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Uncertainty quantification for Wavefield-Reconstruction Inversion using a positive-definite approximated Hessian Zhilong Fang, Chia-Ying Lee, Curt Da Silva, Felix J. Herrmann and Rachel Kuske







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Hessian







Hessian





Hessian













[E. Haber, 2014]

Bayesian theory

Bayesian inference:





$ho_{\mathrm{post}}(\mathbf{m}) \propto ho_{\mathrm{like}}(\mathbf{m} | \mathbf{d}_{obs}) ho_{\mathrm{prior}}(\mathbf{m})$





Prior information



Prior information







Prior information



$ho_{ m prio}$

 $ho_{
m pri}$

$$_{\rm or}(\mathbf{m}) \propto \exp\left(-\|\mathbf{m} - \mathbf{m}_{\rm prior}\|_{\mathbf{\Sigma}_{\rm pri}^{-1}}^2\right)$$

$$\mathbf{hor}(\mathbf{m}) \propto \exp\left(-\|
abla \mathbf{m}\|^2_{\mathbf{\Sigma}_{\mathrm{prior}}^{-1}}
ight)$$



Gaussian distribution assumption:







Gaussian distribution assumption:



$f(\mathbf{m})$ noise $\rho_{\text{like}}(\mathbf{m}|\mathbf{d}_{\text{obs}}) \propto \exp\left(-\|f(\mathbf{m}) - \mathbf{d}_{\text{obs}}\|_{\boldsymbol{\Sigma}_{\text{noise}}}^{2}\right)$



Posterior distribution of FWI:

$ho_{ m post}(\mathbf{m}) \propto \exp\left(-\|\mathbf{PA}(\mathbf{m})^{-1}\mathbf{m}_{\mathbf{m}}^{-1}\mathbf$

$$\mathbf{q} - \mathbf{d}_{obs} \|_{\boldsymbol{\Sigma}_{noise}^{-1}}^2 - \|\mathbf{m} - \mathbf{m}_{prior}\|_{\boldsymbol{\Sigma}_{prior}^{-1}}^2 \right)$$



Posterior distribution of FWI:

$ho_{ m post}(\mathbf{m}) \propto \exp\left(-\|\mathbf{PA}(\mathbf{m})^{-1}\mathbf{m}_{\mathbf{m}}^{-1}\mathbf$

Strong nonlinearity Many local minima

$$\mathbf{q} - \mathbf{d}_{obs} \|_{\boldsymbol{\Sigma}_{noise}^{-1}}^2 - \|\mathbf{m} - \mathbf{m}_{prior}\|_{\boldsymbol{\Sigma}_{prior}^{-1}}^2 \right)$$



Posterior distribution of FWI:

$$\rho_{\text{post}}(\mathbf{m}) \propto \exp\left(-\|\mathbf{PA}(\mathbf{m})^{-1}\mathbf{q} - \mathbf{d}_{\text{obs}}\|_{\boldsymbol{\Sigma}_{\text{noise}}^{-1}}^{2} - \|\mathbf{m} - \mathbf{m}_{\text{prior}}\|_{\boldsymbol{\Sigma}_{\text{prior}}^{-1}}^{2}\right)$$
Strong nonlinearity
Many local minima
$$\mathbf{y}$$

$$\mathbf{q}$$



Posterior distribution of FWI:

$$\rho_{\text{post}}(\mathbf{m}) \propto \exp\left(-\|\mathbf{PA}(\mathbf{m})^{-1}\mathbf{q} - \mathbf{d}_{\text{obs}}\|_{\mathbf{\Sigma}_{\text{noise}}^{-1}}^{2} - \|\mathbf{m} - \mathbf{m}_{\text{prior}}\|_{\mathbf{\Sigma}_{\text{prior}}^{-1}}^{2}\right)$$
Strong nonlinearity
Many local minima
$$y = \left(\begin{array}{c} \mathbf{y} \\ \mathbf{y} \\$$



Bayesian and WRI

Posterior distribution of WRI:

$$\rho_{\text{post}}(\mathbf{m}) \propto \\ \exp\left(-\|\mathbf{Pu}(\mathbf{m}) - \mathbf{d}_{\text{obs}}\|_{\boldsymbol{\Sigma}_{\text{noise}}^{-1}}^{2} - \lambda^{2}\|\right)$$

