Adjoint Models as Analytical Tools

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Personal Background

Work on adjoints since 1990
Chief organizer of 7 of the 8 Adjoint Workshops
25 journal articles on adjoint development or applications
Performed adjoint-related work on:
  - Adjoint development validation and efficiency
  - Development of useful adjoints of models with physics
  - Work on synoptic sensitivity analysis
  - Examination of singular vectors (SVs)
  - Work on predictability

Also work on
  - Dynamic balance (21 papers and 5 technical notes)
  - Predictability (8 papers)
  - Data assimilation (7 papers)
1. Sensitivity analysis: The basis for adjoint model applications
2. Examples of adjoint-derived sensitivity
3. Development of an adjoint model directly from computer code
4. Nonlinear validation
5. Efficient solution of optimization problems
6. Singular vectors
7. Other applications
8. Problems with physics
9. Other important considerations
10. Summary
Sensitivity Analysis:
The basis for adjoint model applications

Adjoint in simple terms
Adjoint Sensitivity Analysis for a Discrete Model

The Problem to Consider:

A possibly nonlinear model:

\[ y = m(x) \]  \hspace{1cm} (1)

A differentiable scalar measure of model output fields:

\[ J = J(y) \]  \hspace{1cm} (2)

The result of input perturbations

\[ \Delta J = J(x + x') - J(x) \]  \hspace{1cm} (3)

A 1st-order Taylor series approximation to \( \Delta J \)

\[ J' = \sum_i \frac{\partial J}{\partial x_i} x_i' \]  \hspace{1cm} (4)

The goal is to efficiently determine \( \frac{\partial J}{\partial x_i} \) for all \( i \)
Adjoint Sensitivity Analysis for a Discrete Model

The Tangent Linear Model (TLM)

Apply a 1st-order Taylor series to approximate the model output

\[ y'_i = \sum_j \frac{\partial y_i}{\partial x_j} x'_j \]  \hspace{1cm} (5)

\( \frac{\partial y_i}{\partial x_j} \) is called the **Resolvant** matrix of the TLM or, less accurately, the **Jacobian** of the nonlinear model.

Approximate \( \Delta J \) by a 1st-order Taylor series about \( y' \)

\[ J' = \sum_i \frac{\partial J}{\partial y_i} y'_i \]  \hspace{1cm} (6)
Adjoint Sensitivity Analysis for a Discrete Model

Example of a TLM

Nonlinear discrete model (NLM):

\[ u_{i}^{n+1} = u_{i}^{n} - (\Delta t)u_{i}^{n} \frac{u_{i+1}^{n} - u_{i-1}^{n}}{2(\Delta x)} \quad (7) \]

TLM linearized about the possibly 4-D varying state \( \tilde{u} \):

\[ u_{i}^{',n+1} = u_{i}^{',n} - \frac{\Delta t}{2\Delta x} \left[ u_{i}^{',n} (\tilde{u}_{i+1}^{n} - \tilde{u}_{i-1}^{n}) + \tilde{u}_{i}^{n} (u_{i+1}^{n} - u_{i-1}^{n}) \right] \quad (8) \]
Adjoint Sensitivity Analysis for a Discrete Model

The Adjoint Model
(Adjoint of the TLM or adjoint of the nonlinear model)

Application of the “chain rule” yields

\[
\frac{\partial J}{\partial x_i} = \sum_j \frac{\partial y_j}{\partial x_i} \frac{\partial J}{\partial y_j}
\]  \hspace{1cm} (9)

Contrast with the TLM

\[
y'_i = \sum_j \frac{\partial y_i}{\partial x_j} x'_j
\]  \hspace{1cm} (10)

A. The variables are different in the two equations
B. The order of applications of the variables related to \(x\) and \(y\) differ
C. The indices \(i\) and \(j\) in the matrix operator are reversed
A single impact study yields exact response measures (J) for all forecast aspects with respect to the particular perturbation investigated.

