Polynomial Chaos based Minimum Variance Approach for Characterization of Source Parameters

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Introduction

• Inverse Problem refers to problem of characterizing the system of interest by exploiting measurements resulting for the system (eg. source identification).
  – Source parameters, initial conditions, boundary conditions
  – Uncertainty in the identified source parameters, initial conditions, etc.

• Inverse problems are often ill-posed (eg. optical flow).
  – Tikhonov regularization

• For large scale systems (eg. volcanic plume source ID), the computational cost is significant.
PUFF simulation model

- PUFF is a *Lagrangian* Trajectory Volcanic Ash Tracking Model which initializes and transports a collection of discrete ash particles, representing a sample of the eruption cloud.

- Different types of transport include:
  - Advection: due to the wind field \( W \)
  - Diffusion: due to turbulent dispersion \( Z \)
  - Fallout: due to the gravity and Stoke’s law \( S \)

- **Lagrangian Model:**

\[
R_i(t + \Delta t) = R_i(t) + W(t) \Delta t + Z(t) \Delta t + S_i(t) \Delta t \quad \text{for } i = 1, \ldots \text{Number of particles}
\]

where, \( R_i(t) \) is position vector of \( i^{th} \) ash particle at time \( t \).
PUFF simulation model

- **W(t)** is the local wind velocity which is calculated for each particle by interpolating four dimensional (longitude/latitude/height/time) wind data (obtained from forecast meteorological data) to the particle’s position and time.

- Turbulent dispersion for each particle is modeled with a *random walk* process \( Z(t) \).
  - A *random walk* is a process where a particle takes a step at discrete time intervals in such a manner that each step is independent of the others.

- Turbulent dispersion \( Z(t) \Delta t \) is a vector containing three dimensional Gaussian random numbers with zero mean and specific standard deviation \( \sqrt{\frac{2K}{\Delta t}} \).
  - Diffusion coefficient \( K \) is independent of particle size and local wind dynamics.

- Ash fallout \( S_i(t)=[0 \ 0 \ s_i]^T \) is three dimensional vector where the terminal speed \( s_i \) is approximated by using Stoke’s law and is a function of radius of the particle \( r_i \), dynamic viscosity coefficient \( \eta \), gravitational acceleration \( g \), density of the particle \( \rho_{pi} \), and density of the atmosphere \( \rho_f \):
  
  \[
  s_i = \frac{2}{9} \left( \frac{\rho_{pi} - \rho_f}{\eta} \right) g R_i^2
  \]
To initialize the simulation, we need to specify initial location of ash \([\text{lat}, \text{lon}, z]\), time period of simulation \(t\), and the number of particles \(N\).

Distribution of particles along elevation \(z\) direction can be defined in different ways:
- Initialization

Bent model:

• In this simulation, Bent model has been used instead of mentioned methods for describing the initial distribution of particles along the height.

• BENT solves a cross-sectionally averaged system of equations for continuity, momentum and energy balance as a function of the eruption vent radius and speed of the ejecta.

• BENT assumes a distribution of pyroclasts of different sizes, and the model equations then predict the height distribution of the various sized clasts.

• For this research, the vent size, vent velocity, mean and deviation of particle size form the source parameters which drive the BENT/PUFF model.

Inverse Problem

- The inverse problem requires a forward model and observations
  - The BENT/PUFF advection-diffusion model is used to represent the plume dynamics

Diagram:

1. Parameter $\Theta$ with a given probability distribution
2. Polynomial Chaos Quadrature Sampling from Probability distribution of $\Theta$
3. Propagation of Quadrature points through the dynamic model of the system
4. Observation data from an experiment or simulation
5. Fusion of observation data and prediction data by using Minimum Variance Estimation
6. Estimation of Parameter $\Theta$
Polynomial Chaos:

- Originally used by Norbert Wiener in 1938, to describe the members of the span of Hermite polynomial functionals of standard Gaussian random variables.

- The PC series representation of random variables is used (Ghanem & Spanos, 1991) to model uncertainty in dynamic systems.

- The Hermite polynomial chaos expansion:
  - A Gaussian random variable: \( \omega \in \mathcal{N}(\mu, \sigma^2) = a_0 H_0(\xi) + a_1 H_1(\xi) \)
  - Basis: Hermite polynomials
    - \( H_0 = 1 \)
    - \( H_1 = \xi \in \mathcal{N}(0, 1) \)
    - \( a_0 = \mu \)
    - \( a_1 = \sigma \)

- Generalized (Xiu & Karniadakis, 2002) to use the orthogonal polynomials from the Askey-scheme to model various probability distributions in the scheme, with exponential convergence.

