Tangent linear and adjoint models for variational data assimilation

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Introduction

- 4D-Var is based on minimization of a cost function which measures the distance between the model with respect to the observations and with respect to the background state
- The cost function and its gradient are needed in the minimization.
- The tangent linear model provides a computationally efficient (although approximate) way to calculate the model trajectory, and from it the cost function.
 The adjoint model is a very efficient tool to compute the gradient of the cost function.
- Overview:
 - Brief introduction to 4D-Var with focus on TL/AD aspects
 - General definitions of Tangent Linear and Adjoint models and why they are extremely useful in variational assimilation
 - Writing TL and AD models and testing them
 - Brief mention of automatic differentiation software



<u>4D-Var</u>

In 4D-Var the cost function can be expressed as follows:

$$J = \frac{1}{2} (\mathbf{x}_0 - \mathbf{x}_b)^T \mathbf{B}^{-1} (\mathbf{x}_0 - \mathbf{x}_b) + \frac{1}{2} \sum_{i=0}^n (H_i M_i [\mathbf{x}_0] - \mathbf{y}_i)^T \mathbf{R}_i^{-1} (H_i M_i [\mathbf{x}_0] - \mathbf{y}_i)$$

$$J_b$$

B background error covariance matrix,

R observation error covariance matrix (instrumental + interpolation + observation operator error),

M forward nonlinear forecast model (time evolution of the model state, index i), *H* observation operator (model space \rightarrow observation space).

$$\min J \iff \nabla_{\mathbf{x}_0} J = \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_b) + \sum_{i=0}^n \mathbf{M}'^T[t_i, t_0] \mathbf{H}_i^T \mathbf{R}_i^{-1} \left(H_i M_i [\mathbf{x}_0] - \mathbf{y}_i \right) = 0$$

 \mathbf{H}^{T} = adjoint of observation operator and \mathbf{M}^{T} = adjoint of forecast model.



Incremental 4D-Var at ECMWF

• In incremental 4D-Var, the cost function is minimized in terms of increments:

$$\delta x_i = M'[t_0, t_i] \delta x_0$$

with the model state defined at any time t_i as: $x_i = x_{ti} + \delta x_i, x_{ti} = M(t_0, t_i) x_{t0}$ x_t is the trajectory around which the linearization is performed ($x_t = x_b$ at t=0)

• 4D-Var cost function can then be approximated to the first order by:

$$J(\delta x_0) = \frac{1}{2} \delta x_0^T B^{-1} \delta x_0 + \frac{1}{2} \sum_{i=0}^n (H_i M'[t_0, t_i] \delta x_0 - d_i)^T R^{-1} (H_i M'[t_0, t_i] \delta x_0 - d_i)$$

where $d_i = y_i - H_i(x_{ii})$ is the so-called departure computed using the nonlinear model and observational operator.

• The gradient of the cost function to be minimized is:

min
$$J \iff \nabla_{\delta x_0} J = B^{-1} \delta x_0 + \sum_{i=0}^n M'^T [t_i, t_0] H_i^T R^{-1} (H_i \delta x_i - d_i) = 0$$

M' and H'_i are the tangent linear models which are used in the computations of incremental updates during the minimization (iterative procedure).

 M'^{T} and H_{i}^{T} are the adjoint models which are used to obtain the gradient of the cost function with respect to the initial condition.



Details on linearisation

In the first order approximation, a perturbation δx of the control variable (initial condition) evolves according to the tangent linear model:

$$\delta x_{i} = \left[\frac{\partial M_{i}(x)}{\partial x}\right]_{x_{i-1}} \delta x_{i-1} = M_{i} \delta x_{i-1}$$

where i is the time-step index.