A single adjoint-derived sensitivity yields linearized estimates of the particular measure (J) investigated with respect to all possible perturbations.
Adjoint Sensitivity Analysis for a Discrete Model

Additional Notes

1. Mathematically, the field $\partial J / \partial x$ is said to reside in the dual space of $x$

2. With the change of notation $\hat{x} = \partial J / \partial x$, $M = \partial y / \partial x$, etc.,

$$J' = \hat{y}^T y = \hat{y}^T (Mx) = (\hat{y}^T M) x = (M^T \hat{y})^T x = \hat{x}^T x \quad (11)$$

3. The exact definition of the adjoint depends on the quadratic expression used to define $J'$. If the simple Euclidean norm (or dot product) is used, then for a discrete model, the adjoint is simply a transpose. Such a simple norm may not be appropriate when the dual space fields are to be physical interpreted. (More on this later.)

4. The adjoint is not generally the inverse: in non-trivial atmospheric models, $M^T \neq M^{-1}$.

5. This is all 1st-year calculus and linear algebra. If examination of gradients is useful, then so are the adjoint models used to calculate them.
Adjoint Sensitivity Analysis for a Discrete Model

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Adjoint Sensitivity Analysis for a Discrete Model

Example Model Equations

Nonlinear model:

\[ u_{i}^{n+1} = u_{i}^{n} - (\Delta t)u_{i}^{n} \frac{u_{i+1}^{n} - u_{i-1}^{n}}{2(\Delta x)} \]  

\[ (7) \]

TLM:

\[ u_{i}^{n+1} = u_{i}^{n} - \frac{\Delta t}{2\Delta x} \left[u_{i}^{n}(\tilde{u}_{i+1}^{n} - \tilde{u}_{i-1}^{n}) + \tilde{u}_{i}^{n}(u_{i+1}^{n} - u_{i-1}^{n})\right] \]  

\[ (8) \]

Adjoint model:

\[ \hat{u}_{i}^{n} = \hat{u}_{i}^{n+1} - \frac{(\Delta t)}{2(\Delta x)} \left[(\tilde{u}_{i+1}^{n} - \tilde{u}_{i-1}^{n})\hat{u}_{i}^{n+1} + \tilde{u}_{i-1}^{n}\hat{u}_{i-1}^{n+1} - \tilde{u}_{i+1}^{n}\hat{u}_{i+1}^{n+1}\right] \]  

\[ (12) \]
Adjoint Sensitivity Analysis for a Discrete Model

Example $J$

Consider $J$ for northward moisture flux through a “window”

$J$ for continuous fields

$$J = \int q \, v \, dm$$  \hspace{1cm} (13)

$J$ for discretized model

$$J = \sum w_{i,j,k} \ q_{i,j,k} \ v_{i,j,k}$$  \hspace{1cm} (14)

$$\frac{\partial J}{\partial v_{i,j,k}} = w_{i,j,k} \ \tilde{q}_{i,j,k}$$  \hspace{1cm} (15)

$$\frac{\partial J}{\partial q_{i,j,k}} = w_{i,j,k} \ \tilde{v}_{i,j,k}$$  \hspace{1cm} (16)
References


Although the previous description of an adjoint for a discreet model is correct, it fails to adequately account for issues regarding the discrete representation of physically continuous fields. *(More later.)*
Examples of Adjoint-Derived Sensitivities
Example Sensitivity Field

\[ \frac{\partial J_1}{\partial z} \text{ for } t=-36, \sigma=0.40 \]

Contour interval 0.02 Pa/m  M=0.1 Pa/m

Errico and Vukicevic
1992 MWR
\frac{\partial \overline{qv}}{\partial T_s} (t = -48 \text{ h}) \quad \frac{\partial \overline{qv}}{\partial q} (\sigma = .86, \ t = -48 \text{ h})
From Errico and Vukicevic 1992

$J$ = average surface pressure in a small box centered at $P$

$J$ = barotropic component of vorticity at point $P$

$\frac{\partial J_2}{\partial u}$ for $t = -3$, $\sigma = 0.35$

$\frac{\partial J_3}{\partial u}$ for $t = -3$, $\sigma = 0.35$

**Fig. 11.** The same as Fig. 9, except for sensitivity of $J_2$. The contour interval is 0.006 mb s$^{-1}$.

**Fig. 13.** The same as Fig. 9, except for sensitivity of $J_3$. The contour interval is 0.003 s$^{-1}$.
Sensitivity field for $J=p_s$ with respect to $T$ for an idealized cyclone

From Langland and Errico 1996 *MWR*
Development of Adjoint Model From Line by Line Analysis of Computer Code
Why consider development from code?