Likelihood

where,





$$= \begin{pmatrix} \lambda \Sigma_{\text{pde}}^{-1/2} \mathbf{q} \\ \Sigma_{\text{noise}}^{-1/2} \mathbf{d}_{\text{obs}} \end{pmatrix}$$





Larger # of degrees of freedom



[van Leeuwen, T and Herrmann, F J , 2013]

"more convex"



Bayesian and WRI

Mean and covariance of the model:

$$\mathbb{E}(\mathbf{m}) = \int \mathbf{m}\rho_{\text{post}}(\mathbf{m})d\mathbf{m}$$
$$Cov(\mathbf{m}) = \int (\mathbb{E}(\mathbf{m}) - \mathbf{m})^2 \rho_{\text{po}}$$

 $d\mathbf{m} = d\mathbf{m}$



Quantify the uncertainty

Solution:

Integrate the posterior distribution

Goal : Quantify the uncertainty based on the posterior distribution $ho_{ m post}({f m})$



Quantify the uncertainty

Solution:

Integrate the posterior distribution | Huge computational cost!!!

Goal : Quantify the uncertainty based on the posterior distribution $ho_{ m post}({f m})$



Quantify the uncertainty

Solution:

- Integrate the posterior distribution
- McMC method to sample the posterior distribution

Goal : Quantify the uncertainty based on the posterior distribution $ho_{ m post}({f m})$



McMC method

Metropolis-Hasting Method:



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McMC method

Metropolis-Hasting Method:





McMC method

Metropolis-Hasting Method:





McMC method

Metropolis-Hasting Method:





McMC method

Metropolis-Hasting Method:























[M. Girolami and B. Calderhead, 2011]

McMC method

Langevin McMC method: $\tilde{\pi}_k(\mathbf{m}) \backsim \mathcal{N}(\mathbf{m}_k - \mathbf{L}\mathbf{g}_k, \mathbf{L})$





[M. Girolami and B. Calderhead, 2011]

McMC method

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McMC method



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McMC method



20



McMC method





McMC method



20



McMC method

Newton Type McMC: $\tilde{\pi}_k(\mathbf{m}) \backsim \mathcal{N}(\mathbf{m}_k - \mathbf{H}_k^{-1}\mathbf{g}_k, \mathbf{H}_k^{-1})$



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Computational cost: 1) Low rank approximation of the Hessian. 2) Number of PDE solvers ~ Number of samples.



Quantify the uncertainty

Solution:

- Integrate the posterior distribution
- McMC method to sample the posterior distribution
 - Advantage: the true uncertainty can be quantified
 - Disadvantage: huge computational cost

Goal : Quantify the uncertainty based on the posterior distribution $ho_{ m post}({f m})$



Quantify the uncertainty

Solution:

- Integrate the posterior distribution
- McMC method to sample the posterior distribution
 - Advantage: the true uncertainty can be quantified
 - Disadvantage: huge computational cost

Goal : Quantify the uncertainty based on the posterior distribution $ho_{ m post}({f m})$

• Use an approximate distribution to quantify the uncertainty





Larger # of degrees of freedom



[van Leeuwen, T and Herrmann, F J , 2013]

"more convex"



Quadratic approximation



$f(\mathbf{m}) \approx f(\mathbf{m}_{\text{MAP}}) + \mathbf{g}^T(\mathbf{m} - \mathbf{m}_{\text{MAP}}) + \frac{1}{2}(\mathbf{m} - \mathbf{m}_{\text{MAP}})^T \mathbf{H}(\mathbf{m} - \mathbf{m}_{\text{MAP}}) := \overline{f}(\mathbf{m})$

m



Hessian of WRI

Misfit function of WRI:

$f(\mathbf{m}, \mathbf{u}(\mathbf{m})) = \|\mathbf{P}\mathbf{u} - \mathbf{d}\|^2 + \lambda^2 \|\mathbf{A}(\mathbf{m})\mathbf{u} - \mathbf{q}\|^2$