The perturbation of the cost function around the initial state is:

$$\delta J(x_0, \delta x_0) = \frac{1}{2} \delta x_0^T B^{-1} \delta x_0 + \frac{1}{2} \sum_{i=0}^n (H_i \delta x_i - d_i)^T R_i^{-1} (H_i \delta x_i - d_i) =$$

$$=\frac{1}{2}\delta x_{0}^{T}B^{-1}\delta x_{0} + \frac{1}{2}\sum_{i=0}^{n} \left(H_{i}^{'}M_{i-1}^{'}\dots M_{0}^{'}\delta x_{0} - d_{i}\right)^{T}R_{i}^{-1}\left(H_{i}^{'}M_{i}^{'}M_{i-1}^{'}\dots M_{0}^{'}\delta x_{0} - d_{i}\right)$$

where $H_i^{'}$ is the linearised version of H_i about x_i and $d_i = y_i - H_i(x_i)$ are the departures from observations.



Details of the linearisation (cnt.)

The gradient of the cost function with respect to δx_0 is given by:

$$\nabla_{\delta x_{0}} J = B^{-1} \delta x_{0} + \sum_{i=0}^{n} (H_{i}^{'} M_{i}^{'} M_{i-1}^{'} \dots M_{0}^{'})^{T} R^{-1} (H_{i}^{'} M_{i}^{'} M_{i-1}^{'} \dots M_{0}^{'} \delta x_{0} - d_{i}) =$$

$$= B^{-1} \delta x_{0} + \sum_{i=0}^{n} M_{0}^{'T} \dots M_{i-1}^{'T} M_{i}^{'T} H_{i}^{'T} R^{-1} (H_{i}^{'} M_{i}^{'} M_{i-1}^{'} \dots M_{0}^{'} \delta x_{0} - d_{i}) =$$

$$= B^{-1} \delta x_{0} + \sum_{i=0}^{n} M^{'T} [t_{i}, t_{0}] H_{i}^{'T} R^{-1} (H_{i}^{'} \delta x_{i} - d_{i})$$

The optimal initial perturbation is obtained by finding the value of δx_0 for which:

$$\nabla_{\delta x_0} J = 0$$

The gradient of the cost function with respect to the initial condition is provided by the **adjoint solution** at time t=0. Let's see how...



Definition of adjoint operator

For any linear operator M' there exist an *adjoint* operator M^* such as:

$$\langle x, M'y \rangle = \langle M^*x, y \rangle$$

where \langle , \rangle is an inner scalar product and x, y are vectors (or functions) of the space where this product is defined.

It can be shown that for the inner product defined in the Euclidean space :

$$M^* = M^{T}$$

We will now show that the gradient of the cost function at time t=0 is provided by the solution of the adjoint equations at the same time:

$$\nabla_{\delta x_0} J = -x_0^*$$



Adjoint solution

Usually the initial guess x_0 is chosen to be equal to the background x_b so that the initial perturbation $\delta x_0 = 0$ The gradient of the cost function is hence simplified as:

$$\nabla_{\delta x_0} J = -\sum_{i=0}^n M^{T}[t_i, t_0] H_i^{T} R^{-1} d_i$$

We choose the solution of the adjoint system as follows:

$$\begin{aligned} x_{n+1}^* &= 0 & \text{(arbitrary "final" condition)} \\ x_0^* &= M_1^* x_1^* & \text{(initial condition)} \\ x_i^* &= M_{i+1}^* x_{i+1}^* + H_i^* R^{-1} d_i, i = 1, \dots, n & \text{(iterative solution)} \end{aligned}$$

We then substitute progressively the solution x_i^* into the expression for x_0^*



Adjoint solution (cnt.)

$$x_{0}^{*} = M_{1}^{*}(M_{2}^{*}x_{2}^{*}) + M_{1}^{*}H_{1}^{*}R^{-1}d_{1} =$$

= $M_{1}^{*}(M_{2}^{*}(M_{3}^{*}x_{3}^{*})) + M_{1}^{*}M_{2}^{*}H_{2}^{*}R^{-1}d_{2} + M_{1}^{*}H_{1}^{*}R^{-1}d_{1} =$
= ...