1. Eventually, an adjoint code will be necessary.

2. The code itself is the most accurate description of the model algorithm.

3. If the model algorithm creates different dynamics than the original equations being modeled, for most applications it is the former that are desirable and only the former that can be validated.
Development of Adjoint Model From Line by Line Analysis of Computer Code

Let $A$, $B$, $C$, $D$ be different operators making up $M$ (e.g., advection, dry physics, moist physics, etc.)

Let subscripts denote time steps.

Then, the TLM and Adjoint are described by sequences of linear operators

**TLM:**

$$y' = D_n C_n B_n A_n \ldots D_1 C_1 B_1 A_1 D_0 C_0 B_0 A_0 x'$$

**Adjoint**

$$\hat{x} = A_n^T B_n^T C_n^T D_n^T A_1^T B_1^T C_1^T D_1^T \ldots A_0^T B_0^T C_0^T D_0^T \hat{y}$$
Development of Adjoint Model From Line by Line Analysis of Computer Code

Parent NLM:
\[
Y = X \times (W^A) \\
Z = Y \times X
\]

TLM:
\[
Y_{tlm} = X_{tlm} \times (W^A) + W_{tlm} \times A \times X \times (W^{(A-1)}) \\
Z_{tlm} = Y_{tlm} \times X + X_{tlm} \times Y
\]

Adjoint:
\[
X_{adj} = X_{adj} + Z_{adj} \times Y \\
Y_{adj} = Y_{adj} + Z_{adj} \times X
\]
\[
X_{adj} = X_{adj} + Y_{adj} \times (W^A) \\
W_{adj} = W_{adj} + Y_{adj} \times X \times (W^{(A-1)})
\]
Development of Adjoint Model From Line by Line Analysis of Computer Code

Parent NLM :

\[ Y = X \times (W^A) \]
\[ Z = Y \times X \]

TLM :

\[ Y_{tlm} = X_{tlm} \times (W^A) + W_{tlm} \times A \times X \times (W^{(A-1)}) \]
\[ Z_{tlm} = Y_{tlm} \times X + X_{tlm} \times Y \]

\[ X_{adj} = X_{adj} + Z_{adj} \times Y \]
\[ Y_{adj} = Y_{adj} + Z_{adj} \times X \]

Adjoint :

\[ X_{adj} = X_{adj} + Y_{adj} \times (W^A) \]
\[ W_{adj} = W_{adj} + Y_{adj} \times X \times (W^{(A-1)}) \]
Development of Adjoint Model From Line by Line Analysis of Computer Code

**Automatic Differentiation**

<table>
<thead>
<tr>
<th>Tool</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>TAMC</td>
<td>Ralf Giering (superceded by TAF)</td>
</tr>
<tr>
<td>TAF</td>
<td>FastOpt.com</td>
</tr>
<tr>
<td>ADIFOR</td>
<td>Rice University</td>
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<tr>
<td>TAPENADE</td>
<td>INRIA, Nice</td>
</tr>
<tr>
<td>OPENAD</td>
<td>Argonne</td>
</tr>
<tr>
<td>Others</td>
<td><a href="http://www.autodiff.org">www.autodiff.org</a></td>
</tr>
</tbody>
</table>
1. TLM and Adjoint models are straightforward to derive from NLM code, and actually simpler to develop.
2. Intelligent approximations can be made to improve efficiency.
3. TLM and (especially) Adjoint codes are simple to test rigorously.
4. Some outstanding errors and problems in the NLM are typically revealed when the TLM and Adjoint are developed from it.
5. It is best to start from clean NLM code.
6. The TLM and Adjoint can be formally correct but useless!
Nonlinear Validation

Does the TLM or Adjoint model tell us anything about the behavior of meaningful perturbations in the nonlinear model that may be of interest?
Linear vs. Nonlinear Results in Moist Model

24-hour SV1 from case W1
Initialized with T’=1K
Final ps field shown

Contour interval 0.5 hPa

Errico and Raeder 1999 QJRMS
Linear vs. Nonlinear Results in Moist Model

Non-Conv Precip. ci=0.5mm

Convective Precip. ci=2mm

Non-Conv Precip. ci=0.5mm

Convective Precip. ci=2mm
Linear vs. Nonlinear Results

In general, agreement between TLM and NLM results will depend on:

