A stochastic quasi-Newton McMC method for uncertainty quantification of full-waveform inversion

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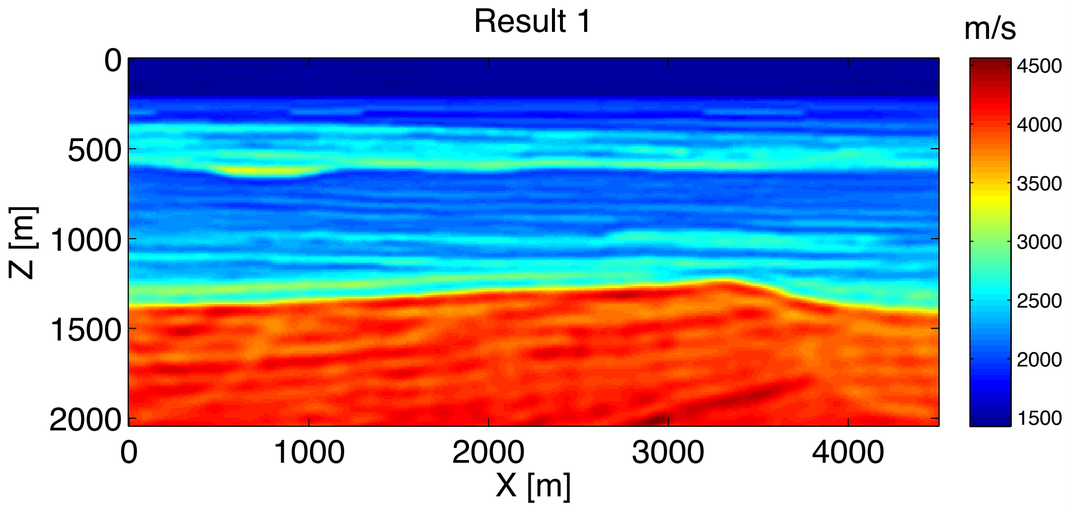
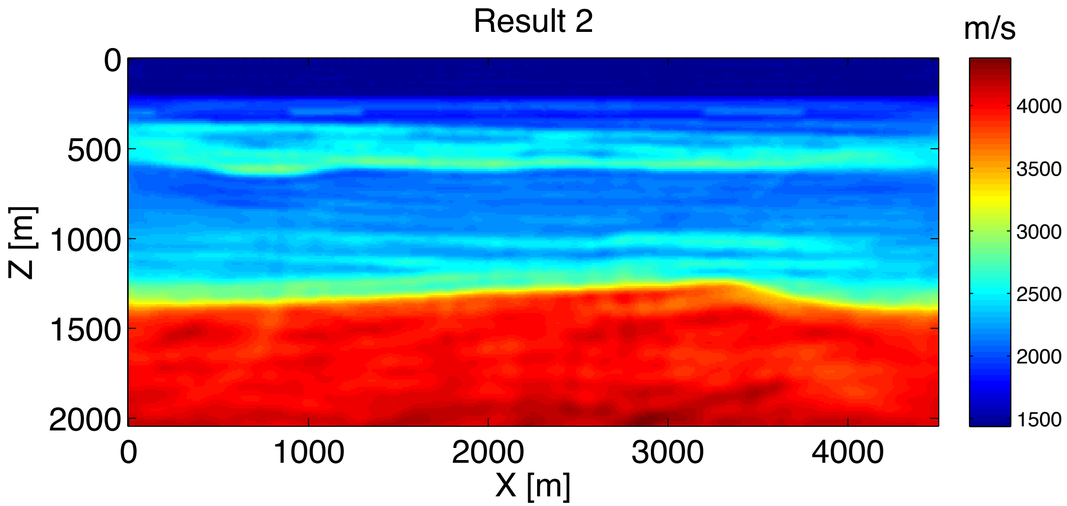
Motivation





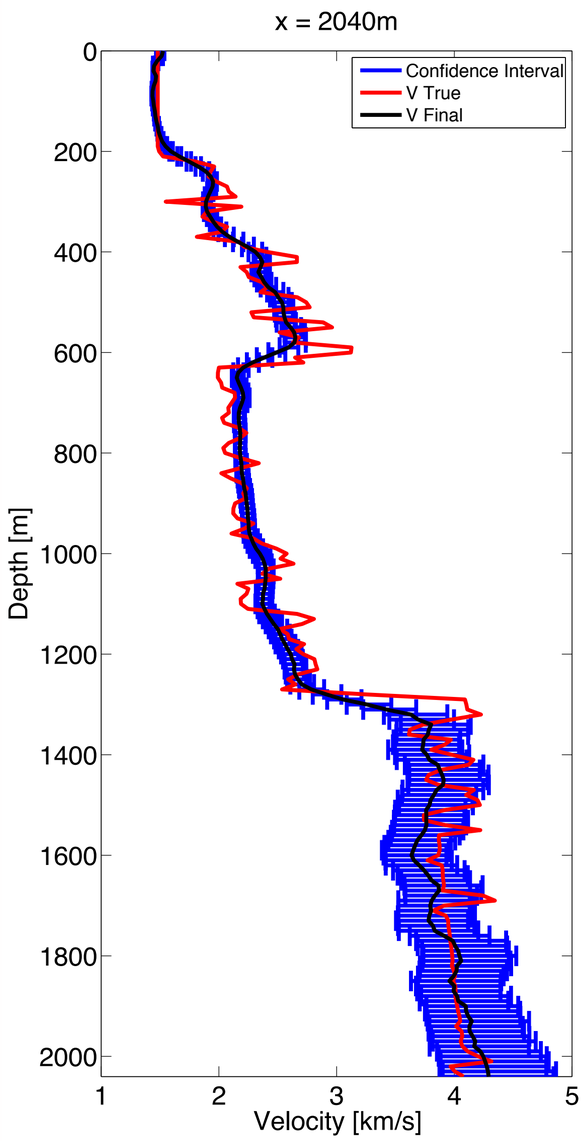
Which one is better?

Misfit?
Eyeball norm?

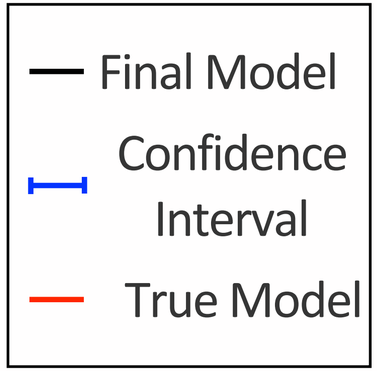
Uncertainty?
Standard Deviation?

Confidence interval

Fast Accurate!!



x = 2040m



Bayesian theory

Deterministic inverse problem:

$$\mathbf{m}^* = \arg\min\left(\frac{1}{2N_s}\sum_{1}^{N_s}\|f_i(\mathbf{m}) - \mathbf{d}_{i\mathrm{obs}}\|_{W_i}^2 + \frac{1}{2}\|\mathbf{m} - \overline{\mathbf{m}}\|_R^2\right)$$

Statistical inverse problem with Bayesian theory:

$$\pi_{post}(\mathbf{m}) := \pi(\mathbf{m}|\mathbf{d}_{obs}) \propto \pi_{prior}(\mathbf{m})\pi(\mathbf{d}_{obs}|\mathbf{m})$$

where $\mathbf{m}$ is the model parameter, and $\mathbf{d}_{obs}$ is the observed data

(James Martin *et al*, 2012)

Bayesian theory

Assume:

$$\text{noise} \sim \mathcal{N}(0, \Gamma_{noise})$$

$$\text{prior model distribution} \sim \mathcal{N}(\mathbf{m}_{prior}, \Gamma_{prior}).$$

Negative log-posterior of the posterior pdf:

$$V(\mathbf{m}) := -\log \pi_{post}(\mathbf{m}) := \frac{1}{2N_s} \sum_{1}^{N_s} \|f_i(\mathbf{m}) - \mathbf{d}_{i\text{obs}}\|^2_{\Gamma^{-1}_{i\text{noise}}} + \frac{1}{2}\|\mathbf{m} - \mathbf{m}_{prior}\|^2_{\Gamma^{-1}_{prior}}$$

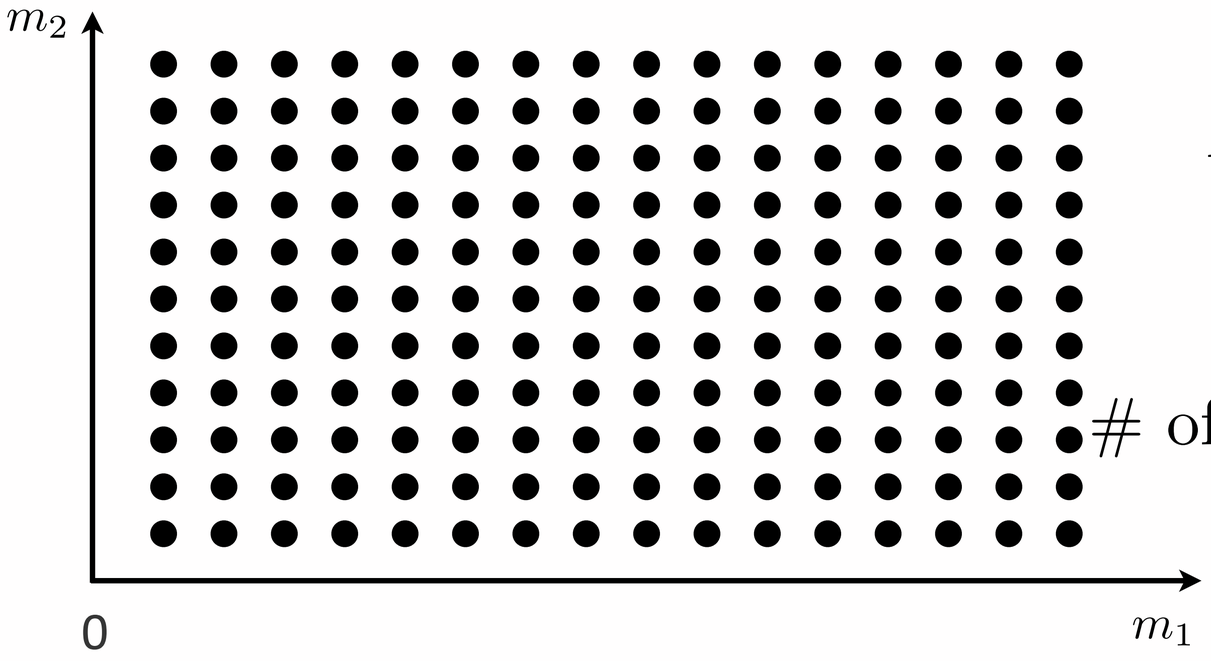
$$\mathbf{m}_{MAP} = \mathbf{m}^*$$

$$\|\mathbf{x}\|^2_{\Gamma^{-1}_{noise}} := \mathbf{x}^T \Gamma^{-1}_{noise} \mathbf{x}$$

Sampling the posterior pdf

How to obtain the posterior probability density function?

- Compute $\pi_{post}(\mathbf{m})$ by discretization? $N = N_{sub\_sample} * N_{para}$



$$N_{para} >> 10^6$$
$$N_{sub\_sample} >> 10^2$$
$$N >> 10^8$$
$$N_s >> 10^2$$

$$\#\text{ of PDE solvers } >> N * N_s$$

Approximate the pdf

How to obtain the posterior probability density function?

- Markov chain Monte Carlo method ? Metropolis - Hasting method

At sample $\mathbf{m}_k$
Draw sample $\mathbf{y}$ from the proposal distribution $\tilde{\pi}_k(\mathbf{m})$

if $\min(1, \dfrac{\pi_{post}(\mathbf{y})\tilde{\pi}_y(\mathbf{m}_k)}{\pi_{post}(\mathbf{m}_k)\tilde{\pi}_k(\mathbf{y})}) > \alpha$

    set $\mathbf{m}_{k+1} = \mathbf{y}$

else

    regenerate $\mathbf{y}$

end

Approximate the pdf

How to obtain the posterior probability density function?

- Stochastic Newton MCMC ?

$$V(\mathbf{m}) := -\log \pi_{post}(\mathbf{m}) := \frac{1}{2N_s}\sum^{N_s} \|f_i(\mathbf{m}) - \mathbf{d}_{i\text{obs}}\|^2_{\Gamma^{-1}_{i\text{noise}}} + \frac{1}{2}\|\mathbf{m} - \mathbf{m}_{prior}\|^2_{\Gamma^{-1}_{prior}}$$

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

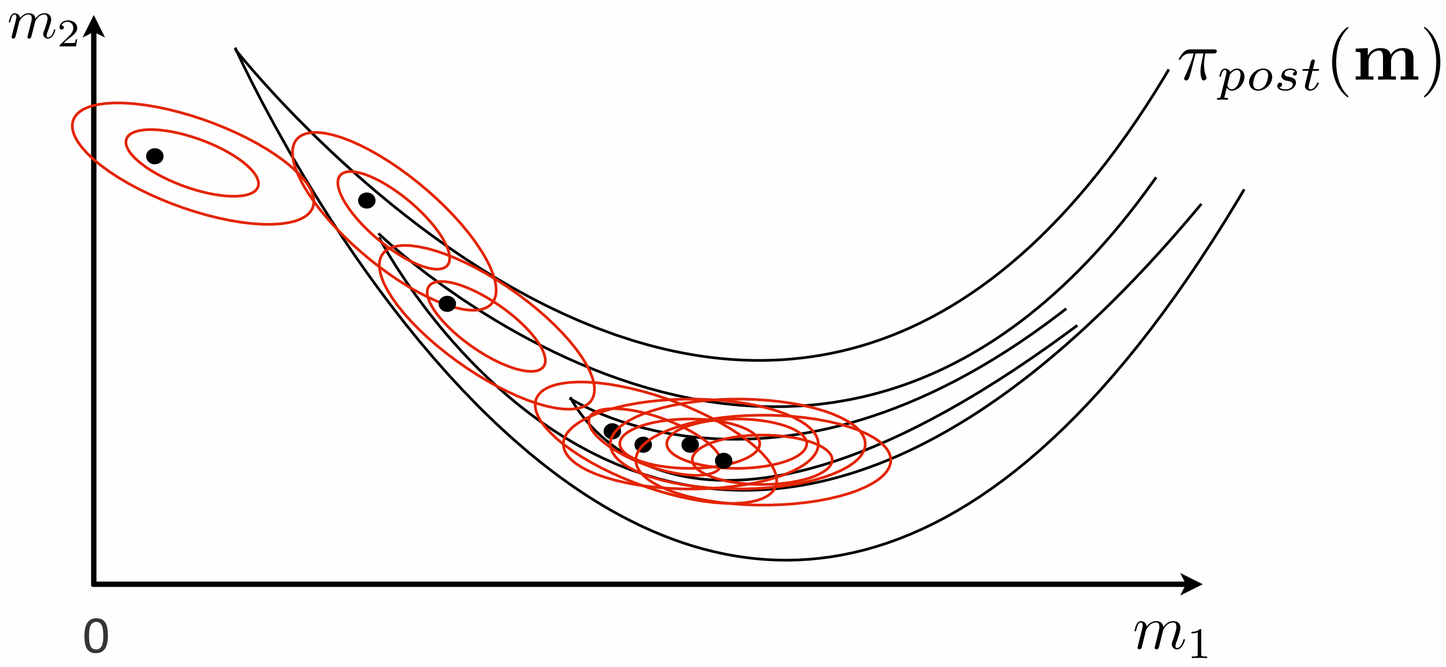
$$\underset{n\times n}{\begin{bmatrix} \mathbf{L}^T \end{bmatrix}} \underset{n\times n}{\begin{bmatrix} \mathbf{H}_{\text{misfit}} \end{bmatrix}} \underset{n\times n}{\begin{bmatrix} \mathbf{L} \end{bmatrix}} \approx \underset{n\times r}{\begin{bmatrix} \mathbf{V}_r \end{bmatrix}} \underset{r\times r}{\begin{bmatrix} \mathbf{D}_r \end{bmatrix}} \underset{r\times n}{\begin{bmatrix} \mathbf{V}_r^T \end{bmatrix}}$$

$$r \ll n$$

(James Martin *et al*, 2012)

Approximate the pdf

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



(James Martin *et al*, 2012)

Approximate the pdf

Challenges:

- Low - rank approximation may not be correct.
- The computational cost of estimating Hessian is huge.
- The computational cost of calculating the posterior distribution probability density function is huge.

$$\text{Computational Cost} \sim \mathcal{O}(N_{\text{sample}} * N_s)$$

BFGS Hessian

At the stage *k*: approximated Hessian $\mathbf{B}_k$ and gradient $\mathbf{g}_k$,

Update $\mathbf{B}_k$ by adding two rank one matries:

$$\mathbf{B}_{k+1} = \mathbf{B}_k + \mathbf{U}_k + \mathbf{V}_k$$

where $\mathbf{B}_{k+1}$ should satisfy

$$\mathbf{B}_{k+1}(\mathbf{x}_{k+1} - \mathbf{x}_k) = \mathbf{g}_{k+1} - \mathbf{g}_k$$

$$\mathbf{y}_k = \mathbf{g}_{k+1} - \mathbf{g}_k$$
$$\mathbf{s}_k = \mathbf{x}_{k+1} - \mathbf{x}_k,$$

No additional computational cost!!!

$$\mathbf{B}_{k+1} = \mathbf{B}_k + \frac{\mathbf{y}_k \mathbf{y}_k^T}{\mathbf{y}_k^T \mathbf{s}_k} - \frac{\mathbf{B}_k \mathbf{s}_k \mathbf{s}_k^T \mathbf{B}_k}{\mathbf{s}_k^T \mathbf{B}_k \mathbf{s}_k}$$

$$\mathbf{B}_{k+1}^{-1} = \left(\mathbf{I} - \frac{\mathbf{s}_k \mathbf{y}_k^T}{\mathbf{y}_k^T \mathbf{s}_k}\right) \mathbf{B}_k^{-1} \left(\mathbf{I} - \frac{\mathbf{y}_k \mathbf{s}_k^T}{\mathbf{y}_k^T \mathbf{s}_k}\right) + \frac{\mathbf{s}_k \mathbf{s}_k^T}{\mathbf{y}_k^T \mathbf{s}_k}$$

l-BFGS Hessian with pseudo GN Hessian as a starter

Limited memory BFGS Hessian:

$$\{\mathbf{s}_i\}_{k-M+1\leq i\leq k}$$
$$\{\mathbf{y}_i\}_{k-M+1\leq i\leq k}$$
$$\mathbf{B}_0^{(k)}$$

$$\longrightarrow$$

$$\mathbf{B}_k$$
$$\mathbf{B}_k^{-1}$$

Choice of $\mathbf{B}_0^{(k)}$: pseudo GN Hessian

(Choi, Y, *et al*, 2012)

Randomized source subsampling

To speed up the computation of posterior pdf:

$$V(\mathbf{m}) := -\log \pi_{post}(\mathbf{m}) := \frac{1}{2N_s}\sum_{1}^{N_s} \|f_i(\mathbf{m}) - \mathbf{d}_{i\mathrm{obs}}\|^2_{\Gamma^{-1}_{i\mathrm{noise}}} + \frac{1}{2}\|\mathbf{m} - \mathbf{m}_{prior}\|^2_{\Gamma^{-1}_{prior}}$$

Randomized source subsampling:

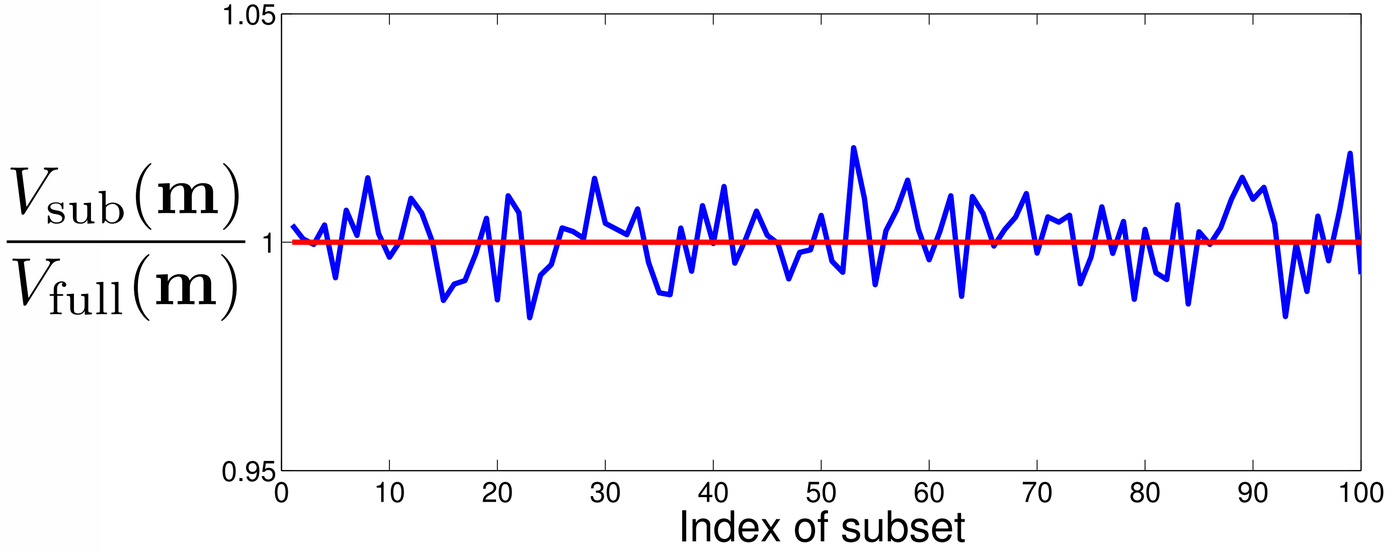
$$\frac{1}{N_s}\sum_{1}^{N_s} \|f_i(\mathbf{m}) - \mathbf{d}_{i\mathrm{obs}}\|^2_{\Gamma^{-1}_{i\mathrm{noise}}} = \frac{1}{\|\mathcal{I}_s\|}\sum_{i\in\mathcal{I}_s} \|f_i(\mathbf{m}) - \mathbf{d}_{i\mathrm{obs}}\|^2_{\Gamma^{-1}_{i\mathrm{noise}}} + \epsilon$$

(Farbod Roosta-Khorasani *et al*, 2013; Eldad *et al,* 2012; Michael P. Friedlander *et al*, 2013, van Leeuwen *et al*, 2013)

Randomized source subsampling

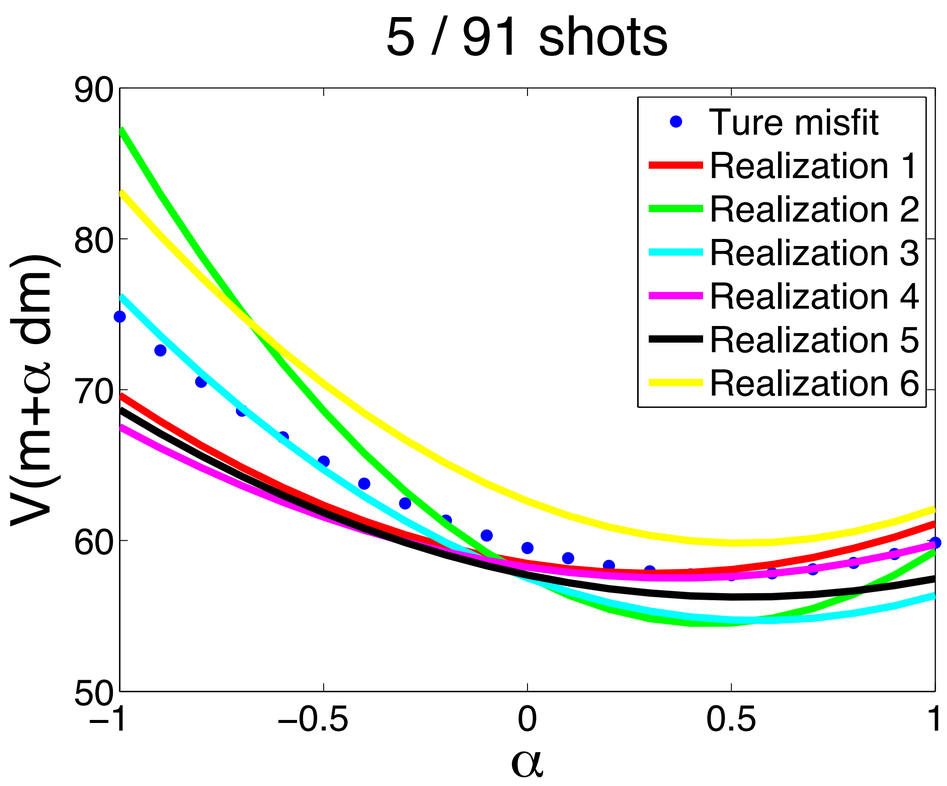
Computational Cost: $\mathcal{O}(N_s) \rightarrow \mathcal{O}(N_{rs}),\ N_{rs} << N_s$

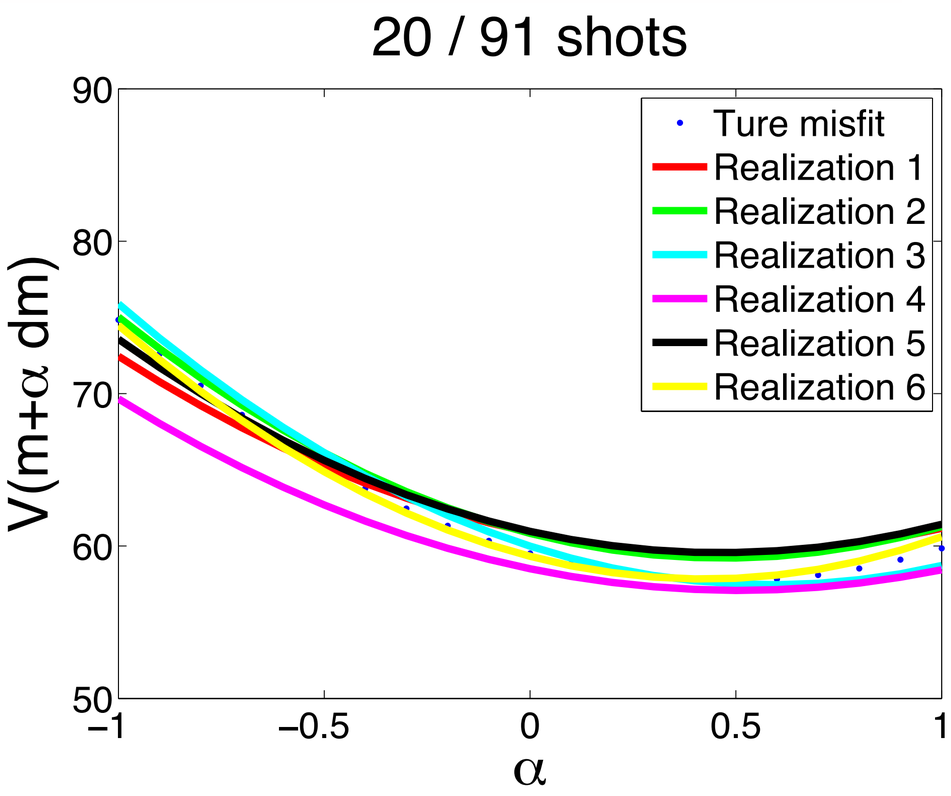
Subset misfit *vs* Full misfit



Randomized source subsampling

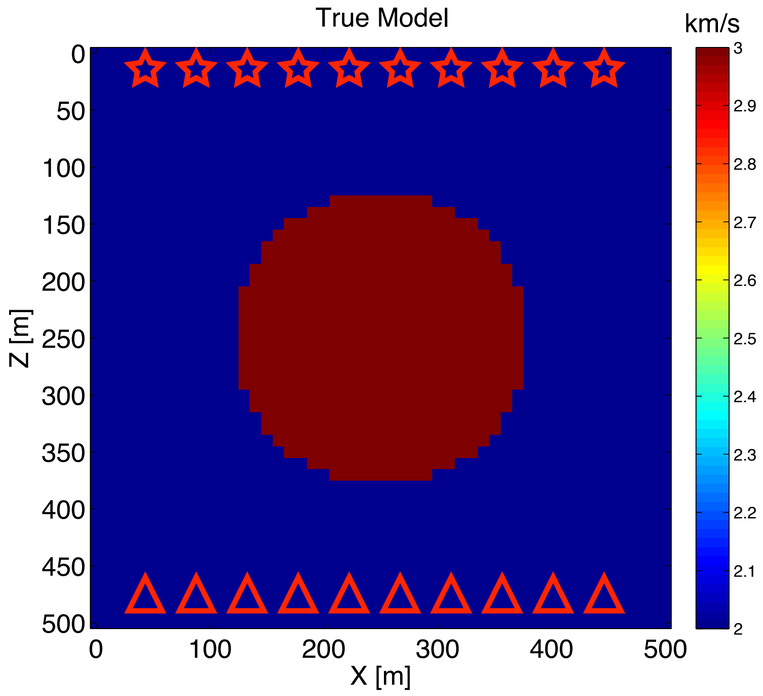
Computational Cost: $\mathcal{O}(N_s) \rightarrow \mathcal{O}(N_{rs})$





Numerical Experiments

Camambert model



☆ - source

△ - receiver

Statistical parameter to be inverted:

Standard deviation : σ

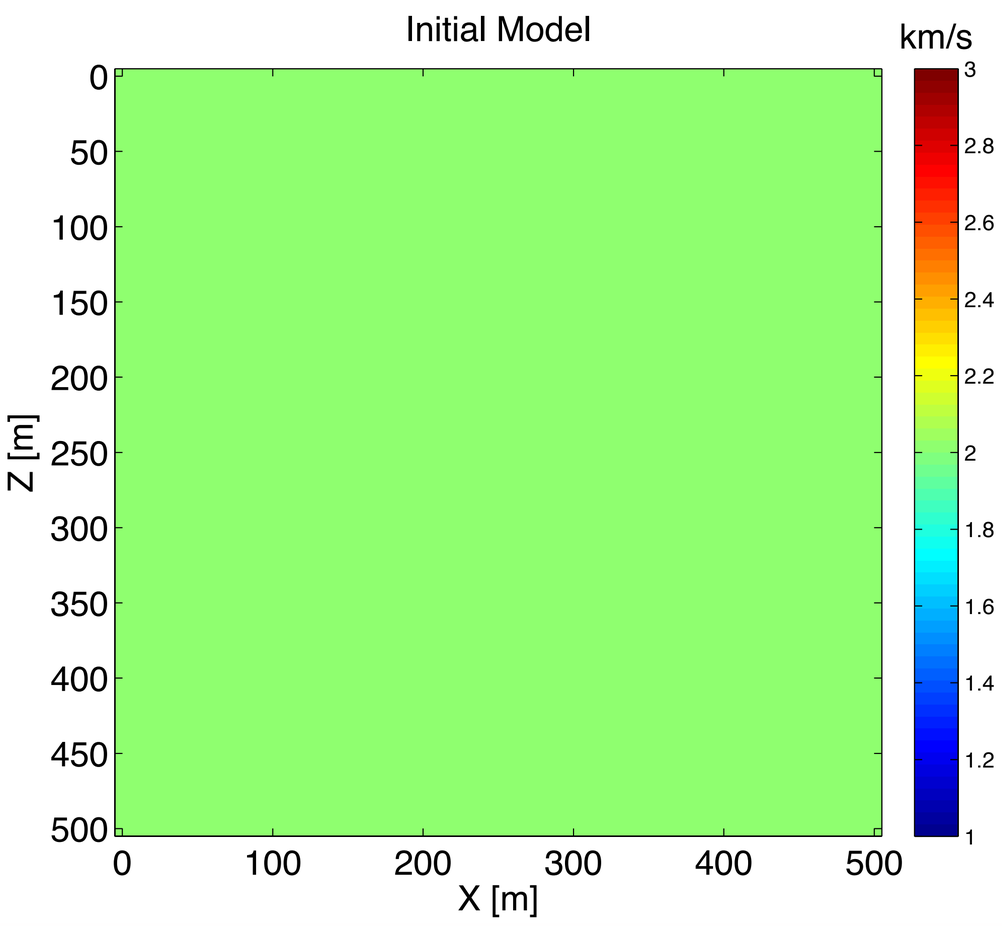
Confidence interval: $P(\mathbf{m} \in \mathrm{I}_{ci}) \geq \alpha$

Acquisition Geometry:

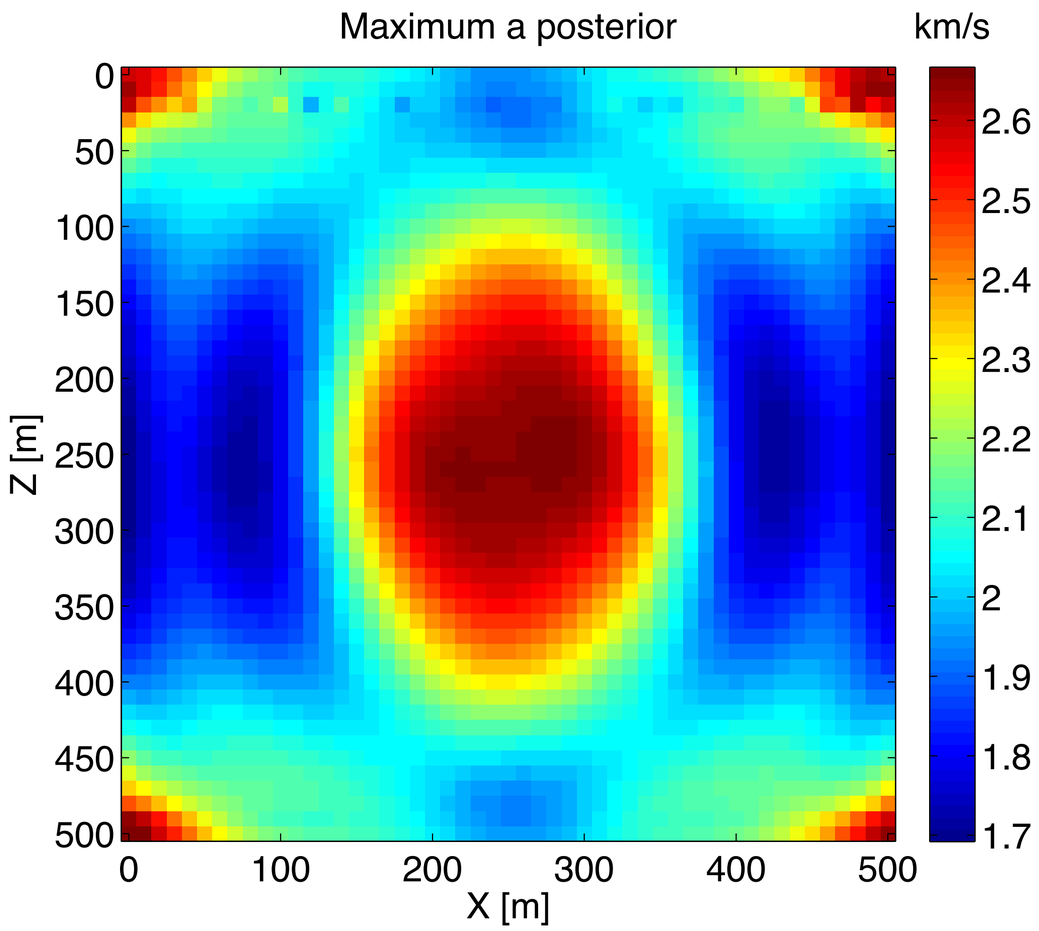
26 shots

51 receivers

10 frequencies

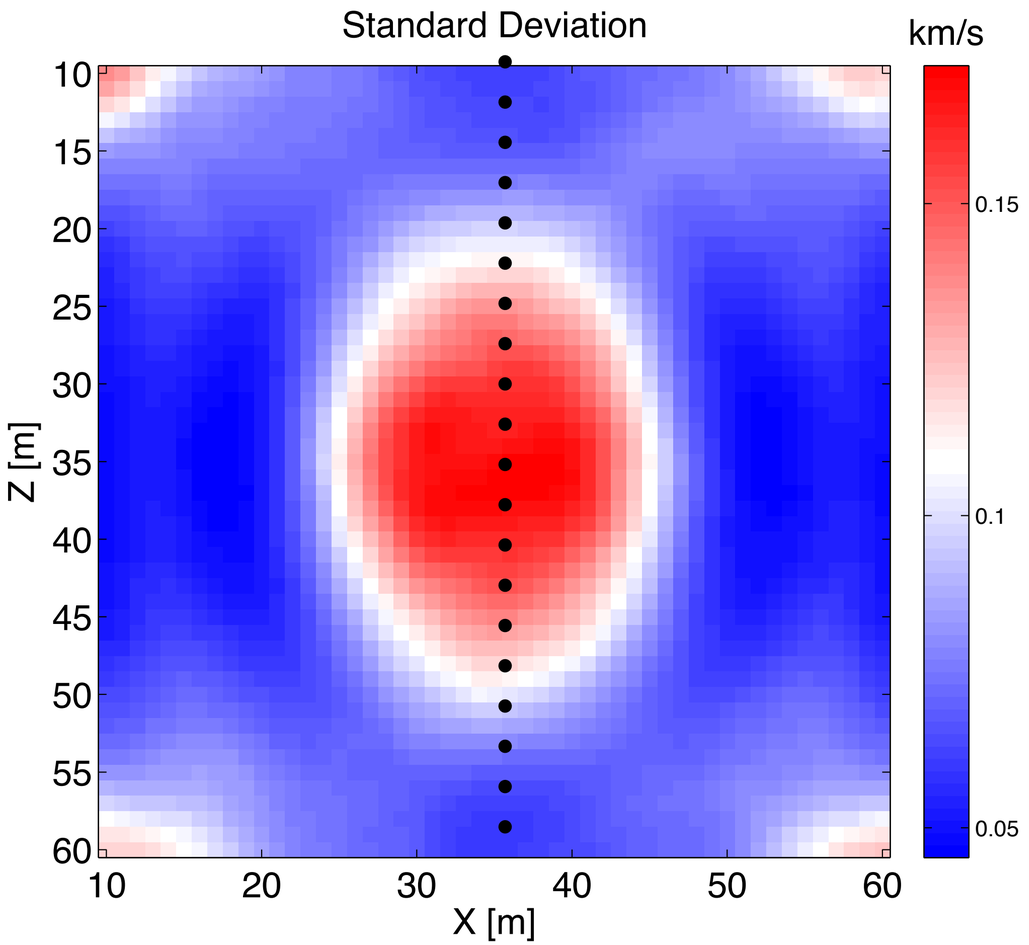


Initial model

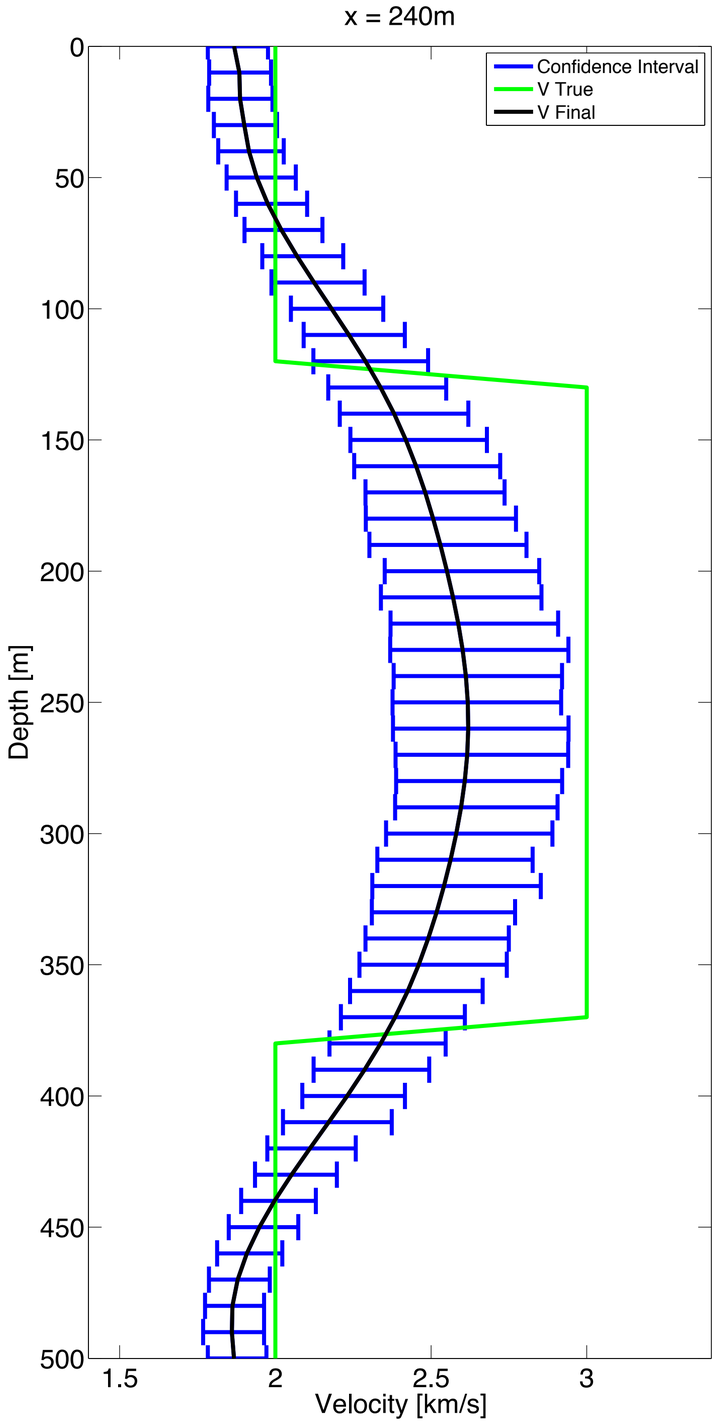


MAP

Nrs = 5



Standard Deviation



$\alpha = 0.9$

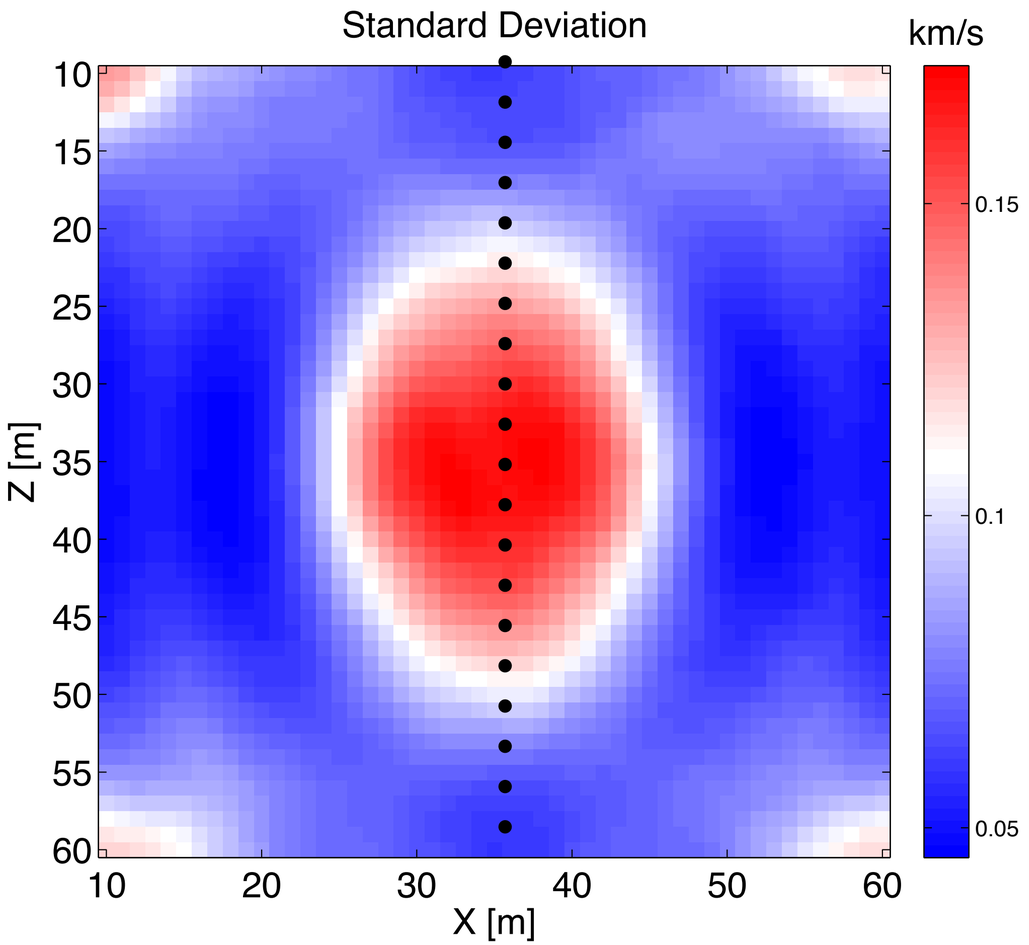
Final Model

Confidence Interval

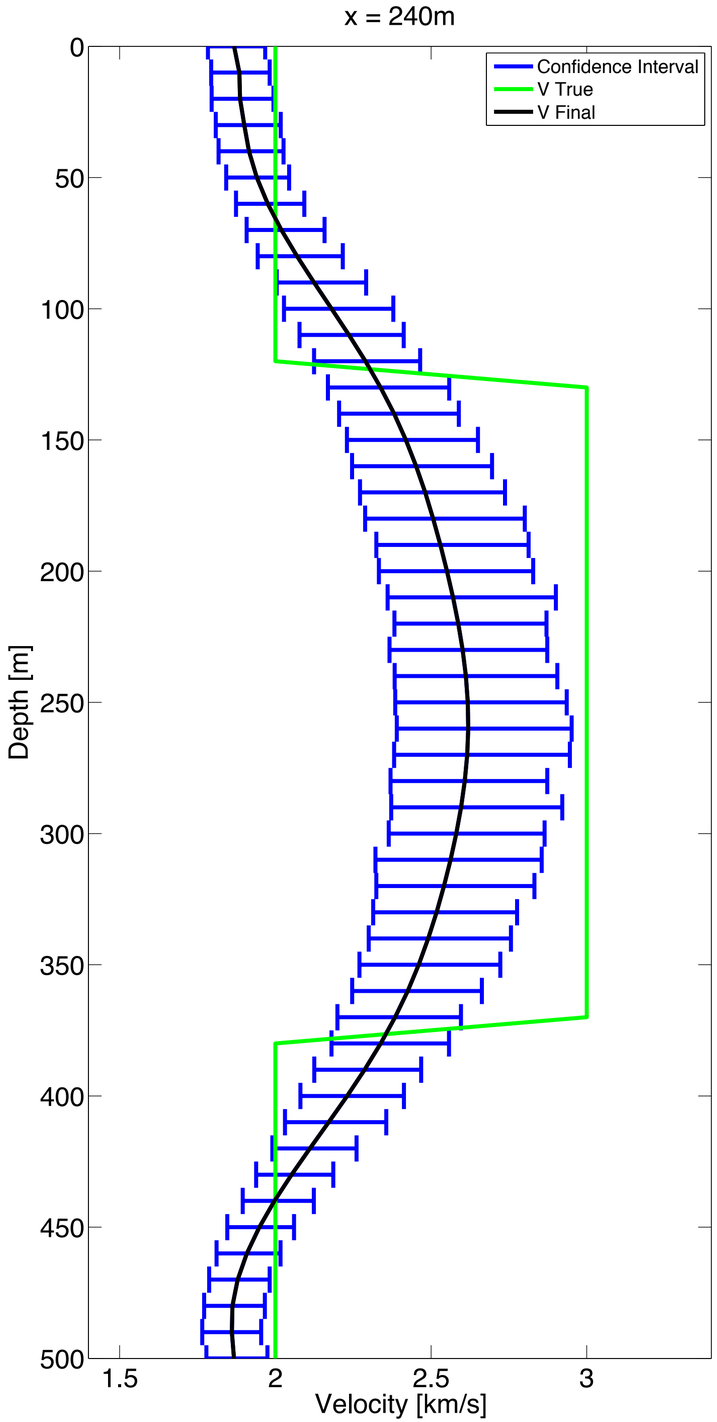
True Model

Confidence Interval

Nrs = 10



Standard Deviation



$\alpha = 0.9$

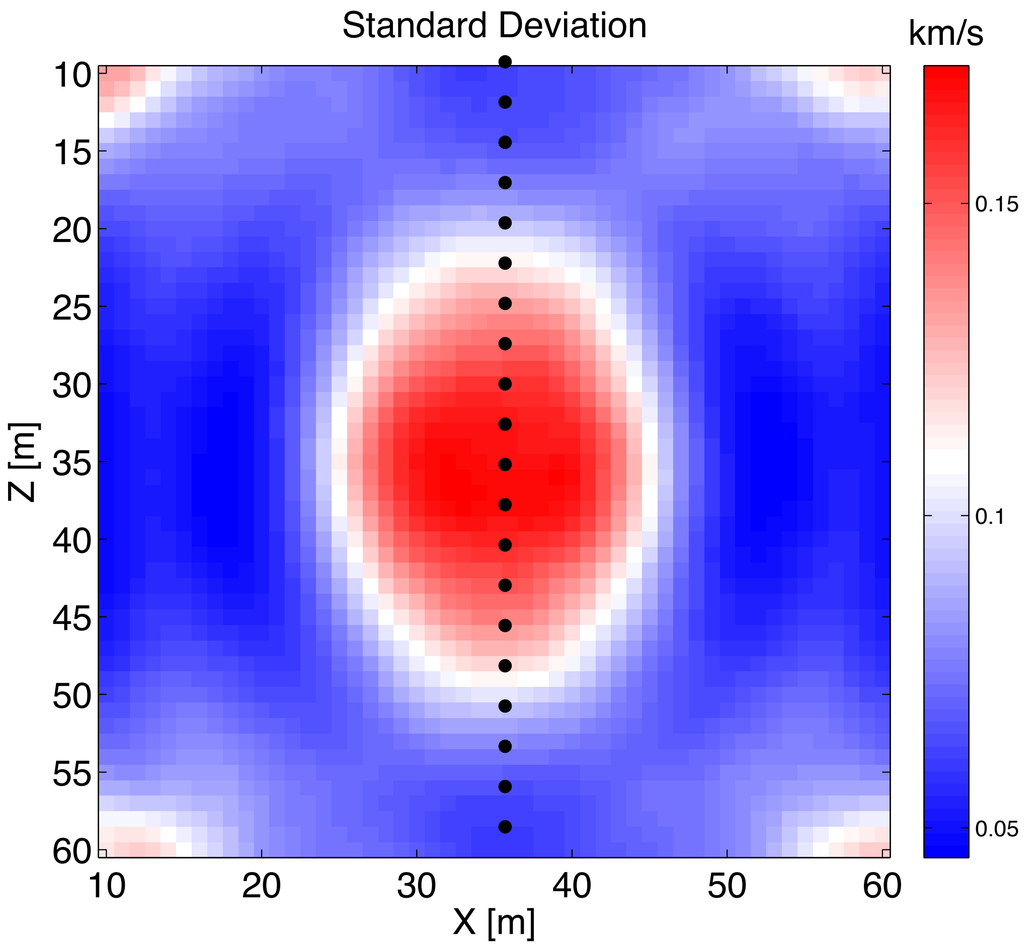
Final Model

Confidence Interval

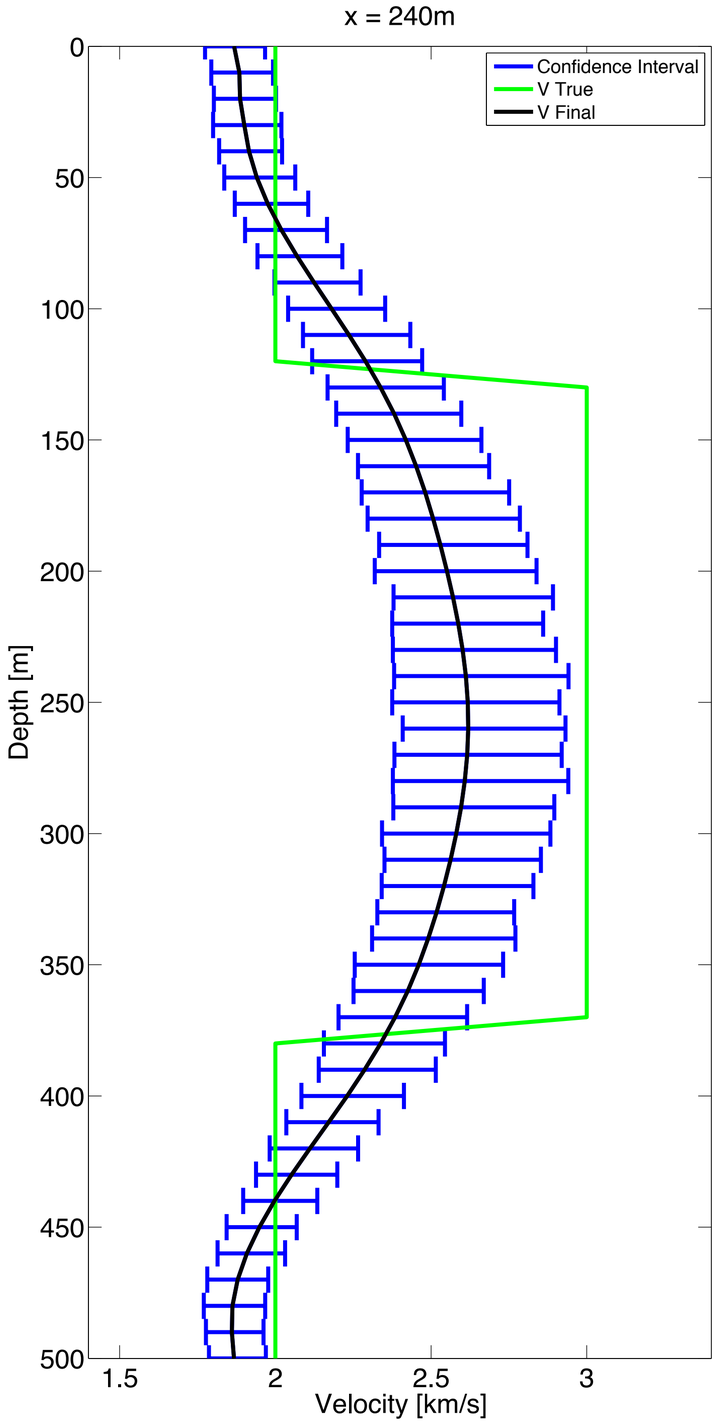
True Model

Confidence Interval

Nrs = 26



Standard Deviation



$\alpha = 0.9$

Final Model

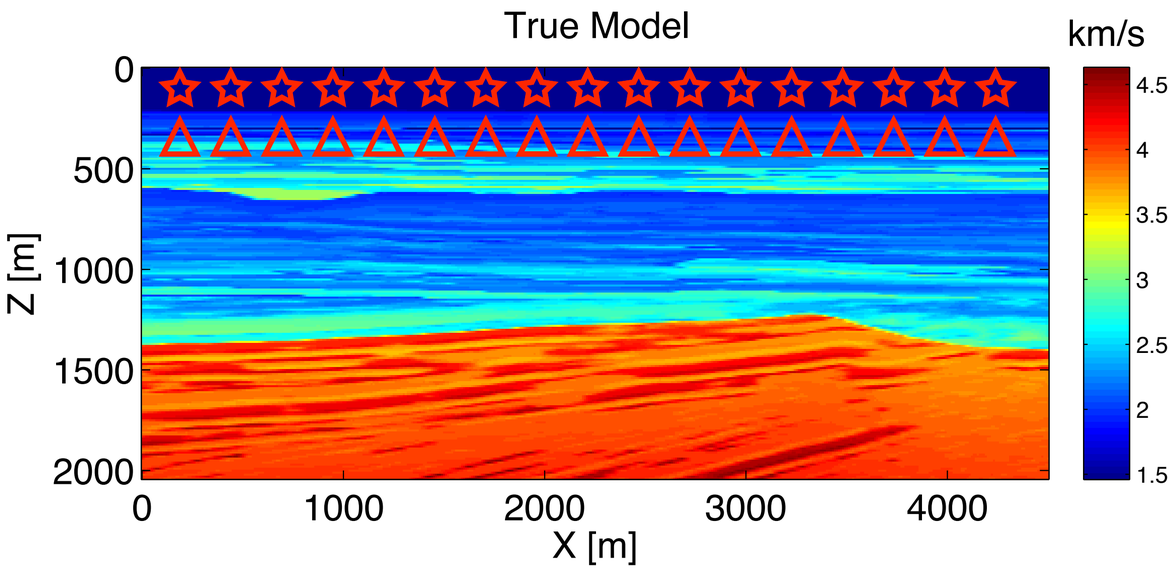
Confidence Interval

True Model

Confidence Interval

Numerical Experiments

BG model



☆ - source

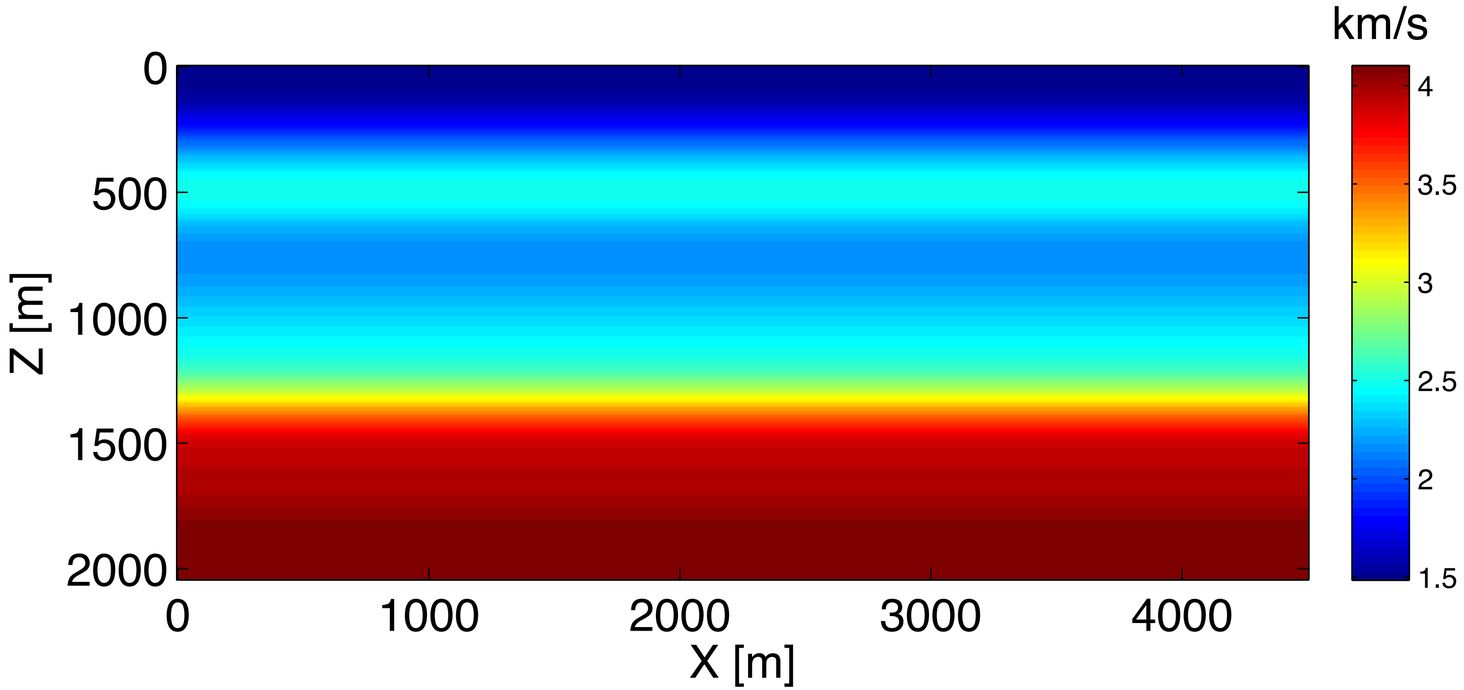
△ - receiver

Acquisition Geometry:

