# Efficient approach for quantifying uncertainty of wavefield reconstruction inversion 

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#### Abstract

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## Motivation

## Noisy acquired data

## Motivation



Uncertainty in data


Risk in oil and gas volume



Prior probability density function (PDF):

$$
\mathbf{m} \longrightarrow \rho_{\text {prior }}(\mathbf{m})
$$

Likelihood PDF: given datad

$$
\mathbf{m} \longrightarrow \rho_{\text {like }}(\mathbf{d} \mid \mathbf{m})
$$

Posterior PDF (Bayes' rule):


$$
\rho_{\text {post }}(\mathbf{m} \mid \mathbf{d})=\rho_{\text {like }}(\mathbf{d} \mid \mathbf{m}) \rho_{\text {prior }}(\mathbf{m})
$$



## Bayesian inference

Mean value of the model:
$\mathbb{E}(\mathbf{m})=\int \mathbf{m} \rho_{\text {post }}(\mathbf{m}) d \mathbf{m}$,
Covariance matrix:

$$
C_{i, j}=\mathbb{E}\left(m_{i} m_{j}\right)-\mathbb{E}\left(m_{i}\right) \mathbb{E}\left(m_{j}\right),
$$

## Bayes w/ FWI





## Bayes w/ FWI

Reduced formulation in the frequency domain:

$$
\begin{aligned}
& F(\mathbf{m})=\mathbf{P A}^{-1} \mathbf{q} \\
& \mathbf{A}=\Delta+\omega^{2} \mathbf{m} \\
& \mathbf{m}: \text { Squared-slowness } \\
& \mathbf{q}: \text { Source } \\
& \omega: \text { Frequency } \\
& \Delta: \text { Laplacian operator } \\
& \mathbf{P}: \text { Projection operator of receiver }
\end{aligned}
$$

## Bayes w/ FWI

## Posterior PDF of FWI:

$$
\rho_{\text {post }}(\mathbf{m} \mid \mathbf{d}) \propto \exp \left(-\frac{1}{2}\left\|\mathbf{P A}(\mathbf{m})^{-1} \mathbf{q}-\mathbf{d}\right\|_{\boldsymbol{\Sigma}_{\text {noise }}^{-1}}^{2}-\frac{1}{2}\left\|\mathbf{m}-\mathbf{m}_{\text {prior }}\right\|_{\boldsymbol{\Sigma}_{\text {prior }}^{-1}}^{2}\right)
$$

## Bayes w/ FWI

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$$
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$$

Strong nonlinearity
Many local minima

## Bayes w/ FWI

## Posterior PDF of FWI:

$$
\rho_{\text {post }}(\mathbf{m} \mid \mathbf{d}) \propto \exp \left(-\frac{1}{2}\left\|\mathbf{P A}(\mathbf{m})^{-1} \mathbf{q}-\mathbf{d}\right\|_{\boldsymbol{\Sigma}_{\text {noise }}^{-1}}^{2}-\frac{1}{2}\left\|\mathbf{m}-\mathbf{m}_{\text {prior }}\right\|_{\boldsymbol{\Sigma}_{\text {prior }}^{-1}}^{2}\right)
$$

Strong nonlinearity ${ }_{-\log \rho_{\text {post }}(\mathbf{m} \mid \mathbf{d})} \uparrow$ Many local minima


Two layer example - FWI



## Bayes w/ FWI

## Local minima:

- difficult to find the maximum a posterior (MAP) estimate
- slow down McMC convergence
- render posterior PDF "less Gaussian"


## Wavefield Reconstruction Inversion - WRI

## Penalty formulation:

$$
\min _{\mathbf{m}, \mathbf{u}} \frac{1}{2}\|\mathbf{P u}-\mathbf{d}\|_{2}^{2}+\frac{\lambda^{2}}{2}\|\mathbf{A}(\mathbf{m}) \mathbf{u}-\mathbf{q}\|_{2}^{2}
$$

## Properties:

- bi-linear w/ respect to $\mathbf{u}$ and $\mathbf{m}$
- larger searching space


## WRI vs FWI

Larger \# of degrees of freedom

"more convex"
less local minima
$\mathbf{u}$
m

## Solving WRI

## Variable projection:

$$
\min _{\mathbf{m}} \frac{1}{2}\|\mathbf{P} \overline{\mathbf{u}}(\mathbf{m})-\mathbf{d}\|_{2}^{2}+\frac{\lambda^{2}}{2}\|\mathbf{A}(\mathbf{m}) \overline{\mathbf{u}}(\mathbf{m})-\mathbf{q}\|_{2}^{2}
$$

where

$$
\overline{\mathbf{u}}(\mathbf{m})=\arg \min _{\mathbf{u}} \frac{1}{2}\|\mathbf{P} \mathbf{u}-\mathbf{d}\|_{2}^{2}+\frac{\lambda^{2}}{2}\|\mathbf{A}(\mathbf{m}) \mathbf{u}-\mathbf{q}\|_{2}^{2}
$$

