Data assimilation and dynamic observers for data-based flow field recovery

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Definition of **data assimilation**

**Data assimilation** is the process by which observations of a system are incorporated into the model state of a numerical model of that system.

(www.wikipedia.org)
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![Diagram of data assimilation process]

- **x**: state
- **y**: observation
- **h(x)**: compressive operator (null-space)
- **h^{-1}(x)**: data assimilation
- **y**: observation
- **x**: state

- ill-posed
- unobserved states?
- existence?
- uniqueness?
Definition of **data assimilation**

**Data assimilation** is the process by which observations of a system are incorporated into the model state of a numerical model of that system.

\[
\mathcal{J} = \| \mathbf{y} - \mathbf{H}(\mathbf{x}) \| \rightarrow \min
\]

**simplest** form: BLUE (best linear unbiased estimator)

\[
\mathbf{H}(\mathbf{x}) \sim \mathbf{h}(\mathbf{x})
\]

observation model

no constraints on dynamical model
**Definition of data assimilation**

Data assimilation is the process by which observations of a system are incorporated into the model state of a numerical model of that system.

(www.wikipedia.org)

$$\dot{x} = f(x, \nu)$$

more information on the dynamic model is required
Classification of **data assimilation**

**Variational** data assimilation (global approach)
- define cost functional
- choose control variables
- optimize by gradient descent
- ... e.g. 3dvar, 4dvar

**Sequential** data assimilation (incremental approach)
- update model as observations become available
- ... e.g. Kalman filter (KF), enKF, dynamic observer
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for **Gaussian** noise and **linear** model

→ classical Kalman filter
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for **nonGaussian** noise and/or **nonlinear** model

→ ensemble Kalman filter

influence of uncertainty
Classification of **data assimilation**

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**sequential** data assimilation (incremental approach)

- update model as observations become available
- ... e.g. Kalman filter (KF), enKF, dynamic observer
- identify a linear state-space model and noise covariances (dynamic observer)
**Variational** data assimilation (global approach)

Data assimilation of mean flows from limited data (*numerical*)

Goal: recover the mean flow of a turbulent flow from *limited* measurements

Approach: variational data assimilation using the RANS equations

\[
\bar{u} \cdot \nabla \bar{u} + \nabla \bar{p} - Re^{-1} \nabla^2 \bar{u} = f^* \\
\nabla \cdot \bar{u} = 0
\]

RANS equ.

With

\[
f^* = -\nabla \cdot R \\
R_{ij} = \bar{u}'_i \bar{u}'_j
\]

Reynolds stresses
**Variational** data assimilation (global approach)

**Data assimilation** of mean flows from limited data (numerical)

We sample the flow field at given measurement locations.

Define a measurement operator

\[
\bar{m} = \mathcal{M} (\bar{u})
\]

high-to-low dimensional map

and a measurement error

\[
\mathcal{E} (\tilde{u}) = \frac{1}{2} \| \bar{m} - \mathcal{M} (\tilde{u}) \|_M^2
\]

with \( \Delta u = \bar{u} - \tilde{u} \)

Note that \( \Delta u \) is not accessible; similar to a **Kalman filter** we have to imply a state-vector error from a measurement error.
**Variational** data assimilation (global approach)

**Data assimilation** of mean flows from limited data (**numerical**)

The shape of the Reynolds stresses in the RANS equations allows solutions of the form

$$\tilde{u}(f, \tilde{p}) = \tilde{u}(f + \nabla \phi, \tilde{p} + \phi)$$

where $\phi$ is a potential field.

We cannot uniquely determine the full Reynolds stresses.

Use a projection onto solenoidal functions to resolve the non-uniqueness issue.
data assimilation of mean flows from limited data (numerical)

We wish to minimize the error measure while observing the RANS equations.