Finally, regrouping and remembering that $x_{n+1}^* = 0$ and that $M^* = M^T$ and $H^* = H^T$ we obtain the following equality:

$$x_{0}^{*} = \sum_{i=0}^{n} M^{T}[t_{i}, t_{0}] H_{i}^{T} R^{-1} d_{i} \implies x_{0}^{*} = -\nabla_{\delta x_{0}} J$$

The **gradient** of **the cost function** with respect to the control variable (initial condition) is obtained by a **backward** integration of the **adjoint model**.



Iterative steps in the 4D-Var Algorithm

- 1. Integrate forward model gives J.
- 2. Integrate adjoint model backwards gives ∇J .
- 3. If $\|\nabla J(x_m)\| \leq \varepsilon$ then stop.
- 4. Compute descent direction D_m (Newton, CG, ...).
- 5. Compute step size ρ_m : $J(x_m + \rho_m D_m) = \min_{\rho} J(x_m + \rho D_m)$.
- 6. Update initial condition: $x_{m+1} = x_m + \rho_m D_m$.



Finding the minimum of cost function J is an iterative minimization procedure





An analysis cycle in 4D-Var



1st ifstraj:

- Non-linear model is used to compute the high-res trajectory (T1279 operational, 12-h forecast)
- High-res departures are computed at exact obs time and location
- Trajectory is interpolated at low res (T159)

1st ifsmin (70 iterations):

- Iterative minimization at T159 resolution
- Tangent linear with simplified physics to calculate the increments δx_i
- Analysis increment at initial time δx_0 is interpolated back linearly from low-res to high-res and it provides a new initial state for the 2nd trajectory run

2nd ifstraj:

• repeat 1st ifstraj and interpolates at T255 resolution

2nd ifsmin (30 iterations):

• repeat 1st ifsmin at T255

Last ifstraj:

• Uses updated initial condition to run another 12-h forecast and stores analysis departures in the Observational Data Base (ODB)



Recap on TL and AD models

• TANGENT LINEAR MODEL

If M is a model such as:

$$\mathbf{x}(t_{i+1}) = M[\mathbf{x}(t_i)]$$

then the tangent linear model of M, called M', is:

$$\delta \mathbf{x}(t_{i+1}) = M'[\mathbf{x}(t_i)] \delta \mathbf{x}(t_i) = \frac{\partial M[\mathbf{x}(t_i)]}{\partial \mathbf{x}} \delta \mathbf{x}(t_i)$$

• ADJOINT MODEL

The adjoint of a linear operator M' is the linear operator M^* such that, for the inner product <,>,

$$orall \mathbf{x}, orall \mathbf{y} \qquad < M' \mathbf{x}, \mathbf{y} > = < \mathbf{x}, \mathbf{M}^* \mathbf{y} >$$

Remarks:

- with the euclidian inner product, $\mathbf{M}^* = M'^T$.
- in variational assimilation, $\nabla_x \mathcal{J} = \mathbf{M}^* \nabla_y \mathcal{J}$, where \mathcal{J} is the cost function.



Simple example of adjoint writing

• non-linear statement

$$x = y + z^{2}$$
$$z = z$$
$$y = y$$
$$x = y + z^{2}$$

• tangent linear statement

$$\delta z = \delta z$$

$$\delta y = \delta y$$

$$\delta x = \delta y + 2z\delta z$$

or in a matrix form:

$$\begin{pmatrix} \delta z \\ \delta y \\ \delta x \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 2z & 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} \delta z \\ \delta y \\ \delta x \end{pmatrix}$$



Simple example of adjoint writing (cnt.)