Hessian of WRI:

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

$\frac{\partial^2 f}{\partial u^2} = \frac{\partial^2 f}{\partial u^2} - \frac{\partial^2 f}{\partial u^2 f}$



Hessian of WRI $\mathbf{H} = \frac{\partial^2 f}{\partial \mathbf{m}^2} - \frac{\partial^2 f}{\partial \mathbf{m} \partial \mathbf{u}} \frac{\partial^2 f}{\partial \mathbf{u}^2}^{-1} \frac{\partial^2 f}{\partial \mathbf{u} \partial \mathbf{m}}$ where, $\frac{\partial^2 \mathbf{f}}{\partial \mathbf{u^2}} = \mathbf{P^T} \mathbf{P} + \lambda^2 \mathbf{A^T} \mathbf{A}$ $\frac{\partial^2 \mathbf{f}}{\partial \mathbf{m}^2} = \lambda^2 \left(\frac{\partial \mathbf{A} \mathbf{u}}{\partial \mathbf{m}}\right)^T \left(\frac{\partial \mathbf{A} \mathbf{u}}{\partial \mathbf{m}}\right)$ $\frac{\partial^{2} \mathbf{f}}{\partial \mathbf{u} \partial \mathbf{m}} = \lambda^{2} \left(\frac{\partial \mathbf{A}^{T} (\mathbf{A} \mathbf{u} - \mathbf{q})}{\partial \mathbf{m}} \right) + \lambda^{2}$ $\frac{\partial^{2} \mathbf{f}}{\partial \mathbf{m}} = \lambda^{2} \left(\frac{\partial \mathbf{A}^{T} (\mathbf{A} \mathbf{u} - \mathbf{q})}{\partial \mathbf{m}} \right)^{T} + \lambda^{2}$ $\partial \mathbf{m} \partial \mathbf{u}$ $\partial \mathbf{m}$

Dense and not positive-definite

$$\mathbf{A}^{\mathbf{Z}} \left(\frac{\partial \mathbf{A} \mathbf{u}}{\partial \mathbf{m}} \right)$$

 $\lambda^{\mathbf{Z}} \left(\frac{\partial \mathbf{A} \mathbf{u}}{\partial \mathbf{m}} \right)^{\mathbf{T}} \mathbf{A}$



Hessian of WRI $\mathbf{H} = \frac{\partial^2 f}{\partial \mathbf{m}^2} - \frac{\partial^2 f}{\partial \mathbf{m} \partial \mathbf{u}} \frac{\partial^2 f}{\partial \mathbf{u}^2}^{-1} \frac{\partial^2 f}{\partial \mathbf{u} \partial \mathbf{m}}$ where, $\frac{\partial^2 \mathbf{f}}{\partial \mathbf{u^2}} = \mathbf{P^T} \mathbf{P} + \lambda^2 \mathbf{A^T} \mathbf{A}$ $\frac{\partial^{2} \mathbf{f}}{\partial \mathbf{m}^{2}} = \lambda^{2} \left(\frac{\partial \mathbf{A} \mathbf{u}}{\partial \mathbf{m}}\right)^{T} \left(\frac{\partial \mathbf{A} \mathbf{u}}{\partial \mathbf{m}}\right)$ $\frac{\partial^{2} \mathbf{f}}{\partial \mathbf{u} \partial \mathbf{m}} = \lambda^{2} \left(\frac{\partial \mathbf{A}^{T} (\mathbf{A} \mathbf{u} - \mathbf{q})}{\partial \mathbf{m}} \right) + \lambda^{2}$ $\frac{\partial^{2} \mathbf{f}}{\partial \mathbf{m}} = \lambda^{2} \left(\frac{\partial \mathbf{A}^{T} (\mathbf{A} \mathbf{u} - \mathbf{q})}{\partial \mathbf{m}} \right)^{T} + \lambda$ $\partial \mathbf{m} \partial \mathbf{u}$ $\partial \mathbf{m}$

