Adjoint Modeling:
A Brief Introduction

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12 December 2021

What is this about?

Adjoint models are popularly known for their use in estimation and optimization (e.g., data assimilation). Studies using adjoint models, adjoint modeling, are increasingly employing these tools for other purposes as well, especially as a means to investigate the workings of dynamic systems, like the ocean, that can be difficult to ascertain otherwise.

Here we briefly describe what an adjoint is, how it is useful, and how it is derived.

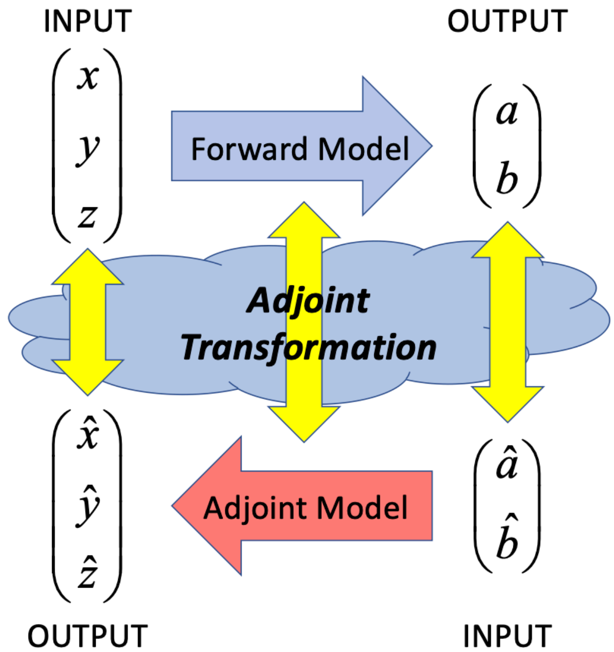
Adjoint is <u>not</u> data assimilation.

What is an adjoint?

Adjoint[1] is a transformation used in studying mathematical relationships. An "adjoint model" refers to an adjoint-transformed version of a model. Here, "model" is simply a set of rules, or a computer program, that takes input and calculates output. To distinguish it from its adjoint, the original pre-transformed model is often referred to as the "forward model" in contrast to its adjoint that computes things "backward" switching roles of what is input and what is output[2] (see diagram below). Adjoint models are particularly useful for computing how forward model output depends on its input, i.e., *<u>sensitivity</u>* (a.k.a. derivative, gradient).

[1] The adjoint here is technically called the Hermitian Adjoint.

[2] Adjoint models are distinct from inverse models that are also "backward." Inverse models solve input from output, whereas adjoint models evaluate dependencies between the two.



A schematic illustration of a forward model and its adjoint. Note the input and output being opposite between the two models.

For illustration, suppose we have a simple “forward model” written as

$$\begin{aligned} a &= x - 2y + 3z \\ b &= 4x - 5z \end{aligned} \quad (1)$$

Here, the model's input is the variables (*x, y, z*) used in the computation on the right-hand-side and its output is the variables (*a, b*) on the left-hand-side assigned (=) to the results of this computation. Now suppose we have a quantity of interest *J* (often called “cost function”, “objective function”, or “target function”) defined in terms of the forward model output,

$$J = 6a - 7b \quad (2)$$

and that we are interested in the sensitivity of this quantity to the model input (x, y, z). In other words, how much would *J* change, if x, y, or z were to change by one?

One way of evaluating this sensitivity is to use the forward model, by changing its input x, y, and z one by one and evaluating how *J* would change each time. For example, *J*’s sensitivity to x can be evaluated by setting x=1 and y=z=0 as input for the forward model (Eq 1) and using its output to evaluate *J* (Eq 2), which result is -22. *J*’s sensitivity to y and z can be obtained similarly, each requiring a separate evaluation of the forward model. Thus, this way of evaluating the sensitivity, the answer of which is (-22, -12, 53), requires <u>three separate evaluations</u> of the forward model, one for each input variable.

The “adjoint model”, in comparison, allows us to evaluate this sensitivity in one step. The adjoint of the forward model (Eq 1) is[3]

$$\begin{aligned}\hat{x} &= \hat{a} + 4\hat{b}\\ \hat{y} &= -2\hat{a}\\ \hat{z} &= 3\hat{a} - 5\hat{b}\end{aligned} \qquad (3)$$

where carets (^) denote variables of the adjoint model (“adjoint variables”). Here, the adjoint model’s input used in the computation on the right-hand-side is $(\hat{a}, \hat{b})$ and its output assigned on the left-hand-side is $(\hat{x}, \hat{y}, \hat{z})$, which are opposite to what they are in the forward model. That is, the adjoint model conducts its computation “backward” compared to the “forward model” as noted above.

Adjoint variables represent sensitivity. Specifically, by setting the adjoint model's input $(\hat{a}, \hat{b})$ to be the sensitivity of *J* to (a, b) (Eq 2),

$$\begin{aligned}\hat{a} &= 6\\ \hat{b} &= -7\end{aligned} \qquad (4)$$

the adjoint model's output $(\hat{x}, \hat{y}, \hat{z})$ gives the sensitivity of *J* to (x, y, z). The result, $(\hat{x}, \hat{y}, \hat{z}) = (\text{-}22, \text{-}12, 53)$, is the same as the previous calculation. However, the present computation requires only one evaluation of the adjoint model (Eq 3) instead of the three that were required by the forward model (Eq 1).