Often the adjoint variables in mathematical formulations are indicated with an asterisk

- adjoint statement
 - transpose matrix

$$\begin{pmatrix} \delta z^* \\ \delta y^* \\ \delta x^* \end{pmatrix} = \begin{pmatrix} 1 & 0 & 2z \\ 0 & 1 & 1 \\ 0 & 0 & 0 \end{pmatrix} \cdot \begin{pmatrix} \delta z^* \\ \delta y^* \\ \delta x^* \end{pmatrix}$$

or in the form of equation set:

$$\delta z^* = \delta z^* + 2z \delta x^*$$

$$\delta y^* = \delta y^* + \delta x^*$$

$$\delta x^* = 0$$

Do not forget the last equation!!! That too is part of the adjoint!

As an alternative to the matrix method, adjoint coding can be carried out using a line-by-line approach.



More practical examples on adjont coding: the Lorenz model

$$\frac{dx_1}{dt} = -px_1 + px_2$$
(1)
$$\frac{dx_2}{dt} = (r - x_3)x_1 - x_2$$
(2)
$$\frac{dx_3}{dt} = x_1x_2 - bx_3$$
(3)

where p is the Prandtl number, r the Rayleigh number, and b the aspect ratio.

- x_1 is the intensity of convection,
- x_2 is the maximum temperature difference
- x_3 is the stratification change due to convection.

Details on the Lorenz model can be found in the references.



The linear code in Fortran

Linearize each line of the code one by one, and set dx/dt=y for simplicity:

y(1) (1)yd(1)	= -p*x(1) + p*x(2) = -p*xd(1) + p*xd(2)	:Nonlinear statement :Tangent linear
y(2) (2)vd(2)	= $x(1)*(r-x(3)) -x(2)$ = $xd(1)*(r-x(3))$:Nonlinear statement
(-,,,,-,,	-x(1)*xd(3) -xd(2)	:Tangent linear

...etc

Remember that \mathbf{p} , \mathbf{r} , \mathbf{b} are constants; $\mathbf{x}(1)$, $\mathbf{x}(2)$ and $\mathbf{x}(3)$ are the independent variables; $\mathbf{y}(1)$, $\mathbf{y}(2)$ and $\mathbf{y}(3)$ are the dependent variables.

We chose the suffix "d" for the tangent linear variable for consistency with the automatic differentation software TAPENADE (see optional practical exercise). Adjoint variables are indicated with the suffix "b". This is just a convention.

Note that in the ECMWF Integrated Forecast System (IFS) the tangent linear and adjoint variables are indicated without any subscripts and the nonlinear trajectory (x) is indicated with the suffix "5" (x5).



Adjoint of one instruction

We start from the tangent linear code:

yd(1) = -p*xd(1) + p*xd(2)

In matrix form, it can be written as:

$$\begin{pmatrix} \delta x_1 \\ \delta x_2 \\ \delta y_1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -p & p & 0 \end{pmatrix} \begin{pmatrix} \delta x_1 \\ \delta x_2 \\ \delta y_1 \end{pmatrix}$$

which can easily be transposed (asterisk indicates adjoint variables):

$$\begin{pmatrix} \delta x_1^* \\ \delta x_2^* \\ \delta y_1^* \end{pmatrix} = \begin{pmatrix} 1 & 0 & -p \\ 0 & 1 & p \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \delta x_1^* \\ \delta x_2^* \\ \delta y_1^* \end{pmatrix}$$

The corresponding adjoint code in FORTRAN is:



Adjoint of one instruction (II)



which can easily be transposed (asterisk indicates transposition):

$$\begin{pmatrix} \delta x_1^* \\ \delta x_2^* \\ \delta x_3^* \\ \delta y_2^* \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & (r-x_3) \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & -x_1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \delta x_1^* \\ \delta x_2^* \\ \delta x_3^* \\ \delta y_2^* \end{pmatrix}$$

The corresponding adjoint code in FORTRAN is:



Trajectory

The trajectory has to be available. It can be:

- saved which costs memory,
- recomputed which costs CPU time.

Depending on the complexity of the code, one option or the other is adopted (or both options at the same time).