Reformulated as an unconstrained variational problem, we get

\[ \mathcal{L}(f, \tilde{u}, \tilde{p}, \tilde{u}^+, p^+) = \mathcal{E}(\tilde{u}) - \langle \tilde{u}^+, \tilde{u} \cdot \nabla \tilde{u} + \nabla \tilde{p} - Re^{-1} \nabla^2 \tilde{u} - f \rangle - \langle \tilde{p}^+, \nabla \cdot \tilde{u} \rangle \]

\[ = \mathcal{E}(\tilde{u}) - \int_{\Omega} \tilde{u}^+ \cdot \tilde{u} \cdot \nabla \tilde{u} + \nabla \tilde{p} \cdot \tilde{u} - Re^{-1} \nabla^2 \tilde{u} \cdot \tilde{u} - f \cdot \tilde{u} \]

Lagrangian error measure constraints

... which introduces Lagrange multipliers (adjoint variables) as independent variable.

scalar product \[ \langle a, b \rangle = \int_{\Omega} a \cdot b \ d\Omega \]
**variational** data assimilation (global approach)

**data assimilation** of mean flows from limited data (**numerical**)

We take first variations to derive the optimality conditions.

\[
\frac{\delta L}{\delta \tilde{u}^+} = 0 \quad \frac{\delta L}{\delta \tilde{p}^+} = 0 \quad \text{RANS-equations}
\]

\[
\frac{\delta L}{\delta \tilde{u}} = 0 \quad \frac{\delta L}{\delta \tilde{p}} = 0 \quad \text{adjoint RANS-equations}
\]

\[
\frac{\delta L}{\delta f} = 0 \quad \text{optimality condition}
\]
**Variational** data assimilation (global approach)

**Data assimilation** of mean flows from limited data (**numerical**)

We take first variations to derive the optimality conditions.

\[
\begin{align*}
\bar{u} \cdot \nabla \bar{u} + \nabla \bar{p} - Re^{-1} \nabla^2 \bar{u} &= f^* \\
\nabla \cdot \bar{u} &= 0
\end{align*}
\]

RANS-equations

\[
\begin{align*}
-\tilde{u} \cdot \nabla \tilde{u}^+ + \tilde{u}^+ \cdot \nabla \tilde{u}^T - \nabla \tilde{p}^+ - Re^{-1} \nabla^2 \tilde{u}^+ &= \frac{\delta \mathcal{E}}{\delta \tilde{u}} \\
\nabla \cdot \tilde{u}^+ &= 0
\end{align*}
\]

Adjoint RANS-equations

\[
\nabla f \mathcal{E} = \tilde{u}^+
\]

Optimality condition
**variational** data assimilation (global approach)

**data assimilation** of mean flows from limited data (numerical)

Rather than solving the equations simultaneously, we iterate according to

The adjoint RANS equations depend on the RANS-solution (variable coefficients and driving). We have to employ *checkpointing*. 
**variational** data assimilation (global approach)

**Data assimilation** of mean flows from limited data (**numerical**)

- Total number of time-steps done
- Stored direct flow field
**Variational** data assimilation (global approach)

**Data assimilation** of mean flows from limited data **(numerical)**

We trade reduced storage requirements for increased simulation time.
Variational data assimilation (global approach)

data assimilation of mean flows from limited data (numerical)

Finally, we choose an error measure in the form

\[
\mathcal{M}(\mathbf{u}) = \mathcal{P}(Q(\mathbf{u}))
\]

... what we measure

... where we measure

for example

\[
Q(\mathbf{u}) = \mathbf{u}
\]

\[
\mathcal{P}(\mathbf{u}) = \int_{\Omega} \mathbf{u}(\mathbf{x}) b_i(\mathbf{x}) \, d\Omega
\]

\[
\frac{\delta \mathcal{E}}{\delta \tilde{\mathbf{u}}} = - \sum_{i=0}^{N} \frac{\delta Q}{\delta \tilde{\mathbf{u}}} b_i \Delta m_i
\]
variational data assimilation (global approach)

data assimilation of mean flows from limited data (numerical)

