

What is Data Assimilation?

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ITT7 (SAMBa Integrative Think Tank)

## What is data assimilation?

## Definition

Data assimilation is a way of combining observations with a numerical model, to create a better guess of the true state.

Used in

- Weather forecasting
- GPS navigation
- Medical imaging
- Seismology
- and many more places.


## Data assimilation setting

We have a state $x_{k} \in \mathbb{R}^{n}$ at time $t_{k}$.
A numerical model $\mathcal{M}_{k}: \mathbb{R}^{n} \rightarrow \mathbb{R}^{n}$ such that

$$
x_{k+1}=\mathcal{M}_{k}\left(x_{k}\right)+\eta_{k} .
$$

A background estimate $x^{b}$ of the truth $x_{0}^{*}$,

$$
x_{0}^{*}=x^{b}+e_{0} .
$$

And observations $y_{k} \in \mathbb{R}^{p_{k}}$ of the state:

$$
y_{k}=\mathcal{H}_{k}\left(x_{k}^{*}\right)+\epsilon_{k},
$$

where $\mathcal{H}_{k}: \mathbb{R}^{n} \rightarrow \mathbb{R}^{p_{k}}$ is an observation operator.
The errors $\eta_{k}, e_{0}, \epsilon_{k}$ are Gaussian with zero mean and covariances $Q_{k} \in \mathbb{R}^{n \times n}, B \in \mathbb{R}^{n \times n}, R_{k} \in \mathbb{R}^{p_{k} \times p_{k}}$ respectively.

## The aim of data assimilation

The goal is to find an estimate $x_{0}$ to the true initial condition $x_{0}^{*}$ which minimises

1. the distance to our background state $x_{0}^{b}$,
2. the distances between the state trajectory $x$ of this initial state, and our observations $y$.

## Different approaches

Different approaches:

- Sequential Data Assimilation
- Variational Data Assimilation


## Kalman Filter

## State and error covariance analysis (corrector step)

Given previous forecast $x_{i}^{F}$ and error covariance matrix $B_{i}^{F}$

$$
\begin{aligned}
\text { State estimate } x_{i}^{A}= & x_{i}^{F}+K_{i}\left(y_{i}-H_{i} X_{i}^{F}\right) \\
\text { where } K_{i}= & B_{i}^{F} H_{i}^{\top}\left(H_{i} B_{i}^{F} H_{i}^{\top}+R_{i}\right)^{-1} \\
& \left(K_{a l} \text { Iman gain }\right) \\
\text { Error covariance estimate } B_{i}^{A}= & \left(1-K_{i} H_{i}\right) B_{i}^{F}
\end{aligned}
$$

## State and error covariance forecast (predictor step)

Given state $x_{i}^{A}$ and error covariance matrix $B_{i}^{A}$
State forecast $x_{i+1}^{F}=M_{i+1, i} X_{i}^{A}$
Error covariance forecast $B_{i+1}^{F}=M_{i+1, i} B_{i}^{A} M_{i+1, i}^{\top}+Q_{i}$

## Different approaches

Different approaches:

- Sequential Data Assimilation
- Variational Data Assimilation


## Variational data assimilation

## Variational data assimilation

We wish to find an estimate $x_{0}$ to $x_{0}^{*}$ which minimises

1. the distance to our background state $x_{0}^{b}$,
2. the distances between the state trajectory $x$ of this initial state, and our observations $y$.

In variational data assimilation, we introduce a cost function J and attempt to minimise that.

$$
J\left(x_{0}\right)=\underbrace{\left\|x_{0}-x_{0}^{b}\right\|}_{J_{b}}+\underbrace{\|y-\mathcal{H}(x)\|}_{J_{0}} .
$$

## Variational data assimilation

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$$

## Variational data assimilation



- Take observations y of the true dynamical system.


## Variational data assimilation



Assimilation Window

- Estimate the initial condition $x_{0}^{b}$, for the numerical model $x_{i+1}=M_{i+1, i}\left(x_{i}\right)$, simulating the true dynamical system .


## Variational data assimilation



- Run the numerical model using the estimated initial condition.


## Variational data assimilation



- Minimise cost function $J\left(x_{0}\right)$ to find an improved initial condition $x^{A}$, i.e.: $\nabla J\left(x^{A}\right)=0$.


## Variational data assimilation



- The numerical model is run using $x^{A}$ as an initial condition.


## Variational data assimilation



- The simulation is continued to create a forecast for the true dynamical system.


## Variational data assimilation



- The process is repeated for new observations.
- This is called cyclic 4DVar.
(Plots from Melina Freitag)


## Variational data assimilation

$$
J\left(x_{0}\right)=\underbrace{\left\|x_{0}-x_{0}^{b}\right\|}_{J_{b}}+\underbrace{\|y-\mathcal{H}(x)\|}_{J_{0}} .
$$



Figure 1: Copyright:ECMwF

## Variational data assimilation

$$
J\left(x_{0}\right)=\underbrace{\left\|x_{0}-x_{0}^{b}\right\|}_{J_{b}}+\underbrace{\|y-\mathcal{H}(x)\|}_{J_{0}} .
$$

Earlier we saw that

$$
x_{0}^{*}=x_{0}^{b}+e_{0}
$$

$e_{0}$ Gaussian with zero mean and covariance $B \in \mathbb{R}^{n \times n}$.
So we take

$$
\begin{aligned}
J_{b} & =\frac{1}{2}\left\|x_{0}-x_{0}^{b}\right\|_{B}^{2} \\
& =\frac{1}{2}\left(x_{0}-x_{0}^{b}\right)^{\top} B^{-1}\left(x_{0}-x_{0}^{b}\right) .
\end{aligned}
$$

## Variational data assimilation

$$
J\left(x_{0}\right)=\underbrace{\left\|x_{0}-x_{0}^{b}\right\|}_{J_{b}}+\underbrace{\|y-\mathcal{H}(x)\|}_{J_{0}} .
$$

With one observation at $x_{0}$,

$$
\begin{aligned}
J_{0} & =\frac{1}{2}\left\|y_{0}-\mathcal{H}_{0}\left(x_{0}\right)\right\|_{R_{0}}^{2} \\
& =\frac{1}{2}\left(y_{0}-\mathcal{H}_{0}\left(x_{0}\right)\right)^{\top} R_{0}^{-1}\left(y_{0}-\mathcal{H}_{0}\left(x_{0}\right)\right)
\end{aligned}
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\end{aligned}
$$

With 4D-Var we consider all observations in our cost function to obtain instead:

$$
\begin{aligned}
J_{0} & =\frac{1}{2} \sum_{k=0}^{N}\left\|y_{k}-\mathcal{H}_{k}\left(x_{k}\right)\right\|_{R_{k}}^{2} \\
& =\frac{1}{2} \sum_{k=0}^{N}\left(y_{k}-\mathcal{H}_{k}\left(x_{k}\right)\right)^{\top} R_{k}^{-1}\left(y_{k}-\mathcal{H}_{k}\left(x_{k}\right)\right)
\end{aligned}
$$

## 4D-Var cost function

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$$
\begin{aligned}
J\left(x_{0}\right) & =\underbrace{\frac{1}{2}\left(x_{0}-x_{0}^{b}\right)^{\top} B^{-1}\left(x_{0}-x_{0}^{b}\right)}_{J_{b}} \\
& +\underbrace{\frac{1}{2} \sum_{k=0}^{N}\left(y_{k}-\mathcal{H}_{k}\left(x_{k}\right)\right)^{\top} R_{k}^{-1}\left(y_{k}-\mathcal{H}_{k}\left(x_{k}\right)\right)}_{J_{0}} .
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& +\underbrace{\frac{1}{2} \sum_{k=0}^{N}\left(y_{k}-\mathcal{H}_{k}\left(\mathcal{M}_{k, 0}\left(x_{0}\right)\right)\right)^{\top} R_{k}^{-1}\left(y_{k}-\mathcal{H}_{k}\left(\mathcal{M}_{k, 0}\left(x_{0}\right)\right)\right)}_{J_{0}} .
\end{aligned}
$$

Where $\mathcal{M}_{k, 0}\left(x_{0}\right)=\mathcal{M}_{k}\left(\mathcal{M}_{k-1}\left(\cdots \mathcal{M}_{1}\left(x_{0}\right)\right)\right)=x_{k}$

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& +\frac{1}{2} \sum_{k=0}^{N}\left(y_{k}-\mathcal{H}_{k}\left(\mathcal{M}_{k, 0}\left(x_{0}\right)\right)\right)^{\top} R_{k}^{-1}\left(y_{k}-\mathcal{H}_{k}\left(\mathcal{M}_{k, 0}\left(x_{0}\right)\right)\right) .
\end{aligned}
$$

## 4D-Var Cost function gradient

$$
\begin{aligned}
\nabla J\left(x_{0}\right) & =B^{-1}\left(x_{0}-x_{0}^{b}\right) \\
& -\sum_{k=0}^{N}\left(H_{k} M_{k, 0}\right)^{T} R_{k}^{-1}\left(y_{k}-\mathcal{H}_{k}\left(\left(\mathcal{M}_{k, 0}\left(x_{0}\right)\right)\right)\right.
\end{aligned}
$$

where $H_{k}$ and $M_{k, 0}$ are the Jacobians of $\mathcal{H}_{k}$ and $\mathcal{M}_{k, 0}$.

## Weak 4D-Var

Weak 4D-Var cost function

$$
\begin{aligned}
J(x) & =\underbrace{\frac{1}{2}\left(x_{0}-x_{0}^{b}\right)^{\top} B^{-1}\left(x_{0}-x_{0}^{b}\right)}_{J_{b}} \\
& +\underbrace{\frac{1}{2} \sum_{k=0}^{N}\left(y_{k}-\mathcal{H}_{k}\left(x_{k}\right)\right)^{\top} R_{k}^{-1}\left(y_{k}-\mathcal{H}_{k}\left(x_{k}\right)\right)}_{J_{o}} \\
& +\underbrace{\frac{1}{2} \sum_{k=1}^{N}\left(x_{k}-\mathcal{M}_{k}\left(x_{k-1}\right)\right)^{T} Q_{k}^{-1}\left(x_{k}-\mathcal{M}_{k}\left(x_{k-1}\right)\right)}_{J_{q}}
\end{aligned}
$$

$$
x=\left[x_{0}^{T}, x_{1}^{T}, \ldots, x_{N}^{T}\right]^{T}
$$

Incremental 4D-Var

## Incremental 4D-Var

Operationally, Incremental 4D-Var is used.

- This is a form of Gauss-Newton iteration, with
- linearised quadratic cost function $\tilde{J}(\delta x)$.

$$
\begin{aligned}
\tilde{J}\left(\delta x^{(\ell)}\right) & =\frac{1}{2}\left(\delta x_{0}^{(\ell)}-b_{0}^{(\ell)}\right)^{\top} B^{-1}\left(\delta x_{0}^{(\ell)}-b_{0}^{(\ell)}\right) \\
& +\frac{1}{2} \sum_{i=0}^{N}\left(d_{i}^{(\ell)}-H_{i} \delta x_{i}^{(\ell)}\right)^{\top} R_{i}^{-1}\left(d_{i}^{(\ell)}-H_{i} \delta x_{i}^{(\ell)}\right) .
\end{aligned}
$$

- Increment at iterate $\ell$,

$$
\delta x_{0}^{(\ell)}=x_{0}^{(\ell+1)}-x_{0}^{(\ell)}
$$

## Incremental 4D-Var

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- Increment at iterate $\ell$,

$$
\delta x_{0}^{(\ell)}=x_{0}^{(\ell+1)}-x_{0}^{(\ell)} .
$$

You can form it into

$$
\mathcal{A} x=b
$$

## More information

For more information and references：
R．M．Asch，M．Bocquet，And M．Nodet，Data Assimilation：Methods， Algorithms and Applications，SIAM，Dec． 2016.
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Title image copvright Star Trek：First Contact．

## Thank you for listening. Any Questions?