The Adjoint Code

Property of adjoints (transposition):

$$(L_n L_{n-1} \dots L_2 L_1)^* = L_1^* L_2^* \dots L_{n-1}^* L_n^*$$

Application: $M_i = L_n L_{n-1} \dots L_2 L_1$ where L_i represents the line *i* of the tangent linear model.

The **adjoint code** is made of the **transpose** of each line of the tangent linear code in **reverse order**.



Adjoint of loops

In the TL code for the Lorenz model we have:

```
DO i=1,3
    xd(i)=xd(i)+dt*yd(i)
ENDDO
```

dt is a constant for our purposes. This loop can be written explicitly:

```
xd(1)=xd(1)+dt*yd(1)
xd(2)=xd(2)+dt*yd(2)
xd(3)=xd(3)+dt*yd(3)
```

We can now transpose and reverse the lines to get the adjoint: yb(3)=yb(3)+dt*xb(3) yb(2)=yb(2)+dt*xb(2) yb(1)=yb(1)+dt*xb(1)

which is equivalent to
DO i=3,1,-1 !Reverse order of indeces!
yb(i)=yb(i)+dt*xb(i)
ENDDO



Conditional statements ("IF" statements)

- What we want is the adjoint of the statements which were actually executed in the direct model.
- We need to know which "branch" of the IF statement was executed
- The result of the conditional statement has to be stored: it is part of the trajectory !!!



Summary of basic rules for line-by-line adjoint coding (1)

Adjoint statements are derived from tangent linear ones in a reversed order

Tangent linear code	Adjoint code
$\delta \mathbf{x} = 0$	$\delta x^* = 0$
$\delta x = A \delta y + B \delta z$	$\delta y^* = \delta y^* + A \delta x^*$
	$\delta z^* = \delta z^* + B \delta x^*$
	$\delta \mathbf{x}^* = 0$
$\delta x = A \delta x + B \delta z$	$\delta z^* = \delta z^* + B \ \delta x^*$
	$\delta x^* = A \delta x^*$
do $k = 1, N$	do $k = N, 1, -1$ (Reverse the loop!)
$\delta x(k) = A \delta x(k-1) + B \delta y(k)$	$\delta x^*(k-1) = \delta x^*(k-1) + A \delta x^*(k)$
end do	$\delta y^*(k) = \delta y^*(k) + B \delta x^*(k)$
Order of operations is important	$\delta x^*(k) = 0$
when variable is updated!	lend do
if (condition) tangent linear code	if (condition) adjoint code

And do not forget to initialize local adjoint variables to zero !



Summary of basic rules for line-by-line adjoint coding (2)

To save memory, the trajectory can be recomputed just before the adjoint calculations (again it depends on the complexity of the model).

Tangent linear code	Trajectory and adjoint code
if $(x > x0)$ then	Trajectory
$\delta \mathbf{x} = \mathbf{A} \delta \mathbf{x} / \mathbf{x}$	$x_{store} = x$ (storage for use in adjoint)
x = A Log(x)	if $(x > x0)$ then
end if	x = A Log(x)
	end if
	Adjoint
	if $(x_{store} > x0)$ then
	$\delta x^* = A \delta x^* / x_{store}$
	end if

The most common sources of error in adjoint coding are:

- 1) Pure coding errors
- 2) Forgotten initialization of local adjoint variables to zero
- 3) Mismatching trajectories in tangent linear and adjoint (even slightly)
- 4) Bad identification of trajectory updates



More facts about adjoints

- The adjoint always exists and it is unique, assuming spaces of finite dimension. Hence, coding the adjoint does not raise questions about its existence, only questions related to the technical implementation.
- In the meteorological literature, the term *adjoint* is often improperly used to denote the adjoint of the tangent linear of a non-linear operator. In reality, the adjoint can be defined for any linear operator. One must be aware that discussions about the *existence of the adjoint* usually should address the existence of the tangent linear model.
- Without re-computation, the cost of the TL is usually about 1.5 times that of the non-linear code, the cost of the adjoint between 2 and 3 times.
- The tangent linear model is not strictly necessary to run a 4D-Var system (but it is needed in the incremental 4D-Var formulation in use operationally at ECMWF). It is also needed as an intermediate step to write and test the adjoint.