For this example, owing to its simplicity, the difference in the amount of computation required to evaluate the sensitivity, between using the forward model and using the adjoint model, is small. But imagine the model being more complex such as the ocean general circulation model used by the Consortium for Estimating the Circulation and Climate of the Ocean (ECCO; https://ecco-group.org; *Wunsch et al., 2009*). In ECCO, a single forward or adjoint model evaluation requires several days of computation on a state-of-the-art supercomputer and input consists of millions of variables. The sensitivity calculation using the forward model will require one forward model evaluation per input variable which altogether will take millions of days to

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[3] In many circumstances, as it is here, the adjoint corresponds to a transpose operation. This can be seen more clearly in matrix notation. Namely, using matrices, Equations (1) and (3) can be written, respectively, as,

$$\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 1 & -2 & 3 \\ 4 & 0 & -5 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \qquad (1')$$

$$\begin{pmatrix} \hat{x} \\ \hat{y} \\ \hat{z} \end{pmatrix} = \begin{pmatrix} 1 & 4 \\ -2 & 0 \\ 3 & -5 \end{pmatrix} \begin{pmatrix} \hat{a} \\ \hat{b} \end{pmatrix} \qquad (3')$$

Note the coefficient matrix on the right-hand-side of the adjoint model (Eq 3’) simply being the transpose of that in the forward model (Eq 1’), i.e., a reversal of rows and columns of the matrix.

complete (that's a couple thousand years!), but the equivalent calculation can be performed with only one evaluation of the adjoint model taking only a few days' time. Thus, it is impractical to use the forward model to evaluate the sensitivity of a model like ECCO's, whereas it is routine using its adjoint. This computational efficiency is what makes an adjoint model indispensable.

Adjoint models efficiently compute sensitivity.

How is an adjoint model useful?

Sensitivity (derivative) is foundational in calculus used in every branch of science and engineering that employs math. Just as how calculus has advanced these disciplines, adjoint-derived sensitivities provide new insight into problems.

Adjoint models were first introduced in oceanography in the context of data assimilation (*Thacker and Long, 1988*). Based on sensitivity of model-data differences, adjoint models are used to fit corresponding forward models to observations. Such approach ("adjoint method") is also at the heart of ECCO's Central Solution and most of its other estimation products. Values of an adjoint's sensitivity also tell us what observations are most effective for monitoring different quantities of interest and are useful in designing observing systems (*Köhl and Stammer, 2004*).

Importantly, adjoints also provide an effective means to investigate the workings of dynamic systems like the ocean. As a tangible example, consider a change in passive tracer, like dye in water, which can tell us how a tracer-tagged water spreads with time (fate of the water). In contrast, the sensitivity of such quantity to tracer concentrations in the past ("adjoint passive tracer"; *Fukumori et al., 2004*), tells us where that tracer-tagged water came from (origin of the water). Quantitative measures of origin and fate elucidate pathways of ocean circulation and provide insight into processes controlling its evolution.

Adjoint models are also employed in directly studying causation and attribution ("adjoint gradient decomposition"; *Fukumori et al., 2015*); in this, sensitivity is used to quantify effects of different elements driving the ocean, thus providing a tool to assess their relative contribution (e.g., wind vs heat flux). In contrast to common practice of using correlation, which quantifies similarities, adjoints reveal causation based on theoretical relationships (first principles) underlying the models.

Adjoints quantify causation that correlation doesn't.

How do you derive an adjoint?

Derivation of adjoint models is conceptionally straightforward but technically challenging owing to the size and complexities of computer programs of most state-of-the-art models. Remarkably, however, there are software that can automatically transform computer programs into their adjoint ("automatic differentiation", "algorithmic differentiation", "AD tools"; *International Conference on Automatic Differentiation, 2004, 2012*). For example, the ocean circulation model used by ECCO, MITgcm (*Marshall et al.,1997*), was purposefully created to use such automatic differentiation tool to generate its adjoint (*Marotzke et al., 1999*). Today, MITgcm remains one of the few state-of-the-art ocean general circulation models that has an adjoint readily available (https://github.com/MITgcm/MITgcm.git). A rigorous process is in place to routinely test the "adjointability" of new features introduced in the model, thus assuring availability of the adjoint for the latest version of MITgcm for use in ocean state estimation and its various applications.

AD tools help generate adjoint models.

Concluding remark

Despite its foundational nature, adjoint modeling is still far uncommon today compared to forward modeling. This difference is due in part to most adjoint models being developed for the purpose of estimation and optimization as opposed to general modeling applications. As the community becomes more familiar with adjoint models, their availability and scope of utilization will likely broaden synergistically. Application of adjoint models is still at a nascent stage and is ripe for innovation.

Adjoint modeling is on the cusp of transformation.

Acknowledgement

This work was carried out at the Jet Propulsion Laboratory, California Institute of Technology, under a contract with the National Aeronautics and Space Administration (NASA).

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