1. Amplitude of perturbations
2. Stability properties of the reference state
3. Structure of perturbations
4. Physics involved
5. Time period over which perturbation evolves
6. Measure of agreement

The agreement of the TLM and NLM is exactly that of the Adjoint and NLM if the Adjoint is exact with respect to the TLM.
References


Efficient solution of optimization problems
Optimal Perturbations

Type I

Maximize

\[ J' = \sum_i \frac{\partial J}{\partial x_i} x_i' \]  \hspace{1cm} (30)

Given the constraint:

\[ C = \frac{1}{2} \sum_i w_i x_i'^2 \]  \hspace{1cm} (31)

Solution Method: Minimize the augmented variable

\[ I = \sum_i \frac{\partial J}{\partial x_i} x_i' + \lambda \left( C - \sum_i w_i x_i'^2 \right) \]  \hspace{1cm} (32)

\[ \frac{\partial I}{\partial x_i'} = \frac{\partial J}{\partial x_i} - \lambda w_i x_i' \]  \hspace{1cm} (33)

Solution:

\[ x_i'(\text{optimal}) = \frac{\lambda}{w_i} \frac{\partial J}{\partial x_i} \]  \hspace{1cm} (34)

\[ \lambda = C \left[ \sum_i \frac{1}{w_i} \left( \frac{\partial J}{\partial x_i} \right)^2 \right]^{-1} \]  \hspace{1cm} (35)
Optimal Perturbations

Type II

Minimize

\[ C = \frac{1}{2} \sum_i w_i x'_i^2 \]  \hspace{1cm} (36)

Given the constraint:

\[ J' = \sum_i \frac{\partial J}{\partial x_i} x'_i \]  \hspace{1cm} (37)

Solution Method (as before)

Solution:

\[ x'_i \text{(optimal)} = \frac{\lambda}{w_i} \frac{\partial J}{\partial x_i} \]  \hspace{1cm} (38)

\[ \lambda = J' \left[ \sum_i \frac{1}{w_i} \left( \frac{\partial J}{\partial x_i} \right)^2 \right]^{-1} \]  \hspace{1cm} (39)
The more general nonlinear optimization problem

Find the local minima of a scalar nonlinear function $J(x)$. 

$$\frac{\partial J}{\partial x}$$

Gradient at point $P$

Contours of $J$ in phase $(x)$ space
Optimal Perturbations

Sample Norms

1. The Energy Norm

\[ E = \frac{1}{2A} \int \left[ u'^2 + v'^2 + \frac{C_p T'^2}{T_r} + \frac{R T_r}{p_{sr}^2} p'_s^2 \right] dA \ d\sigma \quad (46) \]

2. A Variance Weighted Norm

\[ V = \frac{1}{2A} \int \left[ \frac{u'^2}{u'^2} + \frac{v'^2}{v'^2} + \frac{T'^2}{T'^2} + \frac{p'_s^2}{p'_s^2} \right] dA \ d\sigma \quad (47) \]

3. A norm weighted by the inverse of the analysis error covariance matrix

\[ C = \frac{1}{2} \mathbf{x}'^T \mathbf{A}^{-1} \mathbf{x}' \quad (48) \]

Assuming Gaussian error statistics, \( \exp (-C') \propto \text{PDF}(\mathbf{x}') \)
Singular Vectors
Optimal Perturbations

Singular Vectors

Maximize the L2 norm: \[ N = \frac{1}{2} y'^T N y' \] (40)

Given the TLM: \[ y' = Mx' \] (41)

And the constraint: \[ 1 = C = \frac{1}{2} x'^T C x' \] (42)

Solution Method: Minimize the augmented variable \( I(x') \):

\[
I = \frac{1}{2} x'^T M^T N M x' + \lambda^2 \left( C - \frac{1}{2} x'^T C x' \right) \] (43)

\[
\frac{\partial I}{\partial x'} = M^T N M x' - \lambda^2 C x' \] (44)

For \( z = C^{\frac{1}{2}} x' \), the solution is an eigenvalue problem

\[
\lambda^2 z = C^{-\frac{1}{2}} M^T N M C^{-\frac{1}{2}} z \] (45)
Optimal Perturbations
Additional Notes Regarding SVs

1. \( \lambda \) are the **singular values** of the matrix \( \mathbf{N}^{\frac{1}{2}} \mathbf{M} \mathbf{C}^{-\frac{1}{2}} \).

