Intro Inverse Modelling

Thomas Kaminski (http://FastOpt.com)

Thanks to:

Simon Blessing (FastOpt), Peter Rayner (Mebourne Uni)

2\textsuperscript{nd} Advanced Training Course on Atmospheric Remote Sensing, Juelich, October 2014
References and Definitions


# Definitions

<table>
<thead>
<tr>
<th>Name</th>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parameters</td>
<td>$\vec{p}$</td>
<td>Quantities not changed by model, i.e. process parameters, boundary conditions</td>
</tr>
<tr>
<td>State variables</td>
<td>$\vec{v}(t)$</td>
<td>Quantities altered by model from time step to time step</td>
</tr>
<tr>
<td>Control variables</td>
<td>$\vec{x}$</td>
<td>Quantities exposed to optimisation, a combination of subsets of $\vec{p}$ and $\vec{v}(t = 0)$</td>
</tr>
<tr>
<td>Observables</td>
<td>$\vec{o}$</td>
<td>Measurable quantities</td>
</tr>
<tr>
<td>Observation operator</td>
<td>$\mathbf{H}$</td>
<td>Transforms $\vec{v}$ to $\vec{o}$</td>
</tr>
<tr>
<td>Model</td>
<td>$\mathbf{M}$</td>
<td>Predicts $\vec{o}$ given $\vec{p}$ and $\vec{v}(t = 0)$, includes $\mathbf{H}$</td>
</tr>
<tr>
<td>Data</td>
<td>$\vec{d}$</td>
<td>Measured values of $\vec{o}$</td>
</tr>
</tbody>
</table>
Statement of Problem

Given a model $\mathcal{M}$, a set of measurements $\vec{d}$ of some observables $\vec{\sigma}$, and prior information on some control variables $\vec{x}$, produce an updated description of $\vec{x}$.

$\vec{x}$ may include parts of $\vec{p}$ and $\vec{v}(t = 0)$

$$\vec{\sigma} = \mathcal{M}(\vec{x})$$
Information and PDFs

- We seek true value but all input information is approximate.
- Treat model, measurements and priors as PDFs describing distribution of true value.
- Data and prior error easy.
- Model error is difference between actual and perfect simulation for a given $\vec{x}$.
- Arises from errors in equations and errors in those parameters not included in $\vec{x}$. 
Combining PDFs

- Operate in joint parameter and data space
- Estimates are combination of prior, measurement and model (black triangle)
- Estimate is multiplication of PDFs
- Only involves forward models
- Parameter estimate projection of PDF onto X-axis

Figure: Rayner (2010)
Summary statistics from PDF

- Combination of PDFs (upper) and posterior PDF for parameters (lower)
- Can calculate all summary statistics from posterior PDF
- Maximum Likelihood Estimate (MLE) maximum of PDF
Tightening Model Constraint

- Note no viable solution
- If we cannot treat model as soft constraint we must inflate data uncertainty
- Model error hard to characterise
Gaussian Case

\[ G(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \]

Data:
\[ P_d \propto e^{-\frac{(d-1)^2}{2 \cdot 0.6^2}} \]

Parameters:
\[ P_x \propto e^{2 \cdot 0.6^2} \]

Model:
\[ P_M \propto e^{\frac{- (d-x)^2}{2 \cdot 0.6^2}} \]
Prior plus Data
Prior plus Data plus Model
PDFs and cost functions

• MLE most common quantity

• Maximise PDF numerically

• Most common $P(x) \propto e^{-\frac{1}{2}J}$ so maximising $P \leftrightarrow$ minimising $J$

• $J$ usually called the cost (or misfit or objective) function

• Exponentials convenient because multiplying exponentials $\leftrightarrow$ adding exponents
Perfect and imperfect models

### Imperfect Model
- Include observables ($\vec{o}$) in control variables

\[
J = \frac{1}{2} \left( \frac{(\vec{x} - \vec{x}_0)^2}{\sigma_x^2} + \frac{(\vec{o} - \vec{d})^2}{\sigma_{obs}^2} + \frac{(M(\vec{x}) - \vec{o})^2}{\sigma_M^2} \right)
\]

- $\vec{x}_0$ prior estimate for $\vec{x}$, $\sigma$ standard deviations.
- Allows explicit model error
- Different from weak constraint 4D-Var in which model state added to control variables

### Perfect Model
- Observables not included in control vector

\[
J = \frac{1}{2} \left( \frac{(\vec{x} - \vec{x}_0)^2}{\sigma_x^2} + \frac{(M(\vec{x}) - \vec{d})^2}{\sigma_d^2} \right)
\]

- If model imperfect, carried model error in $\sigma_d$:
  \[
  \sigma_d^2 = \sigma_{obs}^2 + \sigma_M^2
  \]
- This is the form usually used in data assimilation
- For linear $M$ there is a closed solution
- Otherwise minimised by iterative algorithm, usually using gradients
- Can calculate posterior $\sigma_x$ by rearranging PDF
Covariances

\[ J = \frac{1}{2} \left( \frac{(\vec{x} - \vec{x}_0)^2}{\sigma_x^2} + \frac{(M(\vec{x}) - \vec{d})^2}{\sigma_d^2} \right) \]

Takes the more general form

\[ J = \frac{1}{2} \left( (\vec{x} - \vec{x}_0)^T C(\vec{x}_0)^{-1}(\vec{x} - \vec{x}_0) + (M(\vec{x}) - \vec{d})^T C(\vec{d})^{-1}(M(\vec{x}) - \vec{d}) \right) \]

• Off-diagonal terms represent correlation in uncertainty

• Persistent instrumental error

• Model error usually correlated

• Errors in initial conditions from previous forecast
Linear Gaussian case

\[
J = \frac{1}{2} \left( (\vec{x} - \vec{x}_0)^T C(\vec{x}_0)^{-1}(\vec{x} - \vec{x}_0) + (M\vec{x} - \vec{d})^T C(\vec{d})^{-1}(M\vec{x} - \vec{d}) \right)
\]

\[
\vec{x}_{opt} = \vec{x}_0 + C(\vec{x}_0)M^T \left( MC(\vec{x}_0)M^T + C(\vec{d}) \right)^{-1} (\vec{d} - M\vec{x}_0)
\]

\[
C(\vec{x})^{-1} = C(\vec{x}_0)^{-1} + M^T C(\vec{d})^{-1} M
\]

\[
= \frac{d^2 J(x_{opt})}{dx^2}
\]

• \(C(\vec{x})\) does not depend on values, only uncertainties and model
How to solve it?

1. Minimisation

Efficient minimisation algorithms use $J(x)$ and the gradient of $J(x)$ in an iterative procedure. Typically the prior value is used as starting point of the iteration. The gradient is helpful as it always points uphill. The adjoint is used to provide the gradient efficiently.

Example: Newton algorithm for minimisation

Gradient: $g(x) = dJ/dx(x)$

Hessian: $H(x) = dg/dx(x) = d^2J/dx^2(x)$

At the minimum, $x_{min}$: $g(x_{min}) = 0$, hence:

$g(x) = g(x) - g(x_{min}) \sim H(x)(x-x_{min})$

rearranging yields:

$(x_{min} - x) \sim -H^{-1}(x) g(x)$

Smart gradient algorithms use an approximation of $H(x)$
How to solve it?
2. Error bars

Hessian quantifies the curvature of the cost function
Use Hessian at minimum to approximate \( C(x)^{-1} \)

Figure taken from Tarantola (1987) -->