## WRI - iterations

## WRI method

for each source $i$
solve $\binom{\mathbf{P}_{i}}{\lambda \mathbf{A}_{i}(\mathbf{m})} \mathbf{u}_{\lambda, i} \approx\binom{\mathbf{d}_{i}}{\lambda \mathbf{q}_{i}}$
$\mathbf{g}=\mathbf{g}+\lambda^{2} \omega^{2} \operatorname{diag}\left(\overline{\mathbf{u}}_{i, \lambda}\right)^{*}\left(A(\mathbf{m}) \overline{\mathbf{u}}_{i, \lambda}-\mathbf{q}_{i}\right)$ end
$\mathbf{m}=\mathbf{m}-\alpha \mathbf{g}$
correlation proxy wavefield \& PDE residual

## Conventional method

for each source $i$
solve $\mathbf{A}_{i}(\mathbf{m}) \mathbf{u}_{i}=\mathbf{q}_{i}$
solve $\mathbf{A}_{i}(\mathbf{m})^{*} \mathbf{v}_{i}=\mathbf{P}_{i}^{*}\left(\mathbf{P}_{i} \mathbf{u}_{i}-\mathbf{d}_{i}\right)$
$\mathbf{g}=\mathbf{g}+\omega^{2} \operatorname{diag}\left(\mathbf{u}_{i}\right)^{*} \mathbf{v}_{i}$
end
$\mathbf{m}=\mathbf{m}-\alpha \mathbf{g}$
correlation wavefield \& data residual

## Bayes w/ WRI

## Posterior PDF of WRI:

$\rho_{\text {post }}(\mathbf{m} \mid \mathbf{d}) \propto$

$$
\exp \left(-\frac{1}{2} \| \underline{\left.\mathbf{P} \overline{\mathbf{u}}(\mathbf{m})-\mathbf{d}\left\|_{\boldsymbol{\Sigma}_{\text {noise }}^{-1}}^{2}-\frac{\lambda^{2}}{2}\right\| \mathbf{A}(\mathbf{m}) \overline{\mathbf{u}}(\mathbf{m})-\mathbf{q} \|^{2}-\underline{\frac{1}{2}\left\|\mathbf{m}-\mathbf{m}_{p}\right\|_{\boldsymbol{\Sigma}_{\text {prior }}^{-1}}^{2}}\right), ~, ~}\right.
$$

Likelihood
Prior
where

$$
\overline{\mathbf{u}}(\mathbf{m})=\arg \min _{\mathbf{m}} \frac{1}{2}\|\mathbf{P u}-\mathbf{d}\|_{\boldsymbol{\Sigma}_{\text {noise }}^{-1}}^{2}+\frac{\lambda^{2}}{2}\|\mathbf{A}(\mathbf{m}) \mathbf{u}-\mathbf{q}\|^{2} .
$$

Two layer example - WRI


$\mathbf{W R I}-\log \rho_{\text {post }}(\mathbf{m} \mid \mathbf{d})$

Two layer example - FWI



## Challenges for large-scale UQ

Evaluations of the posterior PDF

- many PDE solves to evaluate PDF
- expensive PDE solves

High-dimensional space to explore

- numerical integration too expensive
- McMC based methods are impractical
- too many iterations
- converge too slow


## UQ for large-scale problems

Approximate posterior PDF by Gaussians

Sample the Gaussians w/ Randomize Then Optimize (RTO) method

## Quadratic approximation of $-\log \rho_{\text {post }}(\mathbf{m})$

$-\log \rho_{\text {post }}(\mathbf{m})=f(\mathbf{m})$

$$
\approx f\left(\mathbf{m}_{*}\right)+\frac{1}{2}\left(\mathbf{m}-\mathbf{m}_{*}\right)^{\top} \mathbf{H}\left(\mathbf{m}-\mathbf{m}_{*}\right):=\bar{f}(\mathbf{m})
$$

where $\mathbf{H}=\frac{\partial^{2} f}{\partial \mathbf{m}^{2}}$.