2. The set of \( \mathbf{x}' \) form an orthonormal basis with respect to the norm \( \mathbf{C} \).

3. If \( \mathbf{C} \) and \( \mathbf{N} \) are the Euclidean norm \( \mathbf{I} \), then \( \mathbf{x}' = \mathbf{z} \) are the right (or initial) **singular vectors** (or SVs) of \( \mathbf{M} \) and \( \mathbf{y}' = \mathbf{M} \mathbf{x}' \) are the left (or final or evolved) singular vectors of \( \mathbf{M} \). **The same terminology is used even for more general norms.**

4. \( \lambda^2 = N/C \) for each solution.

5. If \( \mathbf{C} \) is the inverse of the error covariance matrix, then the evolved SVs are the EOFs (or PCs) of the forecast error covariance, and truncations using the leading SVs maximize the retained error variance. (Ehrendorfer and Tribbia 1997 JAS)

6. The SVs and \( \lambda^2 \) depend on the norms used; i.e., on how measurements are made. This dependency is removed only by introducing some other constraint or condition.

7. SVs produced for semi–infinite periods are equivalent to Lyupanov vectors (Legras and Vautard, 1995 ECMWF Note).
Gelaro et al.
MWR 2000
NON-LOCAL INITIAL STRUCTURES

From Novakovskaia et al. 2007 and Errico et al. 2007
The Balance of Singular Vectors

\[ \mathbf{v}'(\sigma = 0.55) \quad \mathbf{T}'(\sigma = 0.55) \]

Initial R mode

Contour 2 units

Initial G mode

Contour 1 unit

Errico 2000
How Many SVs are Growing Ones?

- **EM** E-norm Moist Model
- **ED** E-norm Dry Model
- **TM** R-norm Moist Model
- **TD** R-norm Dry Model

Singular Value Squared

Errico et al. Tellus 2001
Other Applications
Other Applications

1. 4DVAR (Tutorial following)
2. Ensemble Forecasting (R. Buizza, T. Palmer)
3. Key analysis errors (F. Rabier, L. Isaksen)
4. Targeting (R. Langland, R. Gelaro)
5. Observation impact estimates (R. Langland, R. Gelaro)
Problems with Physics
Problems with Physics

Consider Parameterization of Stratiform Precipitation

\[ R \] vs. \[ q_s \]

- NLM
- Modified NLM
- TLM
Example of a potentially worse problem introduced by smoothing
Example of a failed adjoint model development

Sensitivity of forecast $J$ with respect to earlier $T$ in lowest model model level

Time = -3 hours; contour int. = 0.00025
Time = -9 hours; contour int. = 10000.

From R. Errico, unpublished MAMS2 development
Tangent linear vs. nonlinear model solutions

Errico and Raeder 1999 QJRMS

$P_s' \text{ (hPa)}$

time (hrs)
Jacobians of Precipitation

RAS scheme

\[ \frac{\partial R}{\partial T} \] dashed

\[ \frac{\partial R}{\partial q} \] solid

ECMWF scheme

BM scheme

Fillion and Mahfouf 1999 *MWR*
Problems with Physics
 Parameterization of Vertical Eddy Diffusion

NLM:

$$\frac{\partial u}{\partial t} = \ldots + \frac{1}{\rho} \frac{\partial}{\partial z} \rho K \frac{\partial u}{\partial z}$$

The $K$ are flow–dependent eddy diffusion coefficients.

TLM:

$$\frac{\partial u'}{\partial t} = \ldots + \frac{1}{\tilde{\rho}} \frac{\partial}{\partial z} \tilde{\rho} \tilde{K} \frac{\partial u'}{\partial z} + \frac{1}{\tilde{\rho}} \frac{\partial}{\partial z} \tilde{\rho} K' \frac{\partial \tilde{u}}{\partial z} + \text{terms for } \rho'$$

Usually a semi–implicit treatment of $\partial u/\partial z$ is used to greatly increase numerical stability. This appear to work in the NLM but is insufficient in the TLM.

