# 3950 Inter-connections among three vector spaces in a 4D-Var system 

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## Introduction

Control parameters, model state and data spaces are three key vector spaces on which a 4D-Var data assimilation system is constructed. Lorenc(2003) showed that the 4D-Var on the control vector space can readily be interpreted as cost function on the state vector space. The recent study by El Akkraoui and Gauthier (2010) revealed a clear connection between cost functions for the state vector space and data vector space and its consequence on the performance of the descent algorithms. In this study, we summarise the interconnections among the cost functions, their gradients and Hessian matrices of a 4D-Var system written in the three vector spaces.

## Purpose of this study

To understand the connections among three 4D-Var formulations written on the three vector spaces (see Figure 1)

Figure 1. Three vector space in 4D-Var formulation: control vector space (c), state vector space ( x ) and data vector space (y)

## Inter-connections among the 4D-Var formulations I

Inter-connections of the three variations of 4D-Var formulations can be best understood in the following forms

Cost function:

$$
\begin{gather*}
J[\delta \mathbf{c}]=\frac{1}{2}\left(\delta \mathbf{c}-\delta \mathbf{c}^{\mathrm{a}}\right)^{\mathrm{T}} \mathbf{A}_{\mathrm{J}}\left(\delta \mathbf{c}-\delta \mathbf{c}^{\mathrm{a}}\right)+\frac{1}{2} \mathbf{d}^{\mathrm{T}} \mathbf{A}_{\mathrm{L}}^{-1} \mathbf{d}  \tag{2a}\\
I[\delta \mathbf{x}]=\frac{1}{2}\left(\delta \mathbf{x}-\delta \mathbf{x}^{\mathrm{a}}\right)^{\mathrm{T}} \mathbf{A}_{\mathrm{I}}\left(\delta \mathbf{x}-\delta \mathbf{x}^{\mathrm{a}}\right)+\frac{1}{2} \mathbf{d}^{\mathrm{T}} \mathbf{A}_{\mathrm{L}}^{-1} \mathbf{d}  \tag{2b}\\
L[\mathbf{w}]=\frac{1}{2}\left(\mathbf{w}-\mathbf{w}^{\mathrm{a}}\right)^{\mathrm{T}} \mathbf{A}_{\mathrm{L}}\left(\mathbf{w}-\mathbf{w}^{\mathrm{a}}\right)-\mathbf{d}^{\mathrm{T}} \mathbf{A}_{\mathrm{L}}^{-1} \mathbf{d} \tag{2c}
\end{gather*}
$$

Gradient:

$$
\begin{gather*}
\nabla_{\delta \mathbf{c}} J[\delta \mathbf{c}]=\mathbf{A}_{\mathrm{J}}\left(\delta \mathbf{c}-\delta \mathbf{c}^{\mathrm{a}}\right)  \tag{3a}\\
\nabla_{\delta \mathbf{x}} I[\delta \mathbf{x}]=\mathbf{A}_{\mathrm{I}}\left(\delta \mathbf{x}-\delta \mathbf{x}^{\mathrm{a}}\right)  \tag{3b}\\
\nabla_{\mathbf{w}} L[\mathbf{w}]=\mathbf{A}_{\mathrm{L}}\left(\mathbf{w}-\mathbf{w}^{\mathrm{a}}\right) \tag{3c}
\end{gather*}
$$

where,

$$
\mathbf{A}_{\mathrm{J}}=\mathbf{Q}^{-1}+\mathbf{G}^{\mathrm{T}} \mathbf{Q}^{-1} \mathbf{G}, \quad \mathbf{A}_{\mathrm{I}}=\mathbf{P}^{-1}+\mathbf{H}^{\mathrm{T}} \mathbf{P}^{-1} \mathbf{H}, \quad \mathbf{A}_{\mathrm{L}}=\mathbf{S}+\mathbf{R}
$$

There are following relationships among the Hessian matrices:

$$
\begin{equation*}
\mathbf{G Q} \mathbf{A}_{J} \mathbf{Q} \mathbf{G}^{\mathrm{T}}=\mathbf{H P} \mathbf{A}_{J} \mathbf{P} \mathbf{H}^{\mathrm{T}}=\mathbf{A}_{\mathrm{L}} \mathbf{R}^{-1} \mathbf{A}_{\mathrm{L}}-\mathbf{A}_{\mathrm{L}} \tag{4}
\end{equation*}
$$

$$
\begin{equation*}
\mathbf{G} \mathbf{Q} \mathbf{A}_{\mathrm{J}}^{2} \mathbf{Q} \mathbf{G}^{\mathrm{T}}=\mathbf{A}_{\mathrm{J}} \mathbf{R}^{-1} \mathbf{G}\left(\mathbf{A}_{\mathrm{J}} \mathbf{R}^{-1} \mathbf{G}\right)^{\mathrm{T}} \tag{5a}
\end{equation*}
$$

$\mathbf{H P A} \mathbf{A}_{\mathrm{I}} \mathbf{P H}^{\mathrm{T}}=\mathbf{A}_{\mathrm{I}} \mathbf{R}^{-1} \mathbf{H}\left(\mathbf{A}_{\mathrm{I}} \mathbf{R}^{-1} \mathbf{H}\right)^{\mathrm{T}}$

Background: variations in incremental 4D-Var formulation 4D-Var system in incremental formulation can be expressed in a simple vector-matrix form as
(tangent linear) Constraints:

$$
\begin{array}{ll}
\delta \mathbf{x}=\mathbf{M} \delta \mathbf{c} & : \text { forward model } \\
\delta \mathbf{y}=\mathbf{d}-\mathbf{H} \delta \mathbf{x} & \text { : observations }
\end{array} \Leftrightarrow \delta \mathbf{y}=\mathbf{d}-\mathbf{G} \delta \mathbf{c}
$$

where,

$$
\mathbf{d}=\mathbf{y}-\mathbf{G} \mathbf{c}^{\mathrm{b}}, \quad \mathbf{G}=\mathbf{H} \mathbf{M}
$$

I. 4D-Var on control vector space

Cost function:

$$
J[\delta \mathbf{c}]=\frac{1}{2} \delta \mathbf{c}^{\mathrm{T}} \mathbf{Q}^{-1} \delta \mathbf{c}+\frac{1}{2}(\mathbf{G} \delta \mathbf{c}-\mathbf{d})^{\mathrm{T}} \mathbf{R}^{-1}(\mathbf{G} \delta \mathbf{c}-\mathbf{d})
$$

Exact solution:

$$
\begin{equation*}
\delta \mathbf{c}^{\mathrm{a}}=\mathbf{Q} \mathbf{G}^{\mathrm{T}}\left(\mathbf{G} \mathbf{Q} \mathbf{G}^{\mathrm{T}}+\mathbf{R}\right)^{-1} \mathbf{d} \tag{1}
\end{equation*}
$$

where,

$$
\mathbf{Q}=\left\langle\delta \mathbf{c} \delta \mathbf{c}^{\mathrm{T}}\right\rangle, \quad \mathbf{R}=\left\langle\delta \mathbf{y} \delta \mathbf{y}^{\mathrm{T}}\right\rangle
$$

Two variations of 4D-Var formulations can be derived from equation (1) II. 4D-Var on state vector space:

Cost function: $I[\delta \mathbf{x}]=\frac{1}{2} \delta \mathbf{x}^{\mathrm{T}} \mathbf{P}^{-1} \delta \mathbf{x}+\frac{1}{2}(\mathbf{H} \delta \mathbf{x}-\mathbf{d}) \mathbf{P}^{-1}(\mathbf{H} \delta \mathbf{x}-\mathbf{d})^{\mathrm{T}}$
Exact solution:

$$
\delta \mathbf{x}^{\mathrm{a}}=\mathbf{P} \mathbf{H}^{\mathrm{T}}\left(\mathbf{H} \mathbf{P} \mathbf{H}^{\mathrm{T}}+\mathbf{R}\right)^{-1} \mathbf{d}
$$

where,

$$
\mathbf{P}=\left\langle\delta \mathbf{x} \delta \mathbf{x}^{\mathrm{T}}\right\rangle=\mathbf{M} \mathbf{Q} \mathbf{M}^{\mathrm{T}}
$$

III. 4D-Var on data vector space (PSAS):

Cost function:

$$
L[\mathbf{w}]=\frac{1}{2} \mathbf{w}^{\mathrm{T}}(\mathbf{S}+\mathbf{R})^{-1} \mathbf{w}-\mathbf{w}^{\mathrm{T}} \mathbf{d}
$$

Exact solution:

$$
\mathbf{w}^{\mathrm{a}}=(\mathbf{S}+\mathbf{R})^{-1} \mathbf{d}
$$

where,
$\mathbf{S}=\mathbf{G} \mathbf{Q} \mathbf{G}^{\mathrm{T}}=\mathbf{H P} \mathbf{H}^{\mathrm{T}} \quad$ :representer matrix (Bennett, 1992)

Inter-connections among the 4D-Var formulations II
From equations (2),(3),(4) and (5), inter-connections among the three variations of 4D-Var formulations can be established:

$$
J\left[\delta \mathbf{c}^{\mathrm{a}}\right]=I\left[\delta \mathbf{x}^{\mathrm{a}}\right]=-L\left[\mathbf{w}^{\mathrm{a}}\right]
$$

$$
J[\mathbf{w}]=I[\mathbf{w}]=\frac{1}{2}\left\|\nabla_{\mathbf{w}} \mathrm{L}[\mathbf{w}]\right\|_{\mathbf{R}^{-1}}^{2}-\mathrm{L}[\mathbf{w}]
$$

$$
\left\|\nabla_{\delta \mathbf{c}} \mathbf{J}[\mathbf{w}]\right\|^{2}=\left\|\mathbf{G}^{\mathrm{T}} \mathbf{R}^{-1} \nabla_{\mathbf{w}} \mathrm{L}[\mathbf{w}]\right\|^{2}
$$

$$
\left\|\nabla_{\delta \mathbf{x}} \mathrm{I}[\mathbf{w}]\right\|^{2}=\left\|\mathbf{H}^{\mathrm{T}} \mathbf{R}^{-1} \nabla_{\mathbf{w}} \mathrm{L}[\mathbf{w}]\right\|^{2}
$$

where,

$$
\|\mathbf{b}\|^{2}=\mathbf{b}^{\mathrm{T}} \mathbf{b},\|\mathbf{b}\|_{\mathbf{R}^{-1}}^{2}=\mathbf{b}^{\mathrm{T}} \mathbf{R}^{-1} \mathbf{b}
$$

The above relationships are equal to El Akkraoui and Gauthier (2010) when the formulations are preconditioned.

## References

- Bennett (1992), Inverse methods in physical oceanography, Cambridge University Press, Cambridge, UK, 347pp.
- Lorenc (2003), Modelling of error covariances by 4D-Var data assimilation, QJRMS, 129, 3167-3182.
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