## Approximate posterior PDF

## Gaussian approximation:

$$
\rho_{\mathrm{post}}(\mathbf{m}) \approx \rho_{\mathrm{Gauss}}(\mathbf{m})=\mathcal{N}\left(\mathbf{m}_{*}, \mathbf{H}^{-1}\right)
$$

where

$$
\begin{aligned}
& \mathbf{H}=\mathbf{H}_{\mathrm{l}}+\mathbf{H}_{\mathrm{p}}, \\
& \mathbf{H}_{\mathrm{l}}=\frac{\partial^{2} f_{\mathrm{l}}(\mathbf{m})}{\partial \mathbf{m}^{2}}, \quad f_{\mathrm{l}}(\mathbf{m})=-\log \rho_{\text {like }}(\mathbf{d} \mid \mathbf{m}), \\
& \mathbf{H}_{\mathrm{p}}=\frac{\partial^{2} f_{\mathrm{p}}(\mathbf{m})}{\partial \mathbf{m}^{2}}, \quad f_{\mathrm{p}}(\mathbf{m})=-\log \rho_{\text {prior }}(\mathbf{m}) .
\end{aligned}
$$

## Approximate posterior PDF



## Form Hessian

## Gauss-Newton Hessian:

$$
\mathbf{H}_{1}=\mathbf{G}^{\top} \mathbf{A}^{-\top} \mathbf{P}^{\top}\left(\mathbf{I}+\frac{1}{\lambda^{2} \sigma^{2}} \mathbf{P A}^{-1} \mathbf{A}^{-\top} \mathbf{P}^{\top}\right)^{-1} \mathbf{P} \mathbf{A}^{-1} \mathbf{G}
$$

where $\Sigma_{\text {noise }}=\sigma^{2} \mathbf{I}$ and $\mathbf{G}=\frac{\partial \mathbf{A} \overline{\mathbf{u}}}{\partial \mathbf{m}}$.

## Form Hessian

## Gauss-Newton Hessian:

$$
\begin{aligned}
& \mathbf{H}_{l}=\underbrace{\mathbf{G}^{\top} \mathbf{A}^{-\top} \mathbf{P}^{\top}}_{\mathbf{W}^{\top}} \underbrace{\left.\mathbf{I}+\frac{1}{\lambda^{2} \sigma^{2}} \mathbf{P A}^{-1} \mathbf{A}^{-\top} \mathbf{P}^{\top}\right)^{-1}}_{\mathbf{S}} \mathbf{P} \mathbf{A}^{-1} \mathbf{G}, \\
& \text { where } \Sigma_{\text {noise }}=\sigma^{2} \mathbf{I} \text { and } \mathbf{G}=\frac{\partial \mathbf{A} \overline{\mathbf{u}}}{\partial \mathbf{m}}
\end{aligned}
$$

## GN Hessian of WRI



隺 W
Computational cost:
$n_{\text {freq }} \times\left(n_{\text {src }}+n_{\text {rcv }}\right)$
storage cost:
$n_{\text {freq }} \times n_{\text {grid }} \times\left(n_{\text {src }}+n_{\text {rcv }}\right)$
in parallel !!

## Selection of $\lambda$

## Compute wavefields:

$$
\overline{\mathbf{u}}(\mathbf{m})=\left(\frac{1}{\sigma^{2}} \mathbf{P}^{\top} \mathbf{P}+\lambda^{2} \mathbf{A}(\mathbf{m})^{\top} \mathbf{A}(\mathbf{m})\right)^{-1}\left(\lambda^{2} \mathbf{A}(\mathbf{m})^{\top} \mathbf{q}+\frac{1}{\sigma^{2}} \mathbf{P}^{\top} \mathbf{d}\right)
$$

$\mu_{1}$ : maximum eigenvalue of the matrix $\frac{1}{\sigma^{2}} \mathbf{A}^{-\top} \mathbf{P}^{\top} \mathbf{P} \mathbf{A}^{-1}$,

$$
\begin{aligned}
& \lambda^{2} \gg \mu_{1} \rightarrow \overline{\mathbf{u}}(\mathbf{m}) \approx \mathbf{A}(\mathbf{m})^{-1} \mathbf{q} \\
& \lambda^{2} \ll \mu_{1} \rightarrow \frac{1}{\sigma^{2}} \mathbf{P}^{\top} \mathbf{P}+\lambda^{2} \mathbf{A}(\mathbf{m})^{\top} \mathbf{A}(\mathbf{m}) \text { is ill conditioned }
\end{aligned}
$$

Select $\lambda^{2}=\alpha \mu_{1}$

## UQ for large-scale problems

Approximate posterior PDF by Gaussians

Sample the Gaussians w/ Randomize Then Optimize (RTO) method

## Conventional method

Sample Gaussian distribution:

$$
\rho_{\mathrm{Gauss}}(\mathbf{m}) \propto \exp \left(-\frac{1}{2}\left(\mathbf{m}-\mathbf{m}_{*}\right)^{\top} \mathbf{H}\left(\mathbf{m}-\mathbf{m}_{*}\right)\right)
$$

Cholesky factorization:

$$
\begin{gathered}
\mathbf{H}=\mathbf{L}^{\top} \mathbf{L} \\
\mathbf{m}_{\mathbf{s}}=\mathbf{m}_{*}+\mathbf{L}^{-1} \mathbf{r}, \mathbf{r} \sim \mathcal{N}\left(0, \mathcal{I}_{n_{\text {grid }} \times n_{\text {grid }}}\right)
\end{gathered}
$$

$\mathbf{H}$ should be an explicit matrix, computational cost is $\mathcal{O}\left(n_{\text {grid }}^{3}\right)$.

## RTO method

Re-formulate the posterior distribution with:

$$
\mathbf{H}=\mathbf{H}_{l}+\mathbf{H}_{\mathrm{p}}, \mathbf{H}_{\mathrm{l}}=\mathbf{L}_{\mathrm{l}}^{\top} \mathbf{L}_{\mathrm{l}} \text {, and } \mathbf{H}_{\mathrm{p}}=\mathbf{L}_{\mathrm{p}}^{\top} \mathbf{L}_{\mathrm{p}},
$$

then

$$
\begin{aligned}
\rho_{\text {Gauss }}(\mathbf{m}) \propto \exp ( & -\frac{1}{2}\left(\mathbf{L}_{l} \mathbf{m}-\mathbf{L}_{l} \mathbf{m}_{*}\right)^{\top}\left(\mathbf{L}_{l} \mathbf{m}-\mathbf{L}_{l} \mathbf{m}_{*}\right) \\
& \left.-\frac{1}{2}\left(\mathbf{L}_{\mathrm{p}} \mathbf{m}-\mathbf{L}_{\mathrm{p}} \mathbf{m}_{*}\right)^{\top}\left(\mathbf{L}_{\mathrm{p}} \mathbf{m}-\mathbf{L}_{\mathrm{p}} \mathbf{m}_{*}\right)\right)
\end{aligned}
$$

## RTO method

Generate a sample by solving the optimization problem:

$$
\begin{aligned}
\mathbf{m}_{\mathrm{s}}=\arg \min _{\mathbf{m}} & \left\|\mathbf{L}_{\mathrm{l}} \mathbf{m}-\left(\mathbf{L}_{\mathrm{l}} \mathbf{m}_{*}+\mathbf{r}_{1}\right)\right\|^{2}+ \\
& \left\|\mathbf{L}_{\mathrm{p}} \mathbf{m}-\left(\mathbf{L}_{\mathrm{p}} \mathbf{m}_{*}+\mathbf{r}_{\mathrm{p}}\right)\right\|^{2}
\end{aligned}
$$

where

$$
\mathbf{r}_{1} \sim \mathcal{N}\left(0, \mathcal{I}_{n_{\mathrm{rcv}} \times n_{\mathrm{rcv}}}\right) \text { and } \mathbf{r}_{\mathrm{p}} \sim \mathcal{N}\left(0, \mathcal{I}_{n_{\mathrm{grid}} \times n_{\mathrm{grid}}}\right) .
$$

## RTO method

Factorization of $\mathbf{H}_{1}$ :

$$
\begin{aligned}
\mathbf{H}_{l} & =\mathbf{L}_{l}^{\top} \mathbf{L}_{1}, \\
\mathbf{L}_{l} & =\frac{\left(\mathbf{I}+\frac{1}{\lambda^{2} \sigma^{2}} \mathbf{P A}^{-1} \mathbf{A}^{-\top} \mathbf{P}^{\top}\right)^{-\frac{1}{2}} \mathbf{P A}^{-1} \mathbf{G} .}{n_{\mathrm{rcv}} \times n_{\mathrm{rcv}}}
\end{aligned}
$$

## RTO method

A simple example:
$\mathbf{m}_{\mathrm{MAP}}=\left[\begin{array}{ll}0 & 0\end{array}\right]^{\top}$,
$\mathbf{L}_{\text {like }}=\left[\begin{array}{cc}1 & 6 \\ 2 & 7 \\ 3 & 8 \\ 4 & 9 \\ 5 & 10\end{array}\right], \quad$ and $\quad \mathbf{L}_{\text {prior }}=\left[\begin{array}{ll}1 & 0 \\ 0 & 2\end{array}\right]$.

## Covariance matrix

## RTO method (100000 realizations) vs analytical solution:

$$
\begin{aligned}
\operatorname{Cov}_{\text {anal }} & =\left[\begin{array}{rr}
0.185 & -0.072 \\
-0.072 & 0.031
\end{array}\right] \text { and } \\
\operatorname{Cov}_{\mathrm{RTO}} & =\left[\begin{array}{rr}
0.185 & -0.072 \\
-0.072 & 0.031
\end{array}\right]
\end{aligned}
$$

## Marginal distribution comparison

RTO method with 100000 realizations (red) vs Analytical solution (blue)


## Numerical Experiment - layer model

Depth of sources and receivers: 50 m
Number of sources and receivers: 61
Frequency: 2,3 and 4 Hz
Lambda: 4e4
sigma: 10

(a) True model and prior model

(b) STD of the prior distribution

## Randomized Maximum Likelihood - RML

Generate independent samples from $\rho_{\text {post }}(\mathbf{m})$ by solving:

$$
\begin{aligned}
\min _{\mathbf{m}} & \frac{1}{2}\left(\sigma^{-2}\left\|\mathbf{P} \overline{\mathbf{u}}(\mathbf{m})-\mathbf{d}-\mathbf{r}_{\mathrm{d}}\right\|^{2}+\lambda^{2}\left\|\mathbf{A}(\mathbf{m}) \overline{\mathbf{u}}(\mathbf{m})-\mathbf{q}-\mathbf{r}_{\mathrm{s}}\right\|^{2}\right) \\
& +\frac{1}{2}\left\|\mathbf{m}-\mathbf{m}_{\mathrm{p}}-\mathbf{r}_{\mathrm{p}}\right\|_{\Sigma_{\text {prior }}^{-1}}^{2},
\end{aligned}
$$

where

$$
\begin{aligned}
& \mathbf{r}_{\mathrm{d}} \sim \mathcal{N}\left(0, \sigma^{2} \mathcal{I}_{n_{\mathrm{rcv}} \times n_{\mathrm{rcv}}}\right), \\
& \mathbf{r}_{\mathrm{s}} \sim \mathcal{N}\left(0, \lambda^{-2} \mathcal{I}_{n_{\mathrm{grid}} \times n_{\mathrm{grid}}}\right), \\
& \mathbf{r}_{\mathrm{p}} \sim \mathcal{N}\left(0, \Sigma_{\text {prior }}\right) .
\end{aligned}
$$

STD result comparison

(a) STD of prior distribution


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## Cross section comparison



## BG Compass model

(a) True model

 Frequency: 2-31 Hz
Lambda: 1e4

Depth of sources and receivers: 50

## Number of sources and receivers: 91 / 451

 Central frequency: 15 Hz
(c) STD of prior distribution

## Data

$$
\sigma=34
$$


(a) Data at 2 Hz

(b) Signal to noise ratio

## Prior and initial model



## MAP estimate



## Posterior STD



## Prior STD



## Cross section comparison

- prior



## Cross section comparison

## - posterior vs prior


(a) $x=1000 \mathrm{~m}$

(b) $x=2500 \mathrm{~m}$

(c) $x=4000 \mathrm{~m}$

## Cross section comparison

- $95 \%$ confidence interval vs 10 realizations by RML

(a) $x=1000 \mathrm{~m}$

(b) $x=2500 \mathrm{~m}$

(c) $x=4000 \mathrm{~m}$


## Conclusions

Penalty formulation of posterior PDF

- is a bi-Gaussian PDF
- has a better Gaussian approximation compared to reduced formulation

Efficient sampling method

- Gaussian approximation avoids large computational cost associated with evaluating posterior PDF iteratively
- the implicit GN Hessian operator provides a fast way to compute matrix-vector product
- RTO method does not require an explicit Hessian matrix and expensive Cholesky factorization


## Future work

Application to 3D problems.

Bayesian with constraint prior information.

Effects of different acquisition scenarios to the UQ analysis.

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## Acknowledgements

This research was carried out as part of the SINBAD project with the support of the member organizations of the SINBAD Consortium.


## Acknowledgements



The authors wish to acknowledge the SENAI CIMATEC Supercomputing Center for Industrial Innovation, with support from BG Brasil, Shell, and the Brazilian Authority for Oil, Gas and Biofuels (ANP), for the provision and operation of computational facilities and the commitment to invest in Research \& Development.