Test for tangent linear model

• Taylor formula:

$$\lim_{\lambda \to 0} \frac{M(\mathbf{x} + \lambda \delta \mathbf{x}) - M(\mathbf{x})}{M'(\lambda \delta \mathbf{x})} = 1$$

			-
	λ	RATIO	
	0.1 E-09	$0.9994875881543574\mathrm{E}{+}00$]]
	0.1E-08	$0.9999477148855701\mathrm{E}{+}00$	k machine precision
	0.1 E- 07	$0.9999949234236705\mathrm{E}{+}00$	reached
)	0.1 E-06	$0.9999993501022509\mathrm{E}{+}00$	J
	0.1 E- 05	0.999999999999999999999999999999999999	
	0.1E-04	0.9999999 <mark>9</mark> 111338369E+00	
	0.1 E- 03	$0.9999993179193711E{+}00$	
	0.1 E- 02	$0.9999724488345042\mathrm{E}{+00}$	
	0.1 E-01	$0.9993727842790062 \pm 00$	
	$0.1E{+}00$	$0.9978007454264978E{+}00$	
	$0.1E{+}01$	$0.9683066504549524\mathrm{E}{+00}$	

Perturbation scaling factor



Test for adjoint model

• adjoint identity:

$$\forall \mathbf{x}, \forall \mathbf{y} \in M'.\mathbf{x}, \mathbf{y} > = <\mathbf{x}, \mathbf{M}^*.\mathbf{y} >$$

< F(X) , Y > = -.13765102625251640000E-01 $< X , F^*(Y) > = -.13765102625251680000E-01$

THE DIFFERENCE IS 11.351 TIMES THE ZERO OF THE MACHINE

The adjoint test is truly unforgiving. If you do not have a ratio of the norm close to 1 within the precision of the machine, you know there is a bug in your adjoint. At the end of your debugging you will have a perfect adjoint. If properly tested, the adjoint is the only piece of code on Earth to be entirely bug-free (although you may still have an imperfect tangent linear)!



Test of adjoint in practice...

• Compute perturbed variable (y) using perturbation in input variables (x,z) with the tangent linear code

$$\delta y = \frac{\partial y}{\partial x} \, \delta x + \frac{\partial y}{\partial z} \, \delta z$$

 $NORM _ TL = \left\| \delta y \right\|^2$

Call adjoint routine to obtain gradients in x and z with respect to initial perturbation in x and z
$$(\delta x_0, \delta z_0)$$
 from perturbation in y.

$$\delta x^* = \delta x^* + \left(\frac{\partial y}{\partial x}\right) \delta x^*$$
$$\delta z^* = \delta z^* + \left(\frac{\partial y}{\partial z}\right) \delta z^*$$

Compute the norm from the adjoint calculation, using unperturbed state and gradients:

$$NORM _ AD = \delta x_0 \delta x^* + \delta z_0 \delta z^*$$

 According to the test of adjoint NORM_TL must be equal to NORM_AD to the machine precision!



Automatic differentiation

- Because of the strict rules of tangent linear and adjoint coding, automatic differentiation is possible.
- Existing tools: TAF (TAMC), TAPENADE (Odyssée), ...
 - Reverse the order of instructions,
 - Transpose instructions instantly without typos !!!
 - Especially good in deriving tangent linear codes!
- There are still unresolved issues:
 - It is **NOT** a black box tool,
 - Cannot handle non-differentiable instructions (TL is wrong),
 - Can create huge arrays to store the trajectory,
 - The codes often need to be cleaned-up and optimised.
- Look in the "Supplementary material" for more information!



Useful References

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