Instead, the $K'$ term is generally ignored!
Problems with Physics

1. The model may be non-differentiable.
2. Unrealistic discontinuities should be smoothed after reconsideration of the physics being parameterized.
3. Perhaps worse than discontinuities are numerical instabilities that can be created from physics linearization.
4. It is possible to test the suitability of physics components for adjoint development before constructing the adjoint.
5. Development of an adjoint provides a fresh and complementary look at parameterization schemes.
Other Important Considerations

Physically-based norms and the interpretations of sensitivity fields
\[ \frac{\partial (\text{error "energy"})}{\partial (T_t \text{ 24-hours earlier})} \]

1 \times 1.25 \text{ degree lat-lon}

0.5 \times 0.0625 \text{ degree lat-lon}

From R. Todling
Sensitivities of continuous fields

Consider $J(f(x))$ where $J$ is a scalar function of a set $f_i$ of continuous fields represented by the vector $f$, each defined within a multi-dimensional space $x$. Then, the real functional expression

$$\delta J = \langle \frac{\partial J}{\partial f}, \delta f \rangle$$

should be interpreted as

$$\sum_i \int_S dS(x) \frac{\partial J}{\partial f_i}(x) \delta f_i(x)$$

where $S$ is a volume, mass, or other metric. With this interpretation, $\partial J/\partial f_i$ has physical units of $J \times f_i^{-1} \times S^{-1}$; i.e., it is a kind of sensitivity density.

This field of sensitivity density is relatively independent of the grid on which it is represented, but to estimate the change of $J$ due to a perturbation $\delta f$ applied at grid point $x_G$, the grid volume $dS$ at this point must be considered; i.e.,

$$\frac{\partial J}{\partial f_i}(x_G) = \int_{S(x_G)} dS(x) \frac{\partial J}{\partial f_i}(x)$$

It is safer to base physical interpretations of sensitivity on its density, but then sensitivities to grid point perturbations become less obvious.
Sensitivity of $J$ with respect to $u$ 5 days earlier at $45^\circ$N, where $J$ is the zonal mean of zonal wind within a narrow band centered on 10 hPa and $60^\circ$N. (From E. Novakovskaia)
Rescaling options for a vertical grid

- Delta log p
- Delta p

Levels:
- 1 hPa
- 10 hPa
- 100 hPa
- 500 hPa
- 850 hPa
2 Re-scalings of the adjoint results

Mass weighting

Volume weighting

From E. Novakovskaia
Summary
Misunderstanding #1

False: Adjoint models are difficult to understand.

True: Understanding of adjoints of numerical models primarily requires concepts taught in early college mathematics.
Misunderstanding #2

False: Adjoint models are difficult to develop.

True: Adjoint models of dynamical cores are simpler to develop than their parent models, and almost trivial to check, but adjoints of model physics can pose difficult problems.
Misunderstanding #3

**False:** Automatic adjoint generators easily generate perfect and useful adjoint models.

**True:** Problems can be encountered with automatically generated adjoint codes that are inherent in the parent model. Do these problems also have a bad effect in the parent model?
Misunderstanding #4

**False:** An adjoint model is demonstrated useful and correct if it reproduces nonlinear results for ranges of very small perturbations.

**True:** To be truly useful, adjoint results must yield good approximations to sensitivities with respect to meaningfully large perturbations. This must be part of the validation process.
Misunderstanding #5

False: Adjoint models are not needed because the EnKF is better than 4DVAR and adjoint results disagree with our notions of atmospheric behavior.

True: Adjoint models are more useful than just for 4DVAR. Their results are sometimes profound, but usually confirmable, thereby requiring new theories of atmospheric behavior. It is rare that we have a tool that can answer such important questions so directly!
What is happening and where are we headed?

1. There are several adjoint models now, with varying portions of physics and validation.
2. Utilization and development of adjoint models has been slow to expand, for a variety of reasons.
3. Adjoint models are powerful tools that are under-utilized.
4. Adjoint models are like gold veins waiting to be mined.
Recommendations

1. Develop adjoint models.
2. Include more physics in adjoint models.
3. Develop parameterization schemes suitable for linearized applications.
4. Always validate adjoint results (linearity).
4. Consider applications wherever sensitivities would be useful.