Results: flow past a cylinder

\[ Re = 150 \]
variational data assimilation (global approach)

data assimilation of mean flows from limited data (numerical)

interpolation

measurements

recovered mean flow

error
variational data assimilation (global approach)

data assimilation of mean flows from limited data (numerical)

extrapolation

measurements

recovered mean flow

error
**variational** data assimilation (global approach)

**data assimilation** of mean flows from limited data **(numerical)**

State-vector completion of measurements

Recovered mean flow

Error
**variational** data assimilation (global approach)

**data assimilation** of mean flows from limited data (numerical)

state-vector completion

\[ \| \mathbf{u} \| + \nu \]

measurements

\( \mathbf{u} \) recovered mean flow

\( \mathbf{v} \) error
variational data assimilation (global approach)

data assimilation of mean flows from limited data (experimental)

$Re = 13500$
**Variational** data assimilation (global approach)

**Data assimilation** of mean flows from limited data *(experimental)*

![Diagram showing the process of variational data assimilation](image)
**Variational** data assimilation (global approach)

Data assimilation of mean flows from limited data *(experimental)*

- **Variational** data assimilation (global approach)

Measurements

Recovered mean flow

\[ \nabla \times f \]
**variational** data assimilation (global approach)

Data assimilation of mean flows from limited data (experimental)

measurements

recalled mean flow
**variational** data assimilation (global approach)

**data assimilation** of mean flows from limited data (**experimental**)

measurements
state-vector estimation from low-dimensional data (numerical)

principles of a **Kalman filter**

start with state-space formulation

\[
\begin{align*}
\frac{dX}{dt} &= AX + Bw \\
\hspace{1cm} s &= CX + g
\end{align*}
\]

**continuous**

\[
\begin{align*}
X(n+1) &= AX(n) + Bw(n) \\
\hspace{1cm} s(n) &= CX(n) + g(n)
\end{align*}
\]

**discrete**
**sequential** data assimilation (incremental approach)

**state-vector estimation** from low-dimensional data (**numerical**)

Question: can we estimate the state-vector from the measurements only
Solution: minimize the estimation error under the state-space model constraint

We postulate a state-space model for the estimated state

\[
X_e(n + 1) = AX_e(n) + L [s(n) - CX_e(n)] = A_s X_e(n) + Ls(n)
\]

Kalman filter

modified system matrix \( A_s = A - LC \)

How should we choose L? ... minimize the estimation error \( ||X - X_e|| \)

optimization (variational) yields the Riccati equation

\[
P = APA^+ - APC(CPC^+ + G)^{-1} CPA^+ + BWB^+
\]

from which we obtain the **Kalman gain**

\[
L = APC^+(CPC^+ + G)^{-1}
\]
**sequential** data assimilation (incremental approach)

**state-vector estimation** from low-dimensional data (**numerical**)

The *dynamic observer* identifies (rather than prescribes) the state-space model. … we have

\[
x(n + 1) = Ax(n) + Bu(n) + w(n)
\]

\[
y(n) = Cx(n) + Du(n) + v(n)
\]

To reduce the dimensionality of the system, we project onto a POD basis and only track the POD-coefficients \( Y(n) = \{y_1(n), y_2(n), \cdots, y_N(n)\} \)

\[
Y_e(n + 1) = A_s Y_e(n) + L s(n)
\]

\[
s(n) = C Y_e(n)
\]

modified system matrix \( A = A_s + LC \)
**sequential** data assimilation (incremental approach)

**state-vector estimation** from low-dimensional data (**numerical**)

The **dynamic observer** identifies (rather than prescribes) the state-space model.
**Sequential** data assimilation (incremental approach)

**State-vector estimation** from low-dimensional data (**numerical**)

The **dynamic observer** identifies (rather than prescribes) the state-space model.

- Noise will enter the system identification “colored”.
- Driving signal has to be rich in frequencies (pseudo-random binary signal).
**sequential** data assimilation (incremental approach)

**state-vector estimation** from low-dimensional data (numerical)

The **dynamic observer** identifies (rather than prescribes) the state-space model.

\[ \begin{align*}
  \mathbf{y} &\quad \rightarrow \quad \text{system matrices} \quad \rightarrow \quad y_m \\
  \mathbf{s} \quad &\quad \rightarrow \quad \mathbf{w} \\
  \mathbf{N4SID} &\quad \rightarrow \quad \text{diff}
\end{align*} \]

- Noise will enter the system identification “colored”.
- Driving signal has to be rich in frequencies
sequential data assimilation (incremental approach)

state-vector estimation from low-dimensional data (numerical)

The dynamic observer identifies (rather than prescribes) the state-space model.

- Noise will enter the system identification “colored”.
- Driving signal has to be rich in frequencies (pseudo-random binary signal).
- Output signal has to capture the bulk of the dynamics (# of POD modes).
- Residualization (rather than truncation) of model errors is accomplished.
sequential data assimilation (incremental approach)

state-vector estimation from low-dimensional data (numerical)

The dynamic observer identifies (rather than prescribes) the state-space model.
**sequential** data assimilation (incremental approach)

**state-vector estimation** from low-dimensional data (**numerical**)

The **dynamic observer** identifies (rather than prescribes) the state-space model.

![Graphs showing S, E, y1, y10, and Cp](image-url)

- **S**: Graph showing a time series with a peak at around 5000 and another peak at around 8000.
- **E**: Graph showing a smooth increase from 0 to 0.04, with a peak around 7000.
- **y1**: Graph with oscillations that decrease in amplitude over time, with peaks around 2000 and 8000.
- **y10**: Graph similar to y1 but with a smaller amplitude.
- **Cp**: Graph with oscillations and a peak around 5000.
sequential data assimilation (incremental approach)

state-vector estimation from low-dimensional data (numerical)

The dynamic observer identifies (rather than prescribes) the state-space model.

Alternative: linear stochastic estimation (LSE) uses a least squares approach between input and output.
**sequential** data assimilation (incremental approach)

**state-vector estimation** from low-dimensional data (**numerical**)

The **dynamic observer** identifies (rather than prescribes) the state-space model.

Once the system matrices and noise covariances have been identified, we can apply flow control.

\[ E(t) \]

\[ u(t) \]
**sequential** data assimilation (incremental approach)

**state-vector estimation** from low-dimensional data (**numerical**)

For many materials, we do not have optical access to the flow field in the interior.

We would like to reconstruct the (high-dimensional) interior flow state from (low-dimensional) measurements on the wall.

We need to establish a mapping between interior flow fields and wall quantities, as well as a dictionary of interior structures.

\[
Ra = \frac{\alpha g \Delta H^3}{\kappa \nu} = 8.1 \, 10^5
\]

\[
Pr = \frac{\nu}{\kappa} = 0.025 \quad \text{(liquid gallium or mercury)}
\]

\[
Ek = \frac{\nu}{2\Omega H^2} = 2 \, 10^{-5}
\]

\[
\Gamma = 1.87
\]
**sequential** data assimilation (incremental approach)

**state-vector estimation** from low-dimensional data (numerical)

\[ MQ = T_w \]

\[ MUSV \approx T_w \]

optimization problem

\[ \min_S \| MUSV - T_w \| + \gamma \| \text{diag}(S) \|_1 \]
sequential data assimilation (incremental approach)

state-vector estimation from low-dimensional data (numerical)

work in progress …

- formulation of sparsity-promoting recovery of internal flow field
- experiments (UCLA SpinLab) on liquid gallium and SF$_6$
- extension to rotating magnetoconvection and planetary dynamo systems
Summary

• Data assimilation and dynamic observers are powerful techniques to recover higher-dimensional flow states from low-dimensional measurements.

• They can form the foundation for flow analysis and flow manipulation.

• Challenges lie in the treatment of noise and uncertainties and in the robust recovery of the flow states.

• Techniques from robust statistics and $L_1$ (sparsity-promoting) optimization may lead to useful algorithms.