<table>
<thead>
<tr>
<th>Probability Distribution</th>
<th>Polynomial basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gaussian</td>
<td>Hermite Polynomials</td>
</tr>
<tr>
<td>Gamma</td>
<td>Laguerre polynomials</td>
</tr>
<tr>
<td>Beta</td>
<td>Jacobi polynomials</td>
</tr>
<tr>
<td>Uniform</td>
<td>Legendre polynomials</td>
</tr>
</tbody>
</table>
Inverse Problem:

- Forward Propagation

• **Polynomial Chaos Quadrature:**

  The propagation of uncertainty due to time-invariant but uncertain input parameters can be approximated by a generalization of polynomial chaos.

  \[
  \dot{x}(t, \Theta) = f(t, \Theta, x, u), \quad x(t_0) = x_0
  \]

  where, \( X \in \mathbb{R}^n \) and \( \Theta \in \mathbb{R}^m \) can be written in Polynomial Chaos Expansion as:

  \[
  x_i(t, \Theta) = \sum_{k=0}^{N} x_{ik}(t) \phi_k(\xi) = x_i^T(t) \Phi(\xi) \Rightarrow x(t, \xi) = X_{pc}(t) \Phi(\xi)
  \]

  \[
  \theta_i(\xi) = \sum_{k=0}^{N} \theta_{ik} \phi_k(\xi) = \Theta_i^T \Phi(\xi) \Rightarrow \Theta(t, \xi) = \Theta_{pc} \Phi(\xi) \quad \theta_{ik} = \frac{\langle \theta_i(\xi), \phi_k(\xi) \rangle}{\langle \phi_k(\xi), \phi_k(\xi) \rangle}
  \]

  • By substitution of these equations back into stochastic differential equation, we have

  \[
  e_i(X_{pc}, \xi) = \sum_{k=0}^{N} \dot{x}_{ik}(t) \phi_k(\xi) - f_i(t, X_{pc}(t) \Phi(\xi), \Theta_{pc} \Phi(\xi)), \quad i = 1, 2, \cdots, n
  \]

  • To minimize this error, we use *Galerkin approach* to force its projections on basis functions \( \phi_i(\xi) \)s to be zero.
Inverse Problem:
- Forward Propagation

- Evaluation of projection integrals is not always easy!

\[
\langle e_i(X_{pc}, \xi), \phi_j(\xi) \rangle = \sum_{k=0}^{N} x_{ik} \int_{\xi} \phi_k(\xi) \phi_j(\xi) d\xi - \int_{\xi} f_i(t, X_{pc}(i) \Phi(\xi), \Theta_{pc} \Phi(\xi)) \phi_j(\xi) d\xi = 0 \quad i = 1, \ldots, n, \quad j = 0, \ldots, N
\]

\[
= ?
\]

- To simplify integration process, we use M Quadrature Points

\[
\int \phi_i(\xi) \phi_j(\xi) p(\xi) d\xi \approx \sum_{q=1}^{M} w_q \phi_i(\xi_q) \phi_j(\xi_q)
\]

\[
\int f_i(t, X_{pc}(t) \Phi(\xi), \Theta_{pc} \Phi(\xi)) \phi_j(\xi) p(\xi) d\xi \approx \sum_{q=1}^{M} w_q f_i(t, X_{pc}(t) \Phi(\xi_q), \Theta_{pc} \Phi(\xi_q)) \phi_j(\xi_q)
\]
Inverse Problem:
- Data Assimilation

Minimum Variance Estimator:

\[
\hat{z}_k^+ = \hat{z}_k^- + K_k [\hat{\gamma}_k - E^- [h(x_k)]] \\
\Sigma_k^+ = \Sigma_k^- + K_k \Sigma_{zy} \\
K_k = -\Sigma_{zy}^T (\Sigma_{hh}^- + R_k)^{-1}
\]

Where, \( z_k \) is the augmented state vector of states and parameters and prior and posterior mean and covariance matrices are equal to:

\[
\hat{z}_k^- \triangleq E^- [z_k] = \begin{bmatrix} X_{pc1}^- (t) \\ \Theta_{pc1}^- \end{bmatrix} \\
\Sigma_k^- \triangleq E^- [(z_k - \hat{z}_k^-) (z_k - \hat{z}_k^-)^T] = \begin{bmatrix} \sum_{i=1}^{N} X_{pc1}^{-2} \\ \sum_{i=1}^{N} X_{pc1}^- \Theta_{pc1}^- \\ \sum_{i=1}^{N} \Theta_{pc1}^{-2} \end{bmatrix}
\]

\[
\hat{z}_k^+ \triangleq E^+[z_k] = \begin{bmatrix} X_{pc1}^+ (t) \\ \Theta_{pc1}^+ \end{bmatrix} \\
\Sigma_k^+ \triangleq E^+[ (z_k - \hat{z}_k^-) (z_k - \hat{z}_k^-)^T] = \begin{bmatrix} \sum_{i=1}^{N} X_{pc1}^{+2} \\ \sum_{i=1}^{N} X_{pc1}^+ \Theta_{pc1}^+ \\ \sum_{i=1}^{N} \Theta_{pc1}^{+2} \end{bmatrix}
\]
Inverse Problem:
- Data Assimilation

- \( \tilde{Y}_k \) denotes the sensor output obtained from the following observation model:

\[
y_k \triangleq y(t_k) = h(x_k, \Theta) + \nu_k
\]

with known distribution for the noise \( \nu_k \).

- As well, \( h_k, \Sigma_{zy} \) and \( \Sigma_{zz} \) are defined as:

\[
\hat{h}_k \triangleq E^{-1}[h(x_k, \Theta)] = \sum_{a=1}^{M} w_q \ h(x_k(\xi_q))
\]

\[
\Sigma_{zy} \triangleq E^{-1}[(z_k - \hat{z}_k)(h(x_k) - \hat{h}_k)^T] = \sum_{q=1}^{M} w_q(z_k(\xi_q) - \hat{z}_k)(h_q - \hat{h}_k)^T
\]

\[
\Sigma_{hh} \triangleq E^{-1}[(h(x_k) - \hat{h}_k)(h(x_k) - \hat{h}_k)^T] = \sum_{q=1}^{M} w_q(h_q - \hat{h}_k)(h_q - \hat{h}_k)^T
\]
Simulation:

- For validation purposes, we consider the Eyjafjallajökull eruption scenario.
- PUFF model used to propagate ash parcels in a given wind field (NCEP Reanalysis) through time concentrating on the period 14–16 April 2010.
- Variability in the height and loading of the eruption is introduced through the volcano column model BENT.
- Table 1 lists all source variables together with their assumed uncertainties.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value Range</th>
<th>PDF</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vent Radius, $b_0$ (m)</td>
<td>65 – 150</td>
<td>Uniform, + definite</td>
</tr>
<tr>
<td>Vent Velocity, $w_0$ (m/s)</td>
<td>45 – 124</td>
<td>Uniform, + definite</td>
</tr>
<tr>
<td>Mean Grain Size, $M_{d_{\phi}}$, $\phi$ units</td>
<td>2 boxcars: 1.5 -2 and 3 – 5</td>
<td>Uniform $\in$ R</td>
</tr>
<tr>
<td>$\sigma_{\phi}$, $\phi$ units</td>
<td>2 - 6</td>
<td>Uniform $\in$ R</td>
</tr>
</tbody>
</table>
Simulation

- Forward Propagation:

Probability distribution contours and satellite image

Outer Contour: 0.2 (probability of ash present in enclosed area is >=20%)
Inner Contour: 0.7 (probability of ash present in enclosed area is >=70%)
Colored plume: spatial variation of observed plume ash height
Simulation

- Inverse Problem:
SCIPUFF

SCIPUFF (*Second-order Closure Integrated PUFF*)

- Developed by Titan Corporation, Princeton, NJ under the sponsorship of U. S. Defense Special Weapons Agency (DSWA)

- a Lagrangian transport and diffusion model for atmospheric dispersion applications.

- uses three dimensional Gaussian puff representation for the concentration field of a dispersing contaminant to solve advection-diffusion equation.
Location Uncertainty

- Source of the material is assumed to be uniformly distributed on a square of $[2, 4] \times [2, 4]$ km$^2$.

- Time period of simulation is considered to be 1 hour (3600 sec.)

- 101 x 101 grid is used to record the concentration of Propane during the propagation time period.
**PCQ approach**

- 10x 10 quadrature points are being used to cover the support of source location.
- These quadrature points are propagated by using SCIPUFF model during the time.
- Polynomial basis functions are constructed according to the applied distribution for the uncertain source location.
- Coefficients of PC expansions can be found using the Polynomial Chaos quadrature technique.
- After finding coefficients, PC expansion of the output of the SCIPUFF model is constructed acc. to distribution of uncertain source.
- Large number of realizations of PC expansion is generated.
- **Probability Distribution of concentration > threshold** is equal to the number of PC realizations which are greater than that threshold divided by the total number of realizations.
Inverse Problem:

- Given a *set of observation* data and *a priori information* about the source location, what is the best guess about the actual position of the source?

\[
\tilde{y}_k = h(t_k, c_k(z)) + \nu_k
\]
\[
\nu = N(0, R)
\]

where, \( x \in \mathbb{R}^n \), \( \tilde{y} \in \mathbb{R}^m \), \( n >> m \) and \( Z \in \mathbb{R}^2 \) represent states, observations, and coordination of source location, respectively.
Source Identification
- Numerical Simulations

• 16 sparsely distributed sensors have been considered for observation purposes.
• Observation data are polluted with noise.
• Source location is assumed to be uniformly distributed over $[2,4] \times [2,4]$ km$^2$.
• Actual source location is at point $(3.8, 2.2)$.
• Source uncertainty is assumed to be the only uncertainty in the model dynamics.

• **Polynomial Chaos Quadrature (PCQ) Points** have been used during estimation.
Source Identification using PCQ

- Green squares: Sensor location
- Red points: Quadrature points applied to cover the domain of uncertain source
- White point: actual source location

Noisy Observations
$R = 6.25e^{-22}$

Pure Observations
Conclusion

Polynomial Chaos based minimum variance estimator

• Performs well in estimation of parameters of the system.

• Applicable to any type of probability distribution for the parameters (as opposed to Kalman Filter).

• Applicable to large scale systems (>18000 states in illustrated example, about 4000 grid locations with non-zero ash).

• Has been verified on other examples like source estimation of atmospheric releases by using SCIPUFF model.

• Can be applied as a batch or recursive estimation techniques.