programs that execute relevant functions. Implementing automatic differentiation for programs that incorporate implicit functions, such as the solution to an algebraic or differential equation, however, requires particular care. Contemporary applications typically appeal to either the application of the implicit function theorem or, in certain circumstances, specialized adjoint methods. In this paper we show that both of these approaches can be generalized to any implicit function, although the generalized adjoint method is typically more effective for automatic differentiation. To showcase the relative advantages and limitations of the two methods we demonstrate their application on a suite of common implicit functions.

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Automatic differentiation is a powerful tool for algorithmically evaluating derivatives of functions implemented as computer programs (Griewank and Walther, 2008; Baydin et al., 2018; Margossian, 2019). The method is implemented in an increasing diversity of software packages such as Stan (Carpenter et al., 2015, 2017) and Jax (Bradbury et al., 2018), driving state of the art computational tools such as the aforementioned Stan and TensorFlow (Dillon et al., 2017). Each automatic differentiation package provides a library of differentiable expressions and routines that propagate derivatives through programs comprised of those expressions.

Implicit functions are defined not as explicit expressions but rather by a potentially infinite set of equality constraints that an output must satisfy for a given input. Common examples include algebraic equations, optima, and differential equations. Although defined only implicitly by the constraints they must satisfy, these functions and their derivatives can be evaluated at a given input which puts them within the scope of automatic differentiation.

Many approaches to evaluating the derivatives of implicit functions have been developed, most designed for specific classes of implicit functions. Here we focus on two approaches: direct application of the implicit function theorem and adjoint methods. The former is commonly applied to finite-dimensional systems such as algebraic equations and optimization problems (for example Bell and Burke, 2008; Lorraine, Vicol and Duvenaud, 2019; Gaebler, 2021) while the latter is particularly well-suited to infinite-dimensional systems such as ordinary differential equations (for example Pontryagin et al., 1963; Errico, 1997), algebraic differential equations (Cao et al., 2002), and stochastic differential equations (Li et al., 2020). Adjoint methods have also been derived for some finite-dimensional systems such as difference equations (Betancourt, Margossian and Leos-Barajas, 2020). When they can be derived the performance of adjoint methods often scales better than the performance of implicit function theorem methods; the details of those derivations, however, can change drastically from one system to another.

In this paper we derive implicit function theorem and adjoint methods that implement automatic differentiation for any implicit function regardless of its dimensionality. We begin by reviewing derivatives of real-valued functions – drawing a careful distinction between total, partial, and directional derivatives – and then introduce the basics of automatic differentiation. Next we derive implicit function theorem and adjoint methods for any finite-dimensional implicit function and demonstrate their application to the reverse mode automatic differentiation of general algebraic equations, the special case of difference equations, and optimization problems. Finally we generalize these methods to infinite-dimensional implicit functions with demonstrations on ordinary and algebraic differential equations. In each example we examine the particular challenges that arise with each method.
1. AUTOMATIC DIFFERENTIATION

Before discussing the automatic differentiation of implicit functions, in this section we will review the basics of differentiating real-valued functions and then how derivatives of computer programs can be implemented algorithmically as automatic differentiation.

1.1 A Little Derivative

Differentiation is a pervasive topic, but terminology and notation can vary strongly from field to field. In this section we review the mathematics of derivatives on real spaces and introduce all of the terminology and notation that we will use throughout the paper. We first discuss the parameterization of real spaces and the vector space interpretation that emerges before introducing formal definitions for total and directional derivatives and their properties.

1.1.1 Locations and Directions. An $I$-dimensional real space $\mathbb{R}^I$ models a rigid and smooth continuum of points. Here we will consider a subset of the real numbers $X \subseteq \mathbb{R}^I$ which may or may not be compact.

A parameterization of $X$ decomposes the $I$-dimensional space into $I$ copies of the one-dimensional real line,

$$X \approx \mathbb{R}_1 \times \ldots \times \mathbb{R}_i \times \ldots \times \mathbb{R}_I,$$

which we refer to as a coordinate system. Within a parameterization each point $x \in X$ can be identified by $I$ real numbers denoted parameters or coordinates,

$$x = (x_1, \ldots, x_i, \ldots, x_I).$$

Every real space $X$ admits an infinite number of parameterizations (Figure 1). A one-to-one map from $X$ into itself can be interpreted as a map from one parameterization to another and consequently is often denoted a reparameterization or change of coordinate system.

The choice of any given parameterization endows $X$ with a rich geometry. In particular we can use coordinates to define how to scale any point $x \in X$ by a real number $\alpha \in \mathbb{R}$,

$$\alpha \cdot x = \alpha \cdot (x_1, \ldots, x_i, \ldots, x_I)$$

$$= (\alpha \cdot x_1, \ldots, \alpha \cdot x_i, \ldots, \alpha \cdot x_I)$$

$$= x' \in X,$$

as well as add two points $x, x' \in X$ together,

$$x + x' = (x_1, \ldots, x_i, \ldots, x_I) + (x'_1, \ldots, x'_i, \ldots, x'_I)$$

$$= (x_1 + x'_1, \ldots, x_i + x'_i, \ldots, x_I + x'_I)$$

$$= x'' \in X.$$
Fig 1. Every real space $X$ admits an infinite number of parameterizations, or coordinate systems, each of which are capable of uniquely identifying every point with an ordered tuple of real numbers.

These properties make the parameterization of $X$ a vector space over the real numbers; each point $x \in X$ identifies a unique vector $x$ and the coordinates define a distinguished vector space basis. If we further use the coordinates to define an inner product,

$$\langle x, x' \rangle \equiv \sum_{i=1}^{I} (x_i - x'_i)^2$$

then this vector space becomes a Euclidean vector space, $E(X)$.

This Euclidean vector space structure defines a notion of direction and orientation in $X$. For example any point $x \in X$ can be interpreted as a vector $x$ stretching from the origin at $(0, \ldots, 0, \ldots, 0) \equiv O$ to $x$. Similarly any two points $x, x' \in X$ are connected by the vector

$$\Delta x = x' - x = (x'_1 - x_1, \ldots, x'_i - x_i, \ldots, x'_I - x_I).$$

Equivalently we can think of vectors as a way to translate from one point to another (Figure 2). For example $x$ shifts the origin to $x$,

$$x = (x_1, \ldots, x_i, \ldots, x_I)
= (0 + x_1, \ldots, 0 + x_i, \ldots, 0 + x_I)
= (0, \ldots, 0, \ldots, 0) + (x_1, \ldots, x_i, \ldots, x_I)
= O + x,$$
Fig 2. Given a parameterization of the real space $X$ vectors quantify the direction and distance between points, such as $\mathbf{x}$ between point $x$ and the origin $O$ or $\mathbf{x}' - \mathbf{x}$ between $x$ and $x'$. By following a vector we can also translate from the initial point to the final point.

while $\Delta \mathbf{x}$ shifts from $x$ to $x'$,

$$x' = x + (x' - x) = x + (\mathbf{x}' - \mathbf{x}) = x + \Delta \mathbf{x}.$$  

Consequently once we fix a parameterization each set of coordinates $(x_1, \ldots, x_i, \ldots, x_I)$ can be interpreted as either a location $x \in X$ or a direction $\mathbf{x} \in E(X)$.

1.1.2 Transforming Locations and Directions. Given two real spaces $X \subseteq \mathbb{R}^I$ and $Y \subseteq \mathbb{R}^J$ a real-valued function $f : X \to Y$ maps points in $X$ to points in $Y$. Once a parameterization has been fixed for both spaces such a mapping also induces a map from vectors in $E(X)$ to vectors in $E(Y)$, $F : E(X) \to E(Y)$.

Induced maps that preserve the additive and multiplicative structure of the Euclidean vector space, 

$$F(\alpha \cdot \mathbf{x} + \beta \cdot \mathbf{x}') = \alpha \cdot F(\mathbf{x}) + \beta \cdot F(\mathbf{x}')$$

are said to be linear. Linear maps can be represented by a matrix of real numbers that maps the components of the input vector to the components of the output vector,

$$y_j = \sum_{i=1}^{I} F_{ji} x_i,$$

or in standard linear algebra notation,

$$\mathbf{y} = F(\mathbf{x}) = \mathbf{F} \cdot \mathbf{x}.$$  

We will denote the space of linear maps between $E(X)$ and $E(Y)$ as $L(X,Y)$. 

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*Note: The diagram illustrates the transformation of points and vectors in a 2D space, showing the shift from $x$ to $x'$ and the resulting vector $\Delta \mathbf{x}$.*
1.1.3 The Total Derivative. The total derivative of a function $f : X \to Y$ quantifies the behavior of $f$ in the local neighborhood of an input point $x \in X$. This local behavior provides a way of mapping vectors that represent infinitesimal translations from $x$ to vectors that represent infinitesimal translations from $f(x)$.

More formally the total derivative assigns to each point $x \in X$ a linear transformation between $E(X)$ and $E(Y)$,

$$\frac{d}{dx} : X \to L(X, Y)$$

$$x \mapsto \frac{df}{dx}(x) \equiv J(x),$$

that quantifies the first-order variation of $f$ in the neighborhood of each input $x$. We can then say that the total derivative of $f$ at $x$ is the linear transformation $J(x) : E(X) \to E(Y)$.

In components the total derivative at a point $x \in X$ is specified by a matrix of partial derivative functions evaluated at $x$,

$$J_{ji}(x) = \frac{\partial f_j}{\partial x_i}(x),$$

denoted the Jacobian. The action of the total derivative at $x$ on a vector $v \in E(X)$ is then given by matrix multiplication,

$$J(x)(v) = J(x) \cdot v = \sum_{i=1}^{I} J_{ji}(x) v_i.$$

1.1.4 Directional Derivatives. The total derivative of a function $f$ at a point $x$ applied to a vector $v \in E(X)$, or more compactly $J(x)(v)$, quantifies how much the output of $f$ varies as $x$ is translated infinitesimally in the direction of $v$. Consequently $J(x)(v) = J(x) \cdot v$ is called the forward directional derivative.

The forward directional derivative is often used to construct the linear function between $X$ and $Y$ that best approximates $f$ at $x$. The best approximation evaluated at $x'$ is given by translating $f(x)$ along $J(x)(x' - x)$ (Figure 3)

$$\tilde{f}(x') = f(x) + J(x)(x' - x)$$
$$= f(x) + J(x) \cdot (x' - x),$$

or in components,

$$\tilde{f}_j(x'_1, \ldots, x'_I) = f_j(x_1, \ldots, x_I) + \sum_{i=1}^{I} \frac{\partial f_j}{\partial x_i}(x_1, \ldots, x_I) \cdot (x'_i - x_i).$$
Fig 3. The forward directional derivative of the function $f$ at $x \in X$, $J_f$, propagates infinitesimal perturbations to the input, $x' - x$, to infinitesimal perturbations of the output, $J_f \cdot (x' - x)$. Translating the function output $f(x)$ by $J_f \cdot (x' - x)$ generates the best linear approximation to $f$ at $x$, $f$.

The total derivative also defines an adjoint transformation that maps vectors in $E(Y)$ to vectors in $E(X)$, $J^\dagger(x) : E(Y) \to E(X)$. The matrix components of this adjoint transformation are given by the transpose of the Jacobian matrix,

$$J^\dagger_{ji}(x) = J_{ij}(x).$$

The application of this adjoint transformation to a vector $\alpha \in E(Y)$,

$$\beta = J^\dagger(x)(\alpha) = J^T \cdot \alpha,$$

quantifies how the inputs need to vary around $x$ in order to achieve the given output variation $\alpha$. We will refer to this action as a reverse directional derivative.

1.1.5 The Chain Rule. The chain rule provides an explicit construction for the total derivative of a composite function constructed from many component functions. Consider for example a sequence of functions $f_n : X_n \to X_{n+1}$ and the composite function

$$f = f_N \circ \ldots \circ f_n \circ \ldots \circ f_1 : X_1 \to X_{N+1}.$$

The total derivative of $f$ at any point $x_1 \in X_1$ is given by composing the total derivatives of each component function together in the same order,

$$J_f = J_{f_N}(x_N) \circ \ldots \circ J_{f_n}(x_n) \circ \ldots \circ J_{f_1}(x_1),$$

where $x_n = f_{n-1}(x_{n-1})$. Likewise the components of the composite Jacobian matrix are given by a sequence of matrix products,

$$J_f = J_{f_N}(x_N) \cdot J_{f_n}(x_n) \cdot \ldots \cdot J_{f_1}(x_1).$$
Unfortunately these intermediate matrix products are expensive to evaluate, especially when the intermediate spaces \( X_n \) are high-dimensional. Constructing the full composite Jacobian matrix is usually computationally burdensome.

On the other hand this composite structure is well-suited to the evaluation of directional derivatives. For example the forward directional derivative of a composite function is given by

\[
J_f(v) = (J_{f_N}(x_N) \circ \ldots \circ J_{f_1}(x_1))(v),
\]

or

\[
J_f \cdot v = (J_{f_N}(x_N) \cdot \ldots \cdot J_{f_n}(x_n) \cdot \ldots \cdot J_{f_1}(x_1)) \cdot v.
\]

Because of the associativity of matrix multiplication we can apply each component derivative to \( v \) in sequence and avoid the intermediate compositions entirely,

\[
J_f(v) = J_{f_N}(x_N)(\cdots J_{f_n}(x_n)(\cdots (J_{f_1}(x_1)(v)) \cdots) \cdots),
\]

or

\[
J_f \cdot v = J_{f_N}(x_N)(\cdots \cdot J_{f_n}(x_n)(\cdots \cdot J_{f_1}(x_1) \cdot v) \cdots) \cdots.
\]

In other words we can evaluate the total forward directional derivative iteratively,

\[
\begin{align*}
v_1 &= J_{f_1}(x_1)(v) \\
v_2 &= J_{f_2}(x_2)(v_1) \\
&\vdots \\
v_n &= J_{f_n}(x_n)(v_{n-1}) \\
&\vdots \\
v_{N-1} &= J_{f_{N-1}}(x_{N-1})(v_{N-2}) \end{align*}
\]

\[
J_f(x)(v) = v_N = J_{f_N}(x_N)(v_{N-1}),
\]

or in components,

\[
\begin{align*}
v_1 &= J_{f_1}(x_1) \cdot v \\
v_2 &= J_{f_2}(x_2) \cdot v_1 \\
&\vdots \\
v_n &= J_{f_n}(x_n) \cdot v_{n-1} \\
&\vdots \\
v_{N-1} &= J_{f_{N-1}}(x_{N-1}) \cdot v_{N-2} \end{align*}
\]

\[
J_f(x) \cdot v = v_N = J_{f_N}(x_N) \cdot v_{N-1}.
\]

The evaluation of each intermediate directional derivative requires only a matrix-vector product which is substantially less expensive to implement than the matrix-matrix products needed to evaluate the composite Jacobian.
The reverse directional derivative can be evaluated sequentially as well,

\[ \alpha_N = J^T_{fN}(x_N)(\alpha) \]
\[ \alpha_{N-1} = J^T_{fN-1}(x_{N-1})(\alpha_N) \]
\[ \cdots \]
\[ \alpha_{N-n} = J^T_{fN-n}(x_{N-n})(\alpha_{N-n+1}) \]
\[ \cdots \]
\[ \alpha_2 = J^T_{f2}(x_2)(\alpha_3) \]
\[ J^T_f(x)(\alpha) = \alpha_1 = J^T_{f1}(x_1)(\alpha_2), \]

or in components,

\[ \alpha_N = J^T_{fN}(x_N) \cdot \alpha \]
\[ \alpha_{N-1} = J^T_{fN-1}(x_{N-1}) \cdot \alpha_N \]
\[ \cdots \]
\[ \alpha_{N-n} = J^T_{fN-n}(x_{N-n}) \cdot \alpha_{N-n+1} \]
\[ \cdots \]
\[ \alpha_2 = J^T_{f2}(x_2) \cdot \alpha_3 \]
\[ J^T_f(x) \cdot \alpha = \alpha_1 = J^T_{f1}(x_1) \cdot \alpha_2. \]

1.2 Express Yourself

Before we can consider how to implement derivatives of real-valued functions in practice we first have to consider how to implement the real-valued functions themselves. Functions \( f : X \rightarrow Y \) are often implemented as computer programs which take in any input value \( x \in X \) and return the corresponding output value \( f(x) \in Y \). These computer programs are themselves implemented as a sequence of expressions, each of which transforms some descendent of the initial value towards the final output value.

If these expressions defined full component functions then we could use the chain rule to automatically propagate directional derivatives through the program as we discussed in the previous section. Well-defined component functions, however, would depend on only the output of the previous component function, while expressions can depend on the output of multiple previous expressions. Because of this expressions do not immediately define valid component functions on their own, and the chain rule does not immediately apply.

That said we can manipulate each expression into a well-defined component function with a little bit of work. First we’ll need to take advantage of the fact that the expressions that
Fig 4. This pseudo-code implements a function $f : \mathbb{R}^3 \rightarrow \mathbb{R}$ that maps every input $x_1 = (x_{1,1}, x_{1,2}, x_{1,3})$ to a real-valued output through three intermediate expressions. The dependencies between these expressions and the input variables forms an expression graph.

A topological sort of an expression graph is any ordering of the nodes such that each expression follows all expressions on which it depends (Figure 5). Such a sorting ensures that if we process the sorted expressions in order then we will evaluate an expression only once all of the expressions on which it depends have already been evaluated.

Any topological sort provides an explicit sequence of expressions, but each expression can still depend on the output of any expression that precedes it in the stack. We can use the ordering to limit this dependence to only the previous output, however, if we can buffer each expression with any of the previous outputs that are used by future expressions. For example this buffering can be implemented by introducing identify expressions that propagate any necessary values forward (Figure 6). Together each initial expression and the added identify expressions define a layer of expressions that depend on only the expressions in the previous layer, so that these layers define a sequence of valid component functions (Figure 7).

Once we’ve derived these component functions we can finally apply the chain rule. In particular we can evaluate forward directional derivatives by propagating an initial vector through the constructed sequence of component functions. At the same time we can evaluate a reverse directional derivative by first evaluating all of the component functions in a forward sweep through the sequence before executing a reverse sweep that propagates a vector in the output space to the input space.
A topological sort of an expression graph is an ordering of the expressions, often called a stack or a tape, that guarantees that when progressing across the stack in order each expression will not be evaluated until all of the expressions on which it depends have already been evaluated.

In order to turn each topologically-sorted expression into a valid component function they must be complemented with identity maps that carry forward intermediate values needed by future expressions. The resulting layers of expressions depend on only expressions in the previous layer.
Reconstructed Component Functions

\[ f_3 : X_3 \subseteq \mathbb{R}^2 \rightarrow X_4 \subseteq \mathbb{R}^1 \]
\[ (x_{3,1}, x_{3,2}) \mapsto (x_{4,1} = x_{3,1}/x_{3,2}) \]

\[ f_2 : X_2 \subseteq \mathbb{R}^3 \rightarrow X_3 \subseteq \mathbb{R}^2 \]
\[ (x_{2,1}, x_{2,2}, x_{2,3}) \mapsto (x_{3,1} = x_{2,1} + x_{2,2}, x_{3,2} = x_{2,3}) \]

\[ f_1 : X_1 \subseteq \mathbb{R}^3 \rightarrow X_2 \subseteq \mathbb{R}^3 \]
\[ (x_{1,1}, x_{1,2}, x_{1,3}) \mapsto (x_{2,1} = x_{1,1}, x_{2,2} = x_{1,2}, x_{2,3} = x_{1,2} \cdot x_{1,3}) \]

Fig 7. Complementing each topologically-sorted expression with the appropriate identity maps defines valid component functions. When composed together these component functions yield the function implemented by the computer program, here \( f = f_3 \circ f_2 \circ f_1 \), and allow for the application of the chain rule to differentiate through the program.

Something interesting happens, however, when we evaluate the total derivative of one of these reconstructed component functions. Let’s denote the action of the component function as \( f_n : (x, x') \mapsto (g(x), I(x')) \), where \( g \) is the action implemented by the initial expression and \( I \) is the identify map that propagates any auxiliary outputs. We can also decompose the input vector \( v \) into components that map onto \( g \) and \( I \), respectively,

\[ v = (v_g, v_I)^T. \]
In this notation the forward directional derivative becomes

\[ J_{f_n}(v) = J_{f_n}((v_g, v_I)^T) \]
\[ = J_{f_n} \cdot (v_g, v_I)^T \]
\[ = \begin{pmatrix} \frac{\partial g}{\partial x} & \frac{\partial g}{\partial x'} \\ \frac{\partial I}{\partial x} & \frac{\partial I}{\partial x'} \end{pmatrix} \cdot \begin{pmatrix} v_g \\ v_I \end{pmatrix} \]
\[ = \begin{pmatrix} \frac{\partial g}{\partial x} \\ 0 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} v_g \\ v_I \end{pmatrix} \]
\[ = \begin{pmatrix} \frac{\partial g}{\partial x} \cdot v_g \\ 0 \end{pmatrix} \]

The only non-vanishing contribution to the directional derivative comes from the initial expression; the vector corresponding to the buffered outputs, \(v_I\), completely decouples from any derivatives that follow. Consequently the only aspect of the reconstructed component function that influences propagation of the forward directional derivative is the forward directional derivative of the expression itself.

In other words we can evaluate the forward directional derivative of a function implemented by a computer program by propagating only the forward directional derivatives of the individual expressions; at no point do we actually have to construct explicit component functions! The action of the adjoint derivative behaves similarly, allowing us to evaluate the reverse directional derivative using only the reverse directional derivatives local to each expression. When considering higher-order derivatives, however, the equivalence between propagating vectors across expressions and full component functions is not always preserved and explicit component functions may be needed. For more see Betancourt (2018).

1.3 Automatic Differentiation

Automatic differentiation exploits the equivalence between propagating vectors across expressions and full component functions to algorithmically evaluate forward and reverse directional derivatives.

Forward mode automatic differentiation implements forward directional derivatives, passing intermediate values and intermediate forward directional derivatives between expressions as the program is evaluated. These intermediate forward directional derivatives are denoted tangents or sensitivities.

Any implementation of a function \(g\) that supports forward mode automatic differentiation must provide not only a map from input values to output values but also a map from...
input tangents to output tangents,
\[ v' = J_g \cdot v. \]

Similarly reverse mode automatic differentiation implements reverse directional derivatives. Here the program must be evaluated first before intermediate reverse directional derivatives are propagated between expressions in the reverse order that the expressions are evaluated. These intermediate reverse directional derivatives are denoted cotangents or adjoints.

Any implementation of a function \( g \) that supports reverse mode automatic differentiation must provide not only a map from input values to output values but also a map from output cotangents to input cotangents,
\[ \alpha' = J_g^T \cdot \alpha. \]

2. AUTOMATIC DIFFERENTIATION OF FINITE-DIMENSIONAL IMPLICIT FUNCTIONS

A finite collection of constraint functions that an output has to satisfy for a given input implicitly defines a map from inputs to outputs, or an implicit function. In this section we discuss how implicit functions are formally defined, how to differentiate these implicitly defined functions, and then finally demonstrate their application on several instructive examples.

2.1 The Finite-Dimensional Implicit Function Theorem

Consider a finite-dimensional real-valued space of known inputs, \( X \), a finite-dimensional real-valued space of unknown outputs, \( Y \), a finite-dimensional real-valued space of constraint values, \( Z \), and the constraint function
\[ c : X \times Y \to Z \]
\[ (x, y) \mapsto c(x, y). \]

The implicit function theorem defines the conditions under which the constraint function implicitly defines a map from \( f : X \to Y \) which satisfies \( c(x, f(x)) = 0 \) for all inputs in a local neighborhood \( x \in U \subset X \).

More formally consider the neighborhoods \( 0 \in W \subset Z \) and \( V \subset Y \) such that the kernel of the constraint function falls into product of \( U \) and \( V \),
\[ c^{-1}(0) = U \times V, \]
and assume that a function \( f : U \to V \) that satisfies \( c(x, f(x)) = 0 \) exists. If the constraint function \( c \) is differentiable across \( U \times V \) then the total derivative of \( c \) evaluated at \( (x, f(x)) \)
is given by

\[
0 = \frac{d}{dx} c(x, f(x)) = \frac{\partial c}{\partial x}(x, f(x)) + \frac{\partial c}{\partial y}(x, f(x)) \circ \frac{df}{dx}(x).
\]

When the dimension of \(Z\) equals the dimension of \(Y\) then the partial derivative \(\frac{\partial c}{\partial y}(x, y)\) might define a bijection from \(V\) to \(W\). If it does then we can solve for the total derivative of the assumed function,

\[
\frac{df}{dx}(x) = -\left(\frac{\partial c}{\partial y}(x, f(x))\right)^{-1} \circ \frac{\partial c}{\partial x}(x, f(x)).
\]

When \(\frac{\partial c}{\partial y}(x, y)\) is bijective this derivative is well-defined, and the existence and uniqueness of ordinary differential equation solutions guarantees that an implicit function that satisfies \(c(x, f(x)) = 0\) is well-defined in the neighborhood around \(x\). In other words the system of constraints defines an implicit function if and only if the partial derivative \(\frac{\partial c}{\partial y}(x, y)\) is invertible.

The implicit function theorem determines when an implicit function is well-defined, but not how to evaluate it. In practice we typically have to rely on numerical methods that heuristically search the output space for a value \(y\) that satisfies \(c(x, y) = 0\) for the given input \(x\).

### 2.2 Evaluating Directional Derivatives of Finite-Dimensional Implicit Functions

To incorporate implicit functions into an automatic differentiation library we need to be able to evaluate not only the output consistent with a given input but also the directional derivatives. Here we consider three general approaches: a trace method that works with a given numerical solver, a method that utilizes intermediate results of the implicit function theorem, and an adjoint method that evaluates the directional derivative directly.

In all three approaches we will consider not the implicit function alone but rather its composition with a summary function that maps the outputs into some real space, \(g : Y \to \mathbb{R}^K\). Often \(g\) will be the identify map, but the flexibility offered by this summary function will facilitate some of the examples that we consider below.

When \(X = \mathbb{R}^I\) and \(Y = Z = \mathbb{R}^J\) the composition of the summary function with the implicit function defines the real-valued function

\[
h = g \circ f : \mathbb{R}^I \to \mathbb{R}^J \to \mathbb{R}^K
\]

and our goal will be to evaluate either the forward directional derivative \(J_{g \circ f}(x)(v)\) or the reverse directional derivative \(J^\dagger_{g \circ f}(x)(\alpha)\).
2.2.1 Trace Method. Each step that an iterative numerical solver takes while searching for a consistent output can be interpreted as a map from the output space to itself given the fixed input \( x \),

\[
\tilde{f}_n : X \times Y \to Y \\
(x, y_{n-1}) \mapsto y_n.
\]

The trace of the solver’s evaluation then defines a composite function,

\[
\tilde{f}(x, y_0) = (\tilde{f}_N(x) \circ \tilde{f}_{N-1}(x) \circ \ldots \circ f_1(x))(y_0)
\]

that maps the input and an initial guess to an approximate solution,

\[
\tilde{f} : X \times Y \to Y \\
(x, y_0) \mapsto \tilde{y}
\]

satisfying \( c(x, \tilde{y}) \approx 0 \).

If each of these intermediate steps are differentiable and supported by an automatic differentiation library then we can evaluate the directional derivatives of \( \tilde{f} \) using automatic differentiation and use them to approximate the directional derivatives of the exact implicit function \( f \). While straightforward to implement this approach can suffer from poor performance in practice, especially as the number of solver iterations grows and propagating derivatives through the composite function becomes slow and memory intensive. See for example (Bell and Burke, 2008) for further discussion of this trace method applied to optimization problems and (Margossian, 2019) for one on algebraic equations.

2.2.2 Finite-Dimensional Implicit Function Theorem. Conveniently the derivative of the implicit function \( f \) is explicitly constructed in the derivation of the implicit function theorem,

\[
\frac{df}{dx}(x) = - \left( \frac{\partial c}{\partial y}(x, f(x)) \right)^{-1} \circ \frac{\partial c}{\partial x}(x, f(x)).
\]

If we can evaluate these derivatives of the constraint function then we can immediately evaluate the derivative for \( f \) once we have numerically solved for the output of the implicit function \( y = f(x) \),

\[
\frac{df}{dx}(x) = - \left( \frac{\partial c}{\partial y}(x, y) \right)^{-1} \circ \frac{\partial c}{\partial x}(x, y).
\]
The Jacobian of the composite function \( g \circ f \) is then given by

\[
J_{g \circ f}(x) = \frac{\partial (g \circ f)}{\partial x}(x) \\
= \frac{dg}{dy}(f(x)) \circ \frac{df}{dx}(x) \\
= -\frac{dg}{dy}(f(x)) \circ \left( \frac{\partial c}{\partial y}(x, f(x)) \right)^{-1} \circ \frac{\partial c}{\partial x}(x, f(x)).
\]

In components this becomes

\[
(J_{g \circ f})_{ik}(x) = \frac{\partial h_k}{\partial x_i}(x) \\
= \sum_{j=1}^{J} \frac{dg_k}{dy_j}(f(x)) \cdot \frac{df_i}{dx}(x) \\
= -\sum_{j=1}^{J} \sum_{j'=1}^{J} \frac{dg_k}{dy_j}(f(x)) \circ \left( \frac{\partial c_{j'}}{\partial y_j}(x, f(x)) \right)^{-1} \circ \frac{\partial c_{j'}}{\partial x_i}(x, f(x)),
\]

or in more compact matrix notation,

\[
J_{g \circ f} = -J_g \cdot C_y^{-1} \cdot C_x,
\]

where

\[
(C_y)_{ij} = \frac{\partial c_i}{\partial y_j}(x, f(x)) \\
(C_x)_{ij} = \frac{\partial c_i}{\partial x_j}(x, f(x)) \\
(J_g)_{ij} = \frac{\partial g_i}{\partial y_j}(f(x)).
\]

In order to incorporate this composite function into forward mode automatic differentiation we need to evaluate the action of the Jacobian contracted against a tangent vector,

\[
(J_{g \circ f}(x) \cdot v)_j = \sum_{i=1}^{I} (J_{g \circ f})_{ij}(x) \cdot v_i \\
= -\sum_{i=1}^{I} \frac{dg_j}{dy}(f(x)) \circ \left( \frac{\partial c}{\partial y}(f(x)) \right)^{-1} \circ \frac{\partial c}{\partial x_i}(x) \cdot v_i,
\]

or equivalently

\[
J_{g \circ f}(x) \cdot v = -J_g \cdot C_y^{-1} \cdot C_x \cdot v.
\]
Similarly to incorporate this composite function into reverse mode automatic differentiation we need to evaluate the action of the Jacobian contracted against a cotangent vector,

$$(J^T_{g \circ f}(x) \cdot \alpha)_i = \sum_{j=1}^{J} (J_{g \circ f})_{ij}(x) \cdot \alpha_j$$

$$= -\sum_{j=1}^{J} \frac{dg_i}{dy}(f(x)) \circ \left( \frac{\partial c}{\partial y}(f(x)) \right)^{-1} \circ \frac{\partial c}{\partial x}(f(x)) \cdot \alpha_j,$$

or

$$J^T_{g \circ f}(x) \cdot \alpha = -C^T_x \cdot (C^{-1}_y)^T \cdot J^T_g \cdot \alpha$$

$$= -C^T_x \cdot (C^{-1}_y)^{-1} \cdot J^T_g \cdot \alpha.$$  

With so many terms there are multiple ways to evaluate these directional derivatives. The forward method, for example, explicitly constructs $J_{g \circ f}(x) = -J_g \cdot C^{-1}_y \cdot C_x$ before evaluating the contractions $J_{g \circ f}(x) \cdot v$ or $J^T_{g \circ f}(x) \cdot \alpha$. With careful use of automatic differentiation, however, we can evaluate the final directional derivatives more efficiently. In particular we don’t need to explicitly construct $J_g$ and $C_x$ at all.

For example when evaluating $J_{g \circ f}(x) \cdot v$ we can avoid $C_x$ by using one sweep of forward mode automatic differentiation to evaluate $u = C_x \cdot v$ directly. Because of the inversion we have to construct the entirety of $C_y$, for example with $J$ sweeps of forward mode or reverse mode automatic differentiation, but we can avoid constructing $(C_y)^{-1}$ by solving for only the linear system

$$C_y \cdot t = u.$$  

Finally we can avoid constructing $J_g$ with one sweep of forward mode automatic differentiation to evaluate $J_g \cdot t$. These steps are outlined in Algorithm 1.

**Algorithm 1** Forward mode automatic differentiation of finite-dimensional implicit function.

1: **input:** constraint function, $c$; summary function, $g$; tangent, $v$. Note: we assume we have a differentiable program for all the input functions.
2: $u = C_x \cdot v$ (one forward mode sweep)
3: $C_y = \partial c / \partial y$ ($J$ forward or reverse mode sweep)
4: $t = C_y^{-1} \cdot u$ (linear solve)
5: $J_{g \circ f} \cdot v = -J_g \cdot t$ (one forward sweep)
6: **return:** $J_{g \circ f} \cdot v$

Similar optimizations are also possible when evaluating the reverse directional derivative $J^T_{g \circ f}(x) \cdot \alpha$. We first evaluate $\beta = J^T_g \cdot \alpha$ using one sweep of reverse mode automatic differentiation and then construct $C_y$ as above. This allows us to solve the linear system

$$C^T_y \cdot \gamma = \beta.$$
and then evaluate $C_x^T \cdot \beta$ with one more sweep of reverse mode automatic differentiation through the constraint function. These steps are outlined in Algorithm 2.

**Algorithm 2** Reverse mode automatic differentiation of finite-dimensional implicit function.

1: **input**: constraint function, $c$; summary function, $g$; cotangent, $\alpha$. Note: we assume we have a differentiable program for all the input functions.
2: $\beta = J_y^T \cdot \alpha$ (one reverse mode sweep)
3: $C_y = \partial c / \partial y$ ($J$ forward or reverse mode sweep)
4: $\gamma = (C_y^T)^{-1} \beta$ (linear solve)
5: $J_{g \circ f}^T \cdot \alpha = -C_y^T \cdot \gamma$ (one reverse mode sweep)
6: **return**: $J_{g \circ f}^T \cdot \alpha$

Often the form of a particular constraint function results in sparsity structure in $C_x$ and $C_y$ that can be exploited to reduce the cost of the irreducible linear algebraic operations. Identifying this structure and implementing faster operations, however, requires substantial experience with numerical linear algebra.

**2.2.3 The Finite-Dimensional Adjoint Method.** The adjoint method provides a way of directly implementing the contractions that give forward and reverse directional derivatives without explicitly constructing the Jacobian $df/dx(x)$. Adjoint methods have historically been constructed for specific implicit functions but here we present a general construction for any finite-dimensional system of constraints.

We begin by constructing a binary Lagrangian function,

$$\mathcal{L} : X \times Y \to \mathbb{R},$$

whose derivative is equal to the desired contraction when $c(x, y) = 0$. More formally we compose $\mathcal{L}$ with the implicit function defined by the constraints to give the unary function

$$\mathcal{L}(x) = \mathcal{L}(x, f(x)) : x \mapsto \mathbb{R},$$

and then require that

$$\frac{d\mathcal{L}}{dx_i}(x) = (J_{g \circ f} \cdot v)_i(x).$$

for forward mode automatic differentiation or

$$\frac{d\mathcal{L}}{dx_i}(x) = (J_{g \circ f}^T \cdot \alpha)_i(x)$$

for reverse mode automatic differentiation. To simplify the presentation from here on we will focus on only this latter application to reverse mode automatic differentiation.
Next we introduce any mapping $\Lambda : Z \to \mathbb{R}$ that preserves the kernel of the constraint function, $\Lambda \circ c(x, y) = 0$ whenever $c(x, y) = 0$. This allows us to define a second function

$$Q = \Lambda \circ c : X \times Y \to \mathbb{R}$$

with $Q(x, f(x)) = 0$ for all $x \in X$.

These two functions together then define an augmented Lagrangian function,

$$\mathcal{J} = \mathcal{L} + Q : X \times Y \to \mathbb{R}.$$

Substituting $y = f(x)$ gives a unary function,

$$\mathcal{J}(x) = \mathcal{J}(x, f(x))$$

$$= \mathcal{L}(x, f(x)) + Q(x, f(x)).$$

The second term, however, vanishes by construction so that $\mathcal{J}(x)$ reduces to $\mathcal{L}(x)$ and

$$\frac{d\mathcal{J}}{dx_i}(x) = \frac{d\mathcal{L}}{dx_i}(x) = (\mathcal{J}^T \circ f \cdot \alpha)_i(x).$$

While the contribution from $C(x, f(x))$ vanishes, its inclusion into the augmented Lagrangian introduces another way to evaluate the desired directional derivative. The total derivative of the unary augmented Lagrangian is

$$\frac{d\mathcal{J}}{dx_i}(x) = \frac{d\mathcal{J}}{dx_i}(x, f(x))$$

$$= \frac{d\mathcal{L}}{dx_i}(x, f(x)) + \frac{dQ}{dx_i}(x, f(x))$$

$$= \frac{\partial \mathcal{L}}{\partial x_i}(x, f(x)) + \left( \frac{\partial \mathcal{L}}{\partial y}(x, f(x)) \circ \frac{\partial f}{\partial x_i} \right)(x)$$

$$+ \frac{\partial Q}{\partial x_i}(x, f(x)) + \left( \frac{\partial Q}{\partial y}(x, f(x)) \circ \frac{\partial f}{\partial x_i} \right)(x)$$

$$= \frac{\partial \mathcal{L}}{\partial x_i}(x, f(x)) + \frac{\partial Q}{\partial x_i}(x, f(x))$$

$$+ \left( \frac{\partial \mathcal{L}}{\partial y}(x, f(x)) + \frac{\partial Q}{\partial y}(x, f(x)) \circ \frac{\partial f}{\partial x_i} \right)(x).$$

Once we’ve identified the solution $y = f(x)$ the first two terms are ordinary partial derivatives that are straightforward to evaluate. The second two terms, however, are tainted by the total derivative of the implicit function, $df/dx$, which is expensive to evaluate as we saw in the previous section.
At this point, however, we can exploit the freedom in the choice of kernel-preserving function \( \Lambda \) and hence \( J \) itself. If we can engineer a \( \Lambda \) such that
\[
\frac{\partial L}{\partial y}(x, f(x)) + \frac{\partial Q}{\partial y}(x, f(x)) = 0
\]
then the contribution from the last two terms, and the explicit dependence on the derivative of the implicit function vanishes entirely!

The adjoint method attempts to solve this adjoint system
\[
\frac{\partial L}{\partial y}(x, f(x)) + \frac{\partial \Lambda}{\partial c}(c(x, f(x))) \circ \frac{\partial c}{\partial y}(x, f(x)) = 0
\]
for a suitable \( \Lambda \) and then evaluate the desired contraction from the remaining two terms,
\[
\frac{dJ}{dx_i}(x) = \frac{\partial L}{\partial x_i}(x, f(x)) + \frac{\partial \Lambda}{\partial c}(c(x, f(x))) \circ \frac{\partial c}{\partial x_i}(x, f(x)).
\]
If a suitable \( \Lambda \) exists, and we can find it, then this two-stage method allows us to evaluate the directional derivative directly without constructing the derivatives of the implicit function.

2.3 Demonstrations

To compare and contrast the two presented methods for evaluating directional derivatives of an implicit function we examine their application on three common implicit systems: algebraic equations, difference equations, and optimization problems.

2.3.1 Algebraic systems. When \( X = \mathbb{R}^I \) and \( Y = \mathbb{R}^J \) a system of \( J \) transverse constraint functions \( c_j(x, y) \) defines an algebraic system and a well-defined implicit function. In Section 2.2.2 we saw that the finite-dimensional implicit function theorem gives the reverse directional derivative
\[
J^T(x) \cdot \alpha = -C_x^T \cdot (C_y^{-1})^T \cdot J_y^T \cdot \alpha.
\]
where
\[
(J_y)_{ij} = \frac{\partial g_j}{\partial y_i}(f(x))
\]
\[
(C_y)_{ij} = \frac{\partial c_i}{\partial y_j}(x, f(x))
\]
\[
(C_x)_{ij} = \frac{\partial c_i}{\partial x_j}(x, f(x)).
\]
Here we will take \( g \) to be the identify function so that \( J_y \) reduces to the identify matrix and the reverse directional derivative simplifies to
\[
J^T(x) \cdot \alpha = -C_x^T \cdot (C_y^{-1})^T \cdot \alpha.
\]
To apply the adjoint method we need to construct a Lagrangian function that satisfies
\[
\frac{dL}{dx_i}(x, f(x)) = (J^T \cdot \alpha)_i(x).
\]
For example we can take
\[
L = f^T(x) \cdot \alpha = \sum_{j=1}^{J} f_j(x) \cdot \alpha_j.
\]
Next we need to augment \(L\) with the contribution from the constraints \(Q\). Because inner products vanish whenever either input is zero we can take
\[
Q = c^T(x, y) \cdot \lambda = \sum_{j=1}^{J} c_j(x, y) \cdot \lambda_j,
\]
for any real-valued, non-zero constants \(\lambda_j\).

With these choices of \(L\) and \(Q\) the adjoint system becomes
\[
0 = \frac{\partial L}{\partial y_j} + \frac{\partial Q}{\partial y_j} = \alpha_j + \sum_{j'=1}^{J} \frac{\partial c_{j'}}{\partial y_j}(x, f(x)) \cdot \lambda_{j'},
\]
or, in matrix notation,
\[
0 = \alpha + C^T_y \cdot \lambda.
\]
Because \(C_y\) is non-singular we can directly solve this for \(\lambda\),
\[
\lambda = -(C^{-1}_y)^T \cdot \alpha.
\]

Substituting this into the remaining terms then gives
\[
(J^T \cdot \alpha)_i(x) = \frac{dJ}{dx_i}(x, f(x))
\]
\[
= \frac{\partial L}{\partial x_i}(x, f(x)) + \frac{\partial Q}{\partial x_i}(x, f(x))
\]
\[
= 0 + \sum_{j'=1}^{J} \lambda_{j'} \cdot \frac{\partial c_{j'}}{\partial x_i}(x, f(x))
\]
\[
= (C^T_x \cdot \lambda)_i
\]
\[
= (-C^T_x \cdot (C^{-1}_y)^T \cdot \alpha)_i,
\]
or
\[ J^T \cdot \alpha = -C_x^T \cdot (C_y^{-1})^T \cdot J_g^T \cdot \alpha. \]
which is exactly the same as the result from the implicit function theorem.

In this general case there isn’t any structure in the constraint functions to exploit and consequently both methods yield equivalent calculations.

### 2.3.2 Difference Equations

To better contrast the two methods let’s consider a more structured system. A discrete dynamical system over the state space \( \mathbb{R}^N \) defines trajectories
\[ y = (y_1, \ldots, y_i, \ldots, y_I), \]
where the individual states \( y_i \in \mathbb{R}^N \) are implicitly defined by the difference equations
\[ y_{i+1} - y_i = \Delta(y_i, x, i), \]
for some initial condition \( y_0 = u(x) \). To simplify the notation we will write
\[ \Delta_i = \Delta(y_i, x, i) \]
from here on.

Organizing these difference equations into constraint equations defines a highly structured algebraic system,
\[
\begin{align*}
y_1 - y_0 - \Delta_0 &= c_1(x, y) = 0 \\
\vdots \\
y_i - y_{i-1} - \Delta_{i-1} &= c_i(x, y) = 0 \\
\vdots \\
y_I - y_{I-1} - \Delta_{I-1} &= c_I(x, y) = 0,
\end{align*}
\]
which then sets the stage for the implicit function machinery.

Formally this system of constraints defines an entire trajectory; the output space is given by \( Y \subset \mathbb{R}^{N \times I} \). Often, however, we are interested not in the entire trajectory but only the final state, \( y_I \in \mathbb{R}^N \). Conveniently we can readily accommodate this by using the summary function to project out the final state,
\[ g : Y = \mathbb{R}^{N \times I} \to \mathbb{R} \\
(y_1, \ldots, y_i, \ldots, y_I) \mapsto y_I. \]

Having defined an implicit system and summary function we can now apply the implicit function theorem and adjoint methods to derive the gradients of the implicitly-defined final
state. Although these two methods yield equivalent results, the adjoint method more directly incorporates the natural structure of the problem without any explicit linear algebra.

**Differentiation with the Implicit Function Theorem.** To apply the implicit function theorem directly we proceed as in 2.3.1 and and compute

\[
J^T \cdot \alpha = -C_x^T \cdot (C_y^{-1})^T \cdot J_g^T \cdot \alpha.
\]

term by term from the right.

Our chosen summary function yields the Jacobian matrix

\[
J_g = \frac{\partial g}{\partial y} = [0_N, \cdots, 0_N, I_N],
\]

where 0\(_N\) is an \(N \times N\) matrix of zeros and \(I_N\) is the \(N \times N\) identity matrix. The first contraction on the right then gives

\[
\beta^T = (J_g^T \cdot \alpha)^T = [0, 0, \cdots, 0, \alpha_1, \alpha_2, \cdots, \alpha_N].
\]

At this point we construct \(C_y\) from the derivatives of the constraint functions,

\[
C_y = \begin{bmatrix}
I_N & 0_N & \cdots \\
C_y^1 & I_N & 0_N & \cdots \\
0_N & C_y^2 & I_N & 0_N & \cdots \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
0_N & \cdots & \cdots & C_y^{I-1} & I_N
\end{bmatrix},
\]

where

\[
C_y^i = \frac{\partial}{\partial y_i}(y_{i+1} - y_i - \Delta_i) = -1 - \frac{\partial \Delta_i}{\partial y_i},
\]

and then solve the linear system

\[
C_y^T \cdot \gamma = \beta.
\]

Because of the structure of the constraints the matrix \(C_y\) is triangular and with enough linear algebra proficiency we would know that we can efficiently solve for \(\gamma\) with backwards elimination. To clarify the derivation we first split the elements of \(\gamma\) into subvectors of length \(N\),

\[
\gamma^T = [\gamma_1, \ldots, \gamma_I].
\]

The linear system can then be written as

\[
\begin{bmatrix}
I_N & C_y^1 & 0_N & \cdots \\
0_N & I_N & C_y^2 & 0_N & \cdots \\
0_N & 0_N & I_N & C_y^3 & 0_N & \cdots \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots \\
0 & \cdots & \cdots & 0 & I_N
\end{bmatrix}
\begin{bmatrix}
\gamma_1 \\
\gamma_2 \\
\gamma_3 \\
\vdots \\
\gamma_I
\end{bmatrix}
= \begin{bmatrix}
0 \\
0 \\
0 \\
\vdots \\
\alpha
\end{bmatrix}.
\]
Starting from the bottom and going up we can solve this system recursively to obtain the backward difference equations

$$
\gamma_i - \left(1 + \frac{\partial \Delta_i}{\partial y_i}\right) \gamma_{i+1} = 0
$$

with terminal condition

$$
\gamma_I = \alpha.
$$

We now evaluate \(C_x\); for \(i > 1\) the derivatives are straightforward,

$$
(C_x)_i = \frac{\partial c_i}{\partial x} = -\frac{\partial \Delta_{i-1}}{\partial x},
$$

but for \(i = 1\) we have to be careful to incorporate the implicit dependence of the initial state, \(y_0 = u(x)\), on \(x\),

$$
(C_x)_1 = \frac{\partial c_1}{\partial x} = \frac{\partial}{\partial x} (y_1 - y_0 - \Delta(y_0, x, 0))
= \frac{\partial}{\partial x} (y_1 - u(x) - \Delta(u(x), x, 0))
= -\frac{\partial u}{\partial x} - \left(\frac{\partial \Delta}{\partial u} + \frac{\partial \Delta}{\partial u} \cdot \frac{\partial u}{\partial x}\right)
= - \left(1 + \frac{\partial \Delta}{\partial u}\right) \frac{\partial u}{\partial x} - \frac{\partial \Delta}{\partial x}.
$$

Finally we multiply \(C_x\) and \(\gamma\) to give

$$
\left(\frac{dy_I}{dx}\right)^T \cdot \alpha = -C_x^T \cdot \gamma
= \left(\frac{\partial u}{\partial x}\right)^T \cdot \left(1 + \frac{\partial \Delta_0}{\partial u}\right)^T \cdot \gamma_1 + \sum_{i=1}^I \left(\frac{\partial \Delta_{i-1}}{\partial x}\right)^T \cdot \gamma_i.
$$

Although the steps are straightforward, implementing them correctly, let alone efficiently, has required careful organization.

**Differentiation with the Adjoint Method.** Because this discrete dynamical system is a special case of an algebraic system we could appeal to the augmented Lagrangian that we constructed in Section 2.3.1 and then repeat the same linear algebra needed for the implicit function theorem method. A more astute choice of Lagrangian, however, allows us to directly exploit the structure of the constraints and the summary function.
Given our choice of summary function we need to construct a Lagrangian function which satisfies
\[
\frac{\partial \mathcal{L}}{\partial x_i}(x, y_I) = \left( \frac{dy_I}{dx_i} \right)^T \cdot \alpha.
\]
Because \( \Delta_i \) is a telescoping series,
\[
y_I = u(x) + \sum_{i=1}^{I} \Delta_i,
\]
a natural choice is
\[
\mathcal{L}(x, y) = y_I^T \cdot \alpha
\]
\[
= u^T(x) \cdot \alpha + \sum_{i=1}^{I} \Delta_i^T \cdot \alpha.
\]
For the constraint term \( \mathcal{C} \) we utilize a similar form as in the general algebraic case,
\[
\mathcal{Q}(x, y) = \sum_{i=1}^{I} c_i^T \cdot \lambda_i
\]
\[
= \sum_{i=1}^{I} [y_i - y_{i-1} - \Delta_{i-1}]^T \cdot \lambda_i,
\]
where \( \lambda_i \in \mathbb{R}^N \).

The adjoint system defined by \( \mathcal{L} \) and \( \mathcal{Q} \) decouples into the equations
\[
0 = \frac{\partial \mathcal{L}}{\partial y_i} + \frac{\partial \mathcal{Q}}{\partial y_i}
\]
\[
= \left( \frac{\partial \Delta_i}{\partial y_i} \right)^T \cdot \alpha + \lambda_{i+1} - \lambda_i - \left( \frac{\partial \Delta_i}{\partial y_i} \right)^T \cdot \lambda_i.
\]
for \( i \in \{1, \ldots, I-1\} \) along with the terminal condition for \( i = I \),
\[
0 = \lambda_I.
\]
In other words the adjoint system defines a \textit{backward difference equation} that we can solve recursively from \( \lambda_I \) to \( \lambda_{I-1} \) all the way to \( \lambda_1 \).

Once we have solved for these adjoint states we can substitute them into the remaining terms to give the desired directional derivative,
\[
\left( \frac{dy_I}{dx} \right)^T \cdot \alpha = \frac{\partial \mathcal{L}}{\partial x} + \frac{\partial \mathcal{Q}}{\partial x}
\]
\[
= \left( \frac{\partial u}{\partial x} \right)^T \cdot \left( 1 + \frac{\partial \Delta_0}{\partial u} \right)^T \cdot (\alpha - \lambda_0) + \sum_{i=1}^{I} \left( \frac{\partial \Delta_i}{\partial x} \right)^T \cdot (\alpha - \lambda_i).
As expected the adjoint method has provided an alternative path to the same result we obtained with the implicit function theorem. Indeed matching the two expressions for \((dy/dx)\cdot \alpha\), suggests taking
\[
\gamma_i = \alpha - \lambda_i,
\]
in which case the intermediate difference equations that arise in both methods are exactly the same as well! The advantage of the adjoint method is that we did not have to construct \(J_g, C_y, \) or \(C_x\), let alone manage their sparsity to ensure the most efficient computation.

Note also that this procedure yields the same result for difference equations derived in (Betancourt, Margossian and Leos-Barajas, 2020) only with fewer steps, and hence fewer opportunities for mistakes.

2.3.3 Optimization. Another common class of finite-dimensional, implicit functions are defined as solutions to optimization problems. Given an objective function \(F : X \times Y \to \mathbb{R}\) we can define the output of the implicit function as the value which maximizes that objective function for a given input,
\[
y = \arg\max_v F(x, v).
\]

In a neighborhood \(U \times V \subset X \times Y\) where \(F(x, -)\) is convex for all \(x \in U\), this implicit function is also defined by the differential constraint
\[
c(x, y) = \frac{\partial F}{\partial y}(x, y) = 0,
\]
which allows us to apply our machinery to evaluate the derivatives of this implicit function. The convexity constraint is key here; without it the constraint function will identify only general extrema which can include not only maxima but also minima and saddle points.

When \(X \subset \mathbb{R}^I\) and \(Y \subset \mathbb{R}^J\) the differential constraint function reduces to an algebraic system and we can directly apply the results of Section 2.3.1. In particular without any assumptions on the objective function there is no difference in the implementation of the implicit function theorem or adjoint methods.

We start by setting the summary function to the identity so that \(J_g = I\) and
\[
\beta = J_g^T \cdot \alpha = \alpha.
\]

Next we compute
\[
(C_y)_{ij} = \frac{\partial c_i}{\partial y_j}(x, y) = \frac{\partial^2 F}{\partial y_i \partial y_j}(x, y),
\]
for example analytically or with higher-order automatic differentiation (Griewank and Walther, 2008; Betancourt, 2018). Conveniently when the optimization is implemented with a higher-order numerical method this Hessian matrix will already be available at the final solution.
Once $C_y$ has been constructed we then solve the linear system

$$\frac{\partial^2 F}{\partial y_i \partial y_j}(x, y) \cdot \gamma = \alpha.$$ 

Finally we construct

$$(C_x)_{ij} = \frac{\partial c_i}{\partial x_j} = \frac{\partial^2 F}{\partial y_i \partial x_j},$$

and then evaluate

$$J^T \cdot \alpha = -C_x^T \cdot \gamma.$$ 

This final contraction defines a second-order directional derivative of the objective function. Conveniently it can be evaluated with higher-order automatic differentiation without having to explicitly construct $C_x$.

These optimization problems become more sophisticated with the introduction of an additional equality constraint so that the output of the implicit function is now defined by the condition

$$y = \arg\max_s F(x, s) \text{ such that } k(x, y) = 0,$$

for the auxiliary constraint function $k : \mathbb{R}^I \times \mathbb{R}^J \to \mathbb{R}^K$.

In order to define an implicit system that consistently incorporates both of these constraints we have to augment the output space. We first introduce the Lagrange multipliers $\mu \in M \subset \mathbb{R}^K$ and the augmented objective function

$$\Phi : X \times Y \times M \to \mathbb{R}
\quad (x, y, \mu) \mapsto F(x, y) + \mu \cdot k(x, y).$$

A consistent solution to the constrained optimization problem is then given by

$$(y, \mu) = \arg\max_{s, m} \Phi(x, s, m).$$

In other words we can incorporate all of the constraints directly on the augmented output space $\zeta = (y, \mu)$ and then project back down to the original output space using the summary function $g : (y, \mu) \mapsto y$.

Within a sufficiently convex neighborhood we can also define the constrained optimization problem with a constraint function over this augmented output space,

$$c(x, \zeta) = \frac{\partial \Phi}{\partial \zeta}(x, \zeta) = 0,$$

which allows us to apply our methods for evaluating directional derivatives.
From the projective summary function we first construct
\[ \beta = J^T g \cdot \alpha. \]
Next we differentiate the constraint function on the augmented output space,
\[ (C_\zeta)_{ij} = \frac{\partial^2 \Phi}{\partial \zeta_i \partial \zeta_j}(x, \zeta), \]
and then solve the linear system
\[ \frac{\partial^2 \Phi}{\partial \zeta_i \partial \zeta_j}(x, \zeta) \cdot \gamma = \beta. \]
Finally we construct
\[ (C_x)_{ij} = \frac{\partial^2 \Phi}{\partial \zeta_i \partial x_j}, \]
and then evaluate
\[ J^T \cdot \alpha = -C_x^T \cdot \gamma. \]
As before this final contraction defines a second-order directional derivative that can be directly evaluated with higher-order automatic differentiation, although this time on the augmented output space.

Inequality constraints introduce an additional challenge. While the Karush-Kuhn-Tucker conditions define an appropriate system of constraints (Karush, 1939; Kuhn and Tucker, 1951), the dimension of the constraint space varies with the input \( x \) as different inequality constraints become active. Moreover even when the objective function and the additional constraint functions are all smooth the implicit function they define might not be differentiable at every \( x \). We leave a detailed treatment of this problem to future work.

3. AUTOMATIC DIFFERENTIATION OF INFINITE-DIMENSIONAL IMPLICIT FUNCTIONS

With care in how derivatives are defined we can immediately generalize the finite dimensional methods for evaluating directional derivatives of implicit functions to infinite dimensional systems, for example systems that implicitly define entire trajectories, fields, or even probability distributions. In this section we review the basics of differentiable, infinite dimensional spaces and the generalization of the implicit function theorem before generalizing the directional derivative evaluation methods and demonstrating them on two instructive examples.
3.1 The Infinite-Dimensional Implicit Function Theorem

The machinery of differential calculus over the real numbers generalizes quite naturally to a Fréchet calculus over Banach vector spaces. In this section we review the key concepts and then use them to construct an infinite-dimensional implicit function theorem. For a more in depth presentation of these topics see for example Kesavan (2020).

3.1.1 Fréchet derivatives. The Fréchet derivative generalizes the concept of a derivative that we introduced for real spaces to the more general Banach vector spaces, or more compactly Banach spaces. Banach spaces include not only finite-dimensional Euclidean vector spaces but also infinite-dimensional function spaces.

Consider two Banach spaces, $X$ and $Y$, and a function $f : X \to Y$ mapping between them. If $f$ is Fréchet differentiable then the Fréchet derivative assigns to each input point $x \in X$ a bounded, linear map

$$\frac{\delta f}{\delta x} : X \to \text{BL}(X,Y),$$

where $\text{BL}(X,Y)$ is the space of bounded, linear functions from $X$ to $Y$. In other words the Fréchet derivative of $f$ evaluated at $x$ defines a bounded, linear map from $X$ to $Y$,

$$\frac{\delta f}{\delta x}(x) : X \to Y.$$

Note that unlike the total derivative we introduced on real spaces the Fréchet derivative is defined directly on a vector space and so there is no distinction between locations and directions.

If $Z$ is a third Banach space then the composition of $f$ with $g : Y \to Z$ defines a map from $X$ to $Z$,

$$g \circ f : X \to Z.$$

The Fréchet derivative of this composition,

$$\frac{\delta(g \circ f)}{\delta x} : X \to Z,$$

follows a chain rule,

$$\frac{\delta(g \circ f)}{\delta x}(x) = \frac{\delta g}{\delta x}(f(x)) \circ \frac{\delta f}{\delta x}(x).$$

A binary map $h : X \times Y \to Z$ also admits a partial Fréchet derivative. For example the partial Fréchet derivative of $h$ with respect to the first input defines a map

$$\frac{\delta h}{\delta x} : X \times Y \to \text{BL}(X, Z).$$
Equivalently the partial Fréchet derivative of \( h \) evaluated at \( (x, y) \) is a bounded, linear map from \( X \) to \( Z \),
\[
\frac{\delta h}{\delta x}(x, y) : X \to Z.
\]
Similarly we can define a partial derivative with respect to the second output as
\[
\frac{\delta h}{\delta y} : X \times Y \to \text{BL}(Y, Z)
\]
with
\[
\frac{\delta h}{\delta y}(x, y) : Y \to Z.
\]

When a binary map like \( h \) is composed with unary maps in each argument then we can use the chain rule to define a notion of a total Fréchet derivative. Let \( h : X \times Y \to Z \), \( f : W \to X \) and \( g : W \to Y \). The component-wise composition \( h(f(\cdot), g(\cdot)) \) then defines a unary map
\[
q = h(f(\cdot), g(\cdot)) : W \to Z,
\]
with the corresponding Fréchet derivative
\[
\frac{\delta q}{\delta w}(w) : W \to Z,
\]
which decomposes into contributions from each argument,
\[
\frac{\delta q}{\delta x}(w) = \frac{\delta h}{\delta x}(f(w), g(w)) \circ \frac{\delta f}{\delta w}(w) + \frac{\delta h}{\delta y}(f(w), g(w)) \circ \frac{\delta g}{\delta w}(w).
\]

3.1.2 The Implicit Function Theorem. The finite dimensional implicit function theorem immediately generalizes to Banach spaces with the use of Fréchet derivatives. Consider a Banach space of known inputs, \( X \), a Banach space of unknown outputs, \( Y \), a Banach space of constraint values, \( Z \), and the constraint function
\[
c : X \times Y \to Z
\]
\[
(x, y) \mapsto c(x, y).
\]
Once again, we examine a particular input, \( x \in X \), and the neighborhoods \( x \in U \subset X \), \( V \subset Y \) and \( W \subset Z \).

If \( c \) is Fréchet differentiable across \( U \times V \) then it defines two partial Fréchet derivatives
\[
\frac{\delta c}{\delta x}(x, y) : U \to W
\]
and
\[
\frac{\delta c}{\delta y}(x, y) : V \to W.
\]
When $\delta c/\delta y(y)$ defines a bijection from $V$ to $W$ we can also define a corresponding inverse operator,

$$\left(\frac{\delta c}{\delta y}(x, y)\right)^{-1} : W \to V.$$ 

In this case the implicit function theorem guarantees that the kernel of the constraint function, $c^{-1}(0)$, implicitly defines a Fréchet differentiable function from the input space to the output space, $f : U \to V$ that satisfies $c(x, f(x)) = 0$.

As in the finite-dimensional case we can calculate the Fréchet derivative of this implicit function by differentiating the constraint function,

$$0 = \frac{\delta c}{\delta x}(x) = \frac{\delta c}{\delta x}(x, y) + \frac{\delta c}{\delta y}(x, y) \circ \frac{\delta y}{\delta x}(x).$$

Because $\delta c/\delta y$ is invertible at $(x, f(x))$ we can immediately solve for $\delta y/\delta x$ to give

$$\frac{\delta f}{\delta x}(x) = - \left(\frac{\delta c}{\delta y}(x, f(x))\right)^{-1} \circ \frac{\delta c}{\delta x}(x, f(x)).$$

Moving forward we will denote $J_f = \delta f/\delta x(x)$ the Fréchet Jacobian.

### 3.2 Evaluating Directional Derivatives of Infinite-Dimensional Implicit Functions

While we can handle infinite dimensional spaces mathematically any practical automatic differentiation implementation will be restricted to finite dimensional inputs and final outputs. To that end we will assume that the input space is real, $X = \mathbb{R}^I$, while allowing the output space $Y$ to be infinite dimensional, for example corresponding to a smooth trajectory or a latent field. We will use the summary function, however, to project that potentially-infinite dimensional output to a finite-dimensional real space, $g : Y \to \mathbb{R}^J$. For example we might consider a dynamical system that defines an entire trajectory but project out only the finite-dimensional final state.

In order to implement such a system in a reverse mode automatic differentiation library we then need to be able to evaluate the reverse directional derivative

$$J_{gof}^\dagger(x)(\alpha) = (J_f^\dagger(x) \circ J_g^\dagger(f(x)))(\alpha).$$

Because $g \circ f$ is a real-to-real map the total action is given by a matrix-vector product,

$$J_{gof}^\dagger(x)(\alpha) = J_{gof}^T \cdot \alpha,$$
but the component operators $J^\dagger_f(x)$ and $J^\dagger_y(f(x))$ will not be unless $Y$ is a finite-dimensional real space.

Here we will consider the generalizations of the three methods for evaluating this directional derivative that we constructed in Section 2.

3.2.1 Trace Method. Although we can’t practically construct a numerical method for an implicit function $f : \mathbb{R}^I \rightarrow Y$ with infinite-dimensional output space, we often can construct numerical methods for the finite-dimensional composition $g \circ f : \mathbb{R}^I \rightarrow \mathbb{R}^J$. Numerical integrators for ordinary and partial differential equations, for example, discretize $Y$ in order to approximate the finite dimensional outputs of $g \circ f$ without having to confront an infinite dimensional space directly.

Because the intermediate calculations of the numerical solver will be finite-dimensional we immediately apply the trace method discussed in Section 2.2.1, automatically differentiating through each iteration of the solve, to approximate $J^\dagger_{g \circ f}(x)(\alpha)$. As in the finite-dimensional case, however, this direct approach is often too computationally expensive and memory intensive to be practical.

3.2.2 Infinite-Dimensional Implicit Function Theorem. In theory the reverse directional derivative is given immediately by the implicit function theorem,

$$J^\dagger_{g \circ f}(x)(\alpha) = (J^\dagger_f(x) \circ J^\dagger_y(f(x)))(\alpha)$$

$$= \left( - \left( \frac{\delta c}{\delta x}(x, f(x)) \right)^\dagger \circ \left( \left( \frac{\delta c}{\delta y}(x, f(x)) \right)^\dagger \right)^{-1} \circ J^\dagger_y(f(x)) \right)(\alpha).$$

Unfortunately whenever $Y$ is infinite-dimensional each of these Fréchet derivatives will be infinite dimensional operators that are difficult, if not impossible, to implement in practice. For example $J^\dagger_y(f(x))$ maps the finite covector $\alpha$ to an infinite dimensional space that can’t be represented in finite memory.

3.2.3 The Infinite-Dimensional Adjoint Method. With a careful use of Fréchet derivatives the adjoint method defined in Section 2.2.3 generalizes to the case where $Y$ and $Z$ are general Banach spaces. As usual we consider a particular input, $x \in X$, and the neighborhoods $x \in U \subset X$, $V \subset Y$, and $W \subset Z$.

We first define a binary Lagrangian functional

$$\mathcal{L} : U \times V \rightarrow \mathbb{R}$$

that gives a unary functional when we substitute the solution of the implicit function,

$$\mathcal{L}(x) = \mathcal{L}(x, f(x))$$
with the Fréchet derivative
\[ \frac{\delta L}{\delta x}(x) = J^\dagger_{g \circ f}(x)(\alpha). \]

Next we introduce a mapping \( \Lambda : W \to \mathbb{R} \) that preserves the kernel of the constraint function, \( \Lambda \circ c(x, y) = 0 \) whenever \( c(x, y) = 0 \). Composing this mapping with the constraint function gives the constraint Lagrangian functional,
\[ Q = \Lambda \circ c : U \times V \to \mathbb{R}, \]
with \( Q(x, f(x)) = 0 \) for all \( x \in U \).

Together these two functionals define an augmented Lagrangian functional,
\[ J = L + Q, \]
along with the corresponding unary functional
\[ J(x) = J(x, f(x)) = L(x, f(x)) + Q(x, f(x)) = L(x, f(x)), \]
because the constraint functional vanishes by construction when evaluated at the solution to the constraint problem.

The total derivative of this augmented unary functional is given by
\[ \frac{\delta J}{\delta x}(x) = \frac{\delta J}{\delta x}(x, f(x)) = \frac{\delta J}{\delta x}(x, f(x)) + \frac{\delta J}{\delta y}(x, f(x)) \circ \frac{\delta f}{\delta x}(x). \]

If we could engineer a map \( \Lambda \) such that the adjoint system \( \frac{\delta J}{\delta y} \) vanishes,
\[ 0 = \frac{\delta J}{\delta y}(x, f(x)) = \frac{\delta L}{\delta y}(x, f(x)) + \frac{\delta Q}{\delta y}(x, f(x)) = \frac{\delta L}{\delta y}(x, f(x)) + \frac{\delta \Lambda}{\delta c}(x, f(x)) \circ \frac{\delta c}{\delta y}(x, f(x)) \]
then the reverse directional derivative would reduce to
\[ J^\dagger_{g \circ f}(x)(\alpha) = \frac{\delta J}{\delta x}(x, f(x)) = \frac{\delta L}{\delta x}(x, f(x)) + \frac{\delta Q}{\delta x}(x, f(x)) = \frac{\delta L}{\delta x}(x, f(x)) + \frac{\delta \Lambda}{\delta c}(x, f(x)) \circ \frac{\delta c}{\delta x}(x, f(x)). \]
Unfortunately if $Y$ is infinite-dimensional then the adjoint system also becomes infinite-dimensional, and the general Fréchet derivatives will typically be too ungainly to implement in practice.

One important exception is when $Y$ is a Sobolev space. Informally a Sobolev space of order $k$ is an infinite-dimensional Banach space comprised of integrable, real-valued functions whose first $k$ derivatives are sufficiently well-defined. What makes Sobolev spaces so useful is that a large class of functionals over these spaces can be written as integrals.

Consider for example the input space $T \subseteq \mathbb{R}$, the output space $S \subseteq \mathbb{R}^N$, and the Sobolev space $Y$ of $k$-times differentiable functions $y : T \to S$, such as those arising from the solutions to $k$-th order ordinary differential equations. Any integral of the form

$$G(y) = \int_T dt \ g \left( t, y(t), \frac{dy}{dt}(t), \ldots, \frac{d^K y}{dt^K}(t) \right)$$

defines a unary, real-valued functional $G : Y \to \mathbb{R}$ whose Fréchet derivative is given by

$$\frac{\delta G}{\delta y}(y) = \frac{\delta}{\delta y} \int_T dt \ g \left( t, y(t), y^{(1)}(t), \ldots, y^{(K)}(t) \right)$$

$$= \int_T dt \left[ \frac{\partial g}{\partial y} \left( t, y(t), y^{(1)}(t), \ldots, y^{(K)}(t) \right) + \sum_{k=1}^{K} \frac{\partial g}{\partial y^{(k)}} \left( t, y(t), y^{(1)}(t), \ldots, y^{(K)}(t) \right) \cdot \delta y^{(k)} \right].$$

Similarly if $X \subseteq \mathbb{R}^I$ then

$$G(x, y) = \int_T dt \ g \left( x, t, y(t), y^{(1)}(t), \ldots, y^{(K)}(t) \right)$$

defines a binary, real-valued functional $G : X \times Y \to \mathbb{R}$. Consequently we can construct a large class of Lagrangian functionals and constraint functionals as integrals,

$$L(x, y) = \int_T dt \ l \left( x, t, y(t), y^{(1)}(t), \ldots, y^{(K)}(t) \right)$$

$$Q(x, y) = \int_T dt \ q \left( x, t, y(t), y^{(1)}(t), \ldots, y^{(K)}(t) \right)$$
with the corresponding augmented Lagrangian,

\[ J(x, y) = \int_T dt \left[ l(x, t, y(t), y^{(1)}(t), \ldots, y^{(K)}(t)) + q(x, t, y(t), y^{(1)}(t), \ldots, y^{(K)}(t)) \right]. \]

The choice of \( l \) needs to verify the condition that

\[ J^\dagger_g \circ f(x) = \frac{\delta}{\delta x} L(x, f(x)) = \delta_{\delta x} \int_T dt \left[ \frac{\partial l}{\partial x} (x, t, y(t), y^{(1)}(t), \ldots, y^{(K)}(t)) \right. \]

\[ + \left. \sum_{k=1}^K \frac{\partial l}{\partial y^{(k)}} (t, y(t), y^{(1)}(t), \ldots, y^{(K)}(t)) \cdot \delta y^{(k)} \right]. \]

Depending on the problems, choosing \( l \) can be straightforward or require a bit more work, as we will see in the examples. The choice of \( q \) needs to satisfy the condition that, for all \( x \in U \),

\[ 0 = Q(x, f(x)) = \int_T dt \ q(x, t, y(t), y^{(1)}(t), \ldots, y^{(K)}(t)). \]

One straightforward strategy is to define the integrand \( q \) such that it vanishes whenever evaluated at the solution, \( (x, f(x)) \). We can accomplish this for example by taking \( q \) to be the Sobolev inner product of the constraint function, \( f \), with an auxiliary function \( \lambda \in \mathbb{Z} \),

\[ q(x, f(x)) = \langle \lambda, c(x, f(x)) \rangle, \]

where \( \langle , \rangle \) denotes the Sobolev inner product. When evaluated at the solution the constraint function \( c \) vanishes so that the above inner product, and hence the integrand \( q \), also vanish.
When using functionals of this form the reverse directional derivative becomes

\[ J_{gof}^T(x)(\alpha) = \frac{\delta J}{\delta x}(x, f(x)) \]

\[ = \int_T dt \left[ \frac{\partial j}{\partial x}(x, t, y(t), y^{(1)}(t), \ldots, y^{(K)}(t)) + \frac{\partial j}{\partial y}(x, t, y(t), y^{(1)}(t), \ldots, y^{(K)}(t)) \cdot \frac{dy}{dx}(t) \right. \]

\[ + \sum_{k=1}^{K} \frac{\partial j}{\partial y^{(k)}}(x, t, y(t), y^{(1)}(t), \ldots, y^{(K)}(t)) \cdot \frac{\delta y^{(k)}}{\delta y} \cdot \frac{dy}{dx}(t) \]

\[ = \int_T dt \left[ \frac{\partial j}{\partial x}(x, t, y(t), y^{(1)}(t), \ldots, y^{(K)}(t)) + \frac{\partial j}{\partial y}(x, t, y(t), y^{(1)}(t), \ldots, y^{(K)}(t)) \right. \]

\[ + \sum_{k=1}^{K} \frac{\partial j}{\partial y^{(k)}}(x, t, y(t), y^{(1)}(t), \ldots, y^{(K)}(t)) \cdot \frac{dy^{(k)}}{dx}(t) \right]. \]

Because the elements of the Sobolev space are continuous we can simplify the terms in the last line by repeated application of Stokes’ Theorem,

\[ \int_T dt \frac{\partial j}{\partial y^{(k)}} \cdot \frac{dy^{(k)}}{dx} = \sum_{k'=0}^{k} (-1)^{k'} \int_T dt \left[ \frac{d^{k'}}{dt^{k'}} \left( \frac{\partial j}{\partial y^{(k)}} \right) \right. \]

\[ + \left. \int_T dt \frac{d^{k'} k}{dt^{k-1}} \left( \frac{\partial j}{\partial y^{(k)}} \right) \right] \frac{dy}{dx} \cdot \frac{dy}{dx}. \]

where we have dropped the arguments to ease the notational burden. Substituting this into the reverse directional derivative gives

\[ J_{gof}^T(x)(\alpha) = \int_T dt \frac{\partial j}{\partial x} \]

\[ + \sum_{k=1}^{K} \sum_{k'=0}^{k} (-1)^{k'} \left[ \frac{d^{k'}}{dt^{k'}} \left( \frac{\partial j}{\partial y^{(k)}} \right) \frac{d^{k-k'-1} k}{dt^{k-1}} \left( \frac{dy}{dx} \right) \right] \frac{dy}{dx} \]

\[ + \int_T dt \left[ \frac{\partial j}{\partial y} + \sum_{k=1}^{K} (-1)^{k} \frac{d^{k}}{dt^{k}} \left( \frac{\partial j}{\partial y^{(k)}} \right) \right] \cdot \frac{dy}{dx}. \]
If we can engineer a $q$ such that $j$ solves the differential adjoint system

$$0 = \sum_{k=1}^{K} \sum_{k'=0}^{k} (-1)^{k'} \left[ \frac{d^{k'}}{dt^{k'}} \left( \frac{\partial j}{\partial y^{(k')}} \right) \frac{d^{k-k'-1}}{dt^{k-k'-1}} \left( \frac{dy}{dx} \right) \right]_{\delta t}$$

$$0 = \frac{\partial j}{\partial y} + \sum_{k=1}^{K} (-1)^{k} \frac{d^{k}}{dt^{k}} \left( \frac{\partial j}{\partial y^{(k)}} \right)$$

then the reverse directional derivative reduces to the manageable form

$$J_{\eta^\dagger}(x)(\alpha) = \int_{T} dt \frac{\partial j}{\partial x} (x, t, y(t), y^{(1)}(t), \ldots, y^{(K)}(t))$$

$$= \int_{T} dt \left[ \frac{\partial l}{\partial x} (x, t, y(t), y^{(1)}(t), \ldots, y^{(K)}(t)) + \frac{\partial q}{\partial x} (x, t, y(t), y^{(1)}(t), \ldots, y^{(K)}(t)) \right].$$

For different choices of $Y$ the form of the functionals, their Fréchet derivatives, and the resulting differential adjoint system will vary, but the basic procedure of the adjoint method remains the same. By considering more sophisticated Sobolev spaces this general adjoint method can be applied to partial differential equations and other more sophisticated infinite-dimensional implicit systems.

### 3.3 Demonstrations

The particular differential adjoint system we have derived in Section 3.2.3 is immediately applicable to implicit systems defined by ordinary differential and algebraic differential equations. In this section we demonstrate that application on two such systems.

#### 3.3.1 Ordinary Differential Equations.

Consider a time interval $T = [0, \tau] \subset \mathbb{R}$ and the $N$-dimensional trajectories that map each time point to an $N$-dimensional state, $y : T \rightarrow \mathbb{R}^{N}$. The space of trajectories that are at least once-differentiable forms a first-order Sobolev space, $Y$.

A linear system of first-order, ordinary differential equations

$$\frac{dy}{dt} = r(x, y, t),$$

along with an initial condition $y(0) = u(x)$, defines a separate constraint for the trajectory behavior at each $t \in T$,

$$c(x, y)(t) = \frac{dy}{dt}(t) - r(x, y)(t)$$

$$c(x, y)(0) = y(0) - u(x).$$
Collecting all of these constraints together defines an infinite-dimensional constraint function \( c : X \times Y \rightarrow Z \) where \( Z \) is also the space of differentiable functions that map from \( T \) to \( \mathbb{R}^N \).

The summary function \( g : y \mapsto y(\tau) \) projects infinite-dimensional trajectories down to their \( N \)-dimensional final states so that the composition \( g \circ f \) maps inputs \( x \in X \) to a final state at time \( t = \tau \). In order to implement this map into a reverse mode automatic differentiation library we need to be able to implement the reverse directional derivative \( J_{g \circ f}^\dagger(x)(\alpha) \).

To implement the adjoint method we need a Lagrangian functional that satisfies

\[
\frac{d\mathcal{L}}{dx_i}(x, f(x)) = \left( \frac{dy}{dx_i}(T) \right)^T \cdot \alpha.
\]

Integrating the defining differential equation gives an integral functional that provides a particularly useful option,

\[
\mathcal{L}(x, y) = u^T(x) \cdot \alpha + \int_0^T dt \ r^T(x, y, t) \cdot \alpha.
\]

Next we need to construct a functional \( Q \) that vanishes when when evaluated at the implicit solution. Integrating over the constraint function gives

\[
Q(x, y) = \left[ y(0) - u(x) \right]^T \cdot \mu + \int_0^T dt \ \left[ \frac{dy}{dt}(t) - r(x, y, t) \right]^T \cdot \lambda(t),
\]

for any function \( \lambda : \mathbb{R} \rightarrow \mathbb{R}^N \) and constant \( \mu \in \mathbb{R}^N \).

Substituting these integral functionals into the differential adjoint system that we derived in Section 3.2.3 yields the system

\[
0 = \left( \frac{dy}{dx}(0) \right)^T \cdot (\mu - \lambda(0)) + \left( \frac{dy}{dx}(\tau) \right)^T \cdot \lambda(\tau)
\]

\[
0 = \left( \frac{\partial r}{\partial y}(x, y, t) \right)^T \cdot (\alpha - \lambda(t)) - \frac{d\lambda}{dt}(t).
\]

The boundary terms vanish if we take \( \mu = \lambda(0) \) and \( \lambda(\tau) = 0 \) while the differential term vanishes for the \( \lambda(t) \) given by integrating \( \lambda(\tau) = 0 \) backwards from \( t = \tau \) to \( t = 0 \). In other words the differential adjoint system defines a linear, first-order ordinary differential equation that reverses time relative to our initial ordinary differential equation.

Once we’ve solved for \( \lambda(t) \) the reverse directional derivative is given by the partial derivatives of the augmented Lagrangian with respect to \( x \),

\[
J_{g \circ f}^\dagger(x)(\alpha) = \left( \frac{\partial u}{\partial x}(x) \right)^T \cdot (\alpha - \lambda(0)) + \int_0^T dt \left( \frac{\partial r}{\partial x}(x, y, t) \right)^T \cdot (\alpha - \lambda(t)).
\]
While we do have to solve both the nominal and adjoint differential equations, these solves require evaluating only finite-dimensional derivatives. We have completely avoided any infinite-dimensional Fréchet derivatives.

3.3.2 Differential Algebraic Equations. Introducing an algebraic constraint to the previous systems defines a differentiable algebraic system, or DAE. A DAE might, for example, impose the constraint that the component states at each time sum to one so that the states can model how the allocation of a conserved quantity evolves over time.

To simplify the derivation we start by decomposing the trajectories $y(t) \in \mathbb{R}^N$ into a differential component, $y^d \in \mathbb{R}^D$, and an algebraic component, $y^a \in \mathbb{R}^A$, with $N = D + A$. A differential algebraic constraint function can similarly be decomposed into a differential constraint function,

$$c^d(x, y^d, \dot{y}^d, t) \in \mathbb{R}^D,$$

where $\dot{y}$ is shorthand for $dy/dt$, and an algebraic constraint function,

$$c^a(x, y^a, t) \in \mathbb{R}^A.$$

with $c = (c^d, c^a)^T$.

If the differential constraint is given by a linear, first-order differential equation then the differential constraint function becomes

$$c^d(x, y^d, \dot{y}^d, t) = \dot{y}^d - r^d(x, y, t)$$

$$c^d(x, y^d, \dot{y}^d, 0) = y(0) - u(x).$$

When the constraints are consistent this differential algebraic system implicitly defines a map from inputs $x \in X$ to $N$-state trajectories, $y \in T \times \mathbb{R}^N$. We can also write this as a map from inputs and times to states,

$$f : X \times T \rightarrow \mathbb{R}^N,$$

such that $c^d(x, f(x), \dot{f}(x), t) = 0$ and $c^a(x, f(x), t) = 0$.

As in the previous example we will consider a summary function that projects the infinite-dimensional trajectories down to their $N$-dimensional final states, $g : y \mapsto y(\tau)$, so that the composition $g \circ f$ maps inputs $x \in X$ to a final state at time $t = \tau$. Our goal is then to evaluate the finite-dimensional reverse directional derivative $J_{g\circ f}(x)(\alpha)$.

As with ordinary differential systems integrating the trajectory provides an appropriate integral functional,

$$\mathcal{L}(x, y) = u^T(x) \cdot \alpha + \int_0^\tau dt \, \dot{y}^T(x, t) \cdot \alpha$$
that satisfies
\[
\frac{dL}{dx}(x, f(x)) = \left( \frac{df}{dx}(x, \tau) \right)^T \cdot \alpha.
\]

Unlike in the ordinary differential case, however, the differential algebraic system does not immediately provide an analytical expression for \(\dot{y}(x)\).

The first-order linear differential equation does provide the derivative of the differential component,
\[
\dot{y}^d = r^d.
\]

In order to obtain the derivative of the algebraic component we have to differentiate the algebraic constraint,
\[
0 = \frac{\partial c^a_{\partial y^a}}{\partial y^a} \dot{y}^d(x, t) + \frac{\partial c^a_{\partial y^a}}{\partial y^a} \dot{y}^a(x, t) + \frac{\partial c^a_{\partial t}}{\partial t}(x, t),
\]
or
\[
\dot{y}^a = - \left[ \frac{\partial c^a}{\partial y^a} \right]^{-1} \left( \frac{\partial c^a}{\partial y^a} \dot{y}^d + \frac{\partial c^a_{\partial y^a}}{\partial y^a} \right),
\]
where we assume \(\partial c^a / \partial y^a\) is square invertible.

The constraint functional \(Q\) is identical to that from the ordinary differential equation system,
\[
C(x, y) = \left[ y(0) - u(x) \right]^T \cdot \mu + \int_0^\tau dt \ c(x, y, t)^T \cdot \lambda(t).
\]

Plugging \(J = \mathcal{L} + Q\) into the results of Section 3.2.3 gives the system
\[
0 = \left[ \frac{dy}{dx}(0) - \frac{du}{dx}(x) \right]^T \cdot \mu + \left( \frac{dy}{dx} \right)^T \cdot \lambda_{D0}(t) \bigg|_0^\tau
\]
\[
0 = \left( \frac{\partial r}{\partial y} (x, y, t) \right)^T \cdot \alpha + \left( \frac{\partial c}{\partial y}(x, y, t) \right)^T \cdot \lambda(t) - \lambda_{D0}(t)
\]
where

$$\lambda_{D0}(t) = \left(\frac{\partial c}{\partial y}(x, y, t)\right)^T \cdot \lambda(t)$$

$$= \left[\frac{\partial c_d}{\partial y_d} \frac{\partial c_d}{\partial y_d} \frac{\partial c_a}{\partial y_a}\right] \cdot \lambda(t)$$

$$= \begin{bmatrix} I_{D \times D} & 0_{D \times A} \\ 0_{A \times D} & 0_{A \times A} \end{bmatrix} \cdot \lambda(t)$$

$$= \begin{bmatrix} \lambda_{1:D}(t) \\ 0_{1 \times A} \end{bmatrix}.$$ 

Decomposing each term in the differential adjoint system into algebraic and a differential components gives

$$\begin{bmatrix} \left(\frac{\partial r}{\partial y_d}(x, y, t)\right)^T T \cdot \alpha + \left(\frac{\partial c_d}{\partial y_d}(x, y, t)\right)^T T \cdot \lambda_d(t) + \left(\frac{\partial c_a}{\partial y_a}(x, y, t)\right)^T T \cdot \lambda_a(t) - \dot{\lambda}_{D0}(t) \\ \left(\frac{\partial r}{\partial y_a}(x, y, t)\right)^T T \cdot \alpha + \left(\frac{\partial c_a}{\partial y_a}(x, y, t)\right)^T T \cdot \lambda_d(t) + \left(\frac{\partial c_a}{\partial y_a}(x, y, t)\right)^T T \cdot \lambda_a(t) \end{bmatrix} = \begin{bmatrix} 0_D \\ 0_A \end{bmatrix}.$$ 

which defines an adjoint DAE

To ensure that the boundary term vanish we need to set $\mu = \lambda_{D0}(0)$ and $\lambda_{D0}(\tau) = 0_N$.

The algebraic component of $\lambda$ at $t = \tau$ is also given by

$$0_A = \left(\frac{\partial r}{\partial y_a}(x, y, \tau)\right)^T T \cdot \alpha + 0 + \left(\frac{\partial c_a}{\partial y_a}(x, y, \tau)\right)^T T \cdot \lambda_a(\tau)$$

$$\lambda_a(\tau) = -\left[\left(\frac{\partial c_a}{\partial y_a}(x, y, \tau)\right)^{-1}\right] \left(\frac{\partial r}{\partial y_a}(x, y, \tau)\right)^T T \cdot \alpha,$$

where we recall our assumption that $\partial c_a/\partial y_a$ is square invertible.

Now we can ensure that the differential term vanishes by integrating this adjoint DAE backwards from the terminal condition $\lambda(\tau) = (\lambda_d(\tau), \lambda_a(\tau))^T$ at $t = \tau$ to an initial condition at $t = 0$.

Once we have solved for $\lambda(t)$ the reverse directional derivative reduces to

$$J^\dagger_{yf}(x)(\alpha) = -\left(\frac{du}{dx_i}\right)^T \cdot \lambda_{D0}(0) + \int_0^\tau dt \left(\frac{\partial r}{\partial x_i}(x, y, t) + \lambda^T \frac{\partial c}{\partial x_i}(x, y, t)\right)^T \cdot \lambda(t).$$

### 4. DISCUSSION

The implicit function theorem allows us to construct an expression for the directional derivatives of an implicit function as a composition of Fréchet derivatives. The adjoint
method computes these directional derivatives directly without evaluating any of the intermediate terms.

When the output of the implicit function is finite-dimensional these differential operators can be implemented with linear algebra, although care and experience is required to ensure that the linear algebra operations are as efficient as possible. While the adjoint method yields the same result, it naturally incorporates any available structure in the implicit system so that optimal performance can be achieved automatically as we saw in our discussion on difference equations (Section 2.3.2).

If the output of the implicit function is infinite-dimensional then the component Fréchet derivatives that make up the directional derivatives of the implicit function can no longer be evaluated directly, making the composition intractable. Implementing the adjoint method also requires Fréchet derivatives which in general we cannot evaluate. In the important special case where the output of the implicit function falls into a Sobolev space, however, we can engineer the augmented Lagrangian so that the Fréchet derivatives reduce to tractable functional derivatives. This is notably the strategy we deploy when in the case of ODEs and DAEs (Section 3.3).

While the adjoint method is more generally applicable it is not as systematic as the implicit function theorem method. The practicality and performance of the method depends on the choice of Lagrangian and constraint functionals. Engineering performant functionals, let alone valid functionals at all, is by no means trivial. Fortunately in many problems the structure of the implicit system guides the design.

Beyond the implicit function theorem and adjoint methods, we may use the trace method which automatically differentiates through the trace of a numerical solver. In most cases this approach leads to computationally expensive and memory intensive algorithms.

For finite-dimensional systems we could also construct a “forward method” that computes the Jacobian \( J = J_{g \circ f} \) before evaluating its action on an input sensitivity or adjoint to form the wanted directional derivatives. As we discussed in Section 2.2.1, however, fully computing \( J \) first is always less efficient that the iterative evaluation of the directional derivative; see also Gaebler (2021).

Although not as general, we can also construct a forward method that fully computes the Jacobian \( J = J_{g_0 \circ f} \) for certain infinite-dimensional problems. This approach notably applies to certain classes of ODEs and DAEs (Appendix A). In these cases the computational trade-offs between the forward method and the adjoint method is more nuanced; which method is more efficient depends on the specific of the problem. For example Rackauckas et al. (2018) compares the forward and adjoint approaches to implementing automatic differentiation for ODEs. For small ODE systems the overhead cost associated with solving the adjoint system can make the method relatively slow, but as the size of the system and the dimension of \( x \) increases the adjoint method benefits from superior scal-
ability. See also Hindmarsh and Serban (2020); Betancourt, Margossian and Leos-Barajas (2020) for additional scaling discussions.

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APPENDIX A: INFINITE-DIMENSIONAL FORWARD METHOD

As in Section 3.2 consider finite-dimensional real input, $X = \mathbb{R}^I$, an infinite-dimensional output space $Y$, and the summary function $g : Y \to \mathbb{R}^J$. The forward method explicitly computes the matrix representation of the full Jacobian, $J_{gof}$, before contracting this matrix with a sensitivity or adjoint vector to implement directional derivatives for automatic differentiation.

The implicit function theorem prescribes a composite expression for $J_{gof}$, but in general we cannot evaluate the intermediate Fréchet derivatives. In certain special cases, however, we can bypass the implicit function theorem and evaluate $J_{gof}$ directly.

As with the adjoint method, we focus on the special case where $Y$ is a Sobolev space. Theoretically we can reduce a key Fréchet derivative to a functional derivative, which we can evaluate by solving a forward differential system. In practice our ability to construct such a system and solve it depends on the specifics of the problem.

Let $Y$ be the order $K$ Sobolev space of functions $T \subset \mathbb{R} \to \mathbb{R}^N$, and suppose that we can construct a functional

$$\mathcal{P} : X \times Y \to \mathbb{R}^J$$

$$x,y \mapsto \mathcal{P}(x,y),$$

which satisfies

$$\frac{\delta \mathcal{P}}{\delta x}(x) = J_{gof}(x).$$

In addition, assume there exists such a functional which takes the form of an integral,

$$\mathcal{P}(x,y) = \int_T dt \ p(x,t,y(t),...).$$

For example if our summary function $g$ is a Sobolev inner product with the implicit func-
\[(g \circ f)(x) = \langle \gamma, f(x) \rangle = \int dt \gamma(t) f(x, t) = \int dt \gamma^T(t) \cdot y(x, t)\]

then we can take
\[p = \gamma^T(t) \cdot y(x, t),\]
and obtain a satisfactory functional \(P\).

Taking the derivative with respect to \(x\) gives,
\[
\frac{\delta P}{\delta x} = \int_T dt \frac{dp}{dx} \left( x, t, y(t), y^{(1)}(t), \cdots, y^{(K)}(t) \right) = \int_T dt \frac{\partial p}{\partial x} + \sum_{k=0}^K \frac{\partial p}{\partial y^{(k)}} \frac{dy^{(k)}}{dx},
\]
where crucially the Fréchet derivative reduces to a functional derivative.

In order to evaluate this integral we need to evaluate the derivatives of the implicit function, \(dy^{(k)}/dx\), at all times \(t \in T\). In theory we could achieve this by fully constructing the first-order Fréchet derivative from the implicit function theorem, repeatedly differentiating it, and then evaluating all of those Fréchet derivatives at each time \(t\).

The need to evaluate Fréchet derivatives, however, makes this approach infeasible in practice. A more viable alternative is to evaluate the derivatives only at specific times, where they reduce to manageable finite-dimensional objects.

By definition our constraint function defines a map \(c : X \times Y \to Z\) where \(Y\) and \(Z\) are both the space of functions which map from \(T\) to \(\mathbb{R}^N\). In this case the constraint function can equivalently be defined as a collection of maps \(X \times Y \to \mathbb{R}^N\) for each \(t \in T\). Denoting these maps as \(c(x, y, t)\) the implicit function \(f : X \to Y\) is defined by the system of constraints,
\[c(x, f(x), t) = 0, \forall t \in T.\]

Fixing \(t\) and then differentiating with respect to the input \(x\) gives
\[
0 = \frac{\partial c}{\partial x}(t) + \sum_{k=0}^K \frac{\partial c}{\partial y^{(k)}} \frac{dy^{(k)}}{dx}(t) = \frac{\partial c}{\partial x}(t) + \sum_{k=0}^K \frac{\partial c}{\partial y^{(k)}} \left( \frac{dy^{(k)}}{dx} \right)(t).
\]
This forward differential system implicitly defines the derivative evaluations at each \( t \) as a differential equation. Once we’ve solved for \( y(t) \) we can, at least in theory, solve this forward differential system for each \( \frac{d}{dx} (y^{(k)}) \) and then evaluate

\[
\int_T dt \sum_{k=0}^{K} \frac{\partial p}{\partial y^{(k)}} \frac{dy^{(k)}}{dx} = \sum_{k=0}^{K} \int_T dt \frac{\partial p}{\partial y^{(k)}} \frac{dy^{(k)}}{dx},
\]

as a sum of one-dimensional numerical quadratures.

If \( c(x, y, t) \) is a linear a function of \( \frac{dy}{dt} \) and does not depend on higher-order derivatives,

\[
c(y, x, t) = \frac{dy}{dt}(t) - f(x, y, t) = 0,
\]

then the forward differential system becomes particularly manageable. In particular the forward differential system is also linear in the first-order derivative with respect to \( t \),

\[
\frac{dc}{dx}(y, x, t) = \frac{d}{dt} \frac{dy}{dx}(t) - \frac{\partial f}{\partial x}(x, y, t) - \frac{\partial f}{\partial y} \frac{dy}{dt}(t) = 0.
\]

In the absence of such a linearity we need to solve for the evaluations of the trajectory \( y \), the first-order derivative \( \frac{dy}{dx} \), and the higher-order derivatives of \( y \) at the given \( x \) and every \( t \) needed for the numerical quadratures.

For a demonstration of this forward approach on certain ODEs and DAEs see (Hindmarsh and Serban, 2020).

Finally similar to the Sobolev adjoint method (Section 3.2.3) the above derivation generalizes immediately to constrained systems over Sobolev spaces of functions \( T \subset \mathbb{R}^M \rightarrow \mathbb{R}^N \), with \( M > 1 \). Here instead of an ordinary differential forward system we recover a partial differential forward system, and the Jacobian is recovered as a sum of multidimensional integrals instead of one-dimensional integrals.

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