Dense and not positive-definite

$$\mathbf{^{2}A^{T}}\left(\frac{\partial \mathbf{Au}}{\partial \mathbf{m}}\right)$$
$$\lambda^{2}\left(\frac{\partial \mathbf{Au}}{\partial \mathbf{m}}\right)^{T}\mathbf{A}$$

$$\lambda \to \infty \text{ or } \mathbf{m} \to \mathbf{m}_t$$

 $\mathbf{A}\mathbf{u} - \mathbf{q} \to 0$



Hessian of WRI $\mathbf{H} = \frac{\partial^2 f}{\partial \mathbf{m}^2} - \frac{\partial^2 f}{\partial \mathbf{m} \partial \mathbf{u}} \frac{\partial^2 f}{\partial \mathbf{u}^2}^{-1} \frac{\partial^2 f}{\partial \mathbf{u} \partial \mathbf{m}}$ where, $\frac{\partial^2 \mathbf{f}}{\partial \mathbf{u^2}} = \mathbf{P^T} \mathbf{P} + \lambda^2 \mathbf{A^T} \mathbf{A}$ $\frac{\partial^{2} \mathbf{f}}{\partial \mathbf{m}^{2}} = \lambda^{2} \left(\frac{\partial \mathbf{A} \mathbf{u}}{\partial \mathbf{m}}\right)^{T} \left(\frac{\partial \mathbf{A} \mathbf{u}}{\partial \mathbf{m}}\right)$ $\frac{\partial^2 \mathbf{f}}{\partial y} = \lambda^2 \left(\frac{\partial \mathbf{A}^T (\mathbf{A} \mathbf{u} - \mathbf{q})}{\partial y} \right)$ $\partial \mathbf{u} \partial \mathbf{m}$ $\partial \mathbf{m}$ \mathbf{T} $\partial \mathbf{A}^{\mathbf{T}}(\mathbf{A}\mathbf{u}-\mathbf{q})$ $\partial^{\mathbf{2}}\mathbf{f}$ $= \lambda$ + $\partial \mathbf{m}$ $\partial \mathbf{m} \partial \mathbf{u}$

Dense and not positive-definite

$$\mathbf{^{2}A^{T}}\left(\frac{\partial \mathbf{Au}}{\partial \mathbf{m}}\right)$$
$$\lambda^{2}\left(\frac{\partial \mathbf{Au}}{\partial \mathbf{m}}\right)^{T}\mathbf{A}$$

$$\lambda \to \infty \text{ or } \mathbf{m} \to \mathbf{m}_t$$

 $\mathbf{A}\mathbf{u} - \mathbf{q} \to 0$



Approximated Hessian:



 $= \lambda^2 \mathbf{G^T} (\frac{1}{\lambda^2} \mathbf{A^{-T} P^T} (\mathbf{I} + \frac{1}{\lambda^2} \mathbf{P} \mathbf{A^{-1} A^{-T} P^T})^{-1} \mathbf{P} \mathbf{A^{-1}}) \mathbf{G}$ n_{r}^{2} $n_r n_g$ diagonal



Approximated Hessian:



 $= \lambda^2 \mathbf{G^T} (\frac{1}{\lambda^2} \mathbf{A^{-T} P^T} (\mathbf{I} + \frac{1}{\lambda^2} \mathbf{P} \mathbf{A^{-1} A^{-T} P^T})^{-1} \mathbf{P} \mathbf{A^{-1}}) \mathbf{G}$ S W















Computational cost: $n_f * (n_s + n_r)$ storage cost: $n_f * n_g * (n_s + n_r)$

 \square

S



Evaluate the Hessian with three different models:

- True model
- Model from inversion
- Initial model





Evaluate the Hessian with three different model:

- True model
- Model from inversion
- Initial model

Evaluate the Hessian with three different λ choices:

•
$$\lambda = 1e0$$

•
$$\lambda = 1e3$$

• $\lambda = 1e6$



Quadratic approximation $f(\mathbf{m}) \approx f(\mathbf{m}_{\beta}) + \mathbf{g}^{T}(\mathbf{m} - \mathbf{m}_{\beta}) + \frac{1}{2}(\mathbf{m} - \mathbf{m}_{\beta})^{T}\mathbf{H}(\mathbf{m} - \mathbf{m}_{\beta}) := \overline{f}(\mathbf{m})$ $\mathbf{m} = \mathbf{m}_{\beta} + \alpha \mathrm{d}\mathbf{m}, \ \beta \in \{t, n, 0\}$





m

Quadratic approximation with approximated Hessian at mt





Quadratic approximation with approximated Hessian at mn





Quadratic approximation with approximated Hessian at mo



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Diagonal part of the Hessian $\mathbf{H} = \lambda^2 \mathbf{G}^{\mathbf{T}} (\frac{1}{\lambda^2} \mathbf{A}^{-\mathbf{T}} \mathbf{P}^{\mathbf{T}} (\mathbf{I} + \frac{1}{\lambda^2} \mathbf{P} \mathbf{A}^{-1} \mathbf{A}^{-\mathbf{T}} \mathbf{P}^{\mathbf{T}})^{-1} \mathbf{P} \mathbf{A}^{-1}) \mathbf{G}$ $= \mathbf{B}^{\mathbf{T}} \mathbf{B}$

Diagonal part of the Hessian: $h_{i,i} = \mathbf{B}(:,i)^{\mathbf{T}} * \mathbf{B}(:,i)$









*

Β



Quadratic approximation with diagonal part of approximated Hessian at m⁺





Quadratic approximation with diagonal part of approximated Hessian at $m_{\mbox{\tiny n}}$



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Quadratic approximation with diagonal part of approximated Hessian at mo



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- The application of the approximated Hessian and its diagonal part: Invert the MAP point with Newton type method (PDE free and matrix free)
 - Quantify the uncertainty of the inversion result (standard deviation)



Workflow – uncertainty quantification



Compute the Hessian at the MAP estimate and generate the Gaussian distribution.

Quantify the uncertainty of the model.



Numerical experiment (Full acquisition)







Model size: 500m x 2000m Source spacing: 80m Receiver spacing: 20m Fixed spread 2km Frequency : 10-31 Hz

Standard deviation of data noise: 0.1 Standard deviation of pde: 0.1 Standard deviation of model: 1 lambda: 1



Numerical experiment (Full acquisition)





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Posterior distribution



Maximum a posterior





Posterior distribution vs Prior distribution





Confidence intervals (90%)



Maximum a posterior

MAP


Confidence intervals (90%)





Confidence intervals

100 random realizations of data:

$$\mathbf{d}_i = \mathbf{F}(\mathbf{m}_t) + \epsilon$$

Inversion results correspond to these data:

 $\mathbf{d}_i
ightarrow \mathbf{m}_{\mathrm{i}}$





Confidence intervals (90%) — Inversion results of 100 random realizations





Numerical experiment (Partial acquisition)



Numerical experiment (Partial acquisition)









Full acquisition



Lateral [m]



Full acquisition





Partial acquisition











Model size: 2000m x 4500m Source spacing: 50m Receiver spacing: 10m Fixed spread 4.5km Frequency : 5~31 Hz

Standard deviation of data noise: 0.5 Standard deviation of pde: 0.5 Standard deviation of model: 1 lambda: 1



BG model





Posterior distribution





Lateral [m]

- Maximum a posterior



Posterior distribution vs Prior distribution





Confidence intervals (90%)



Lateral [m]

- Maximum a posterior



Confidence intervals (90%)





Confidence intervals (90%) — Inversion results of 100 random realizations





Confidence intervals (90%) — Inversion results of 1000 random realizations







Confidence intervals (90%) — Inversion results of 1000 random realizations



V True



Conclusion

- 1. A positive-definite approximated Hessian of WRI is proposed
 - Matrix free
 - Easy to obtain the diagonal part

2. The quadratic function with the approximated Hessian is a good approximate of the original WRI misfit function

3. The results of inverting noisy data still lie in the confidence intervals • This gives us confidence in our confidence intervals



Future work

deterministic WRI.

uncertainty of density.

release of SINBAD.

1. Apply the positive-definite approximated Hessian to the

2. Consider the density into the workflow and quantify the

3. Add the uncertainty quantification workflow into the soft-



Acknowledgements

Thank you for your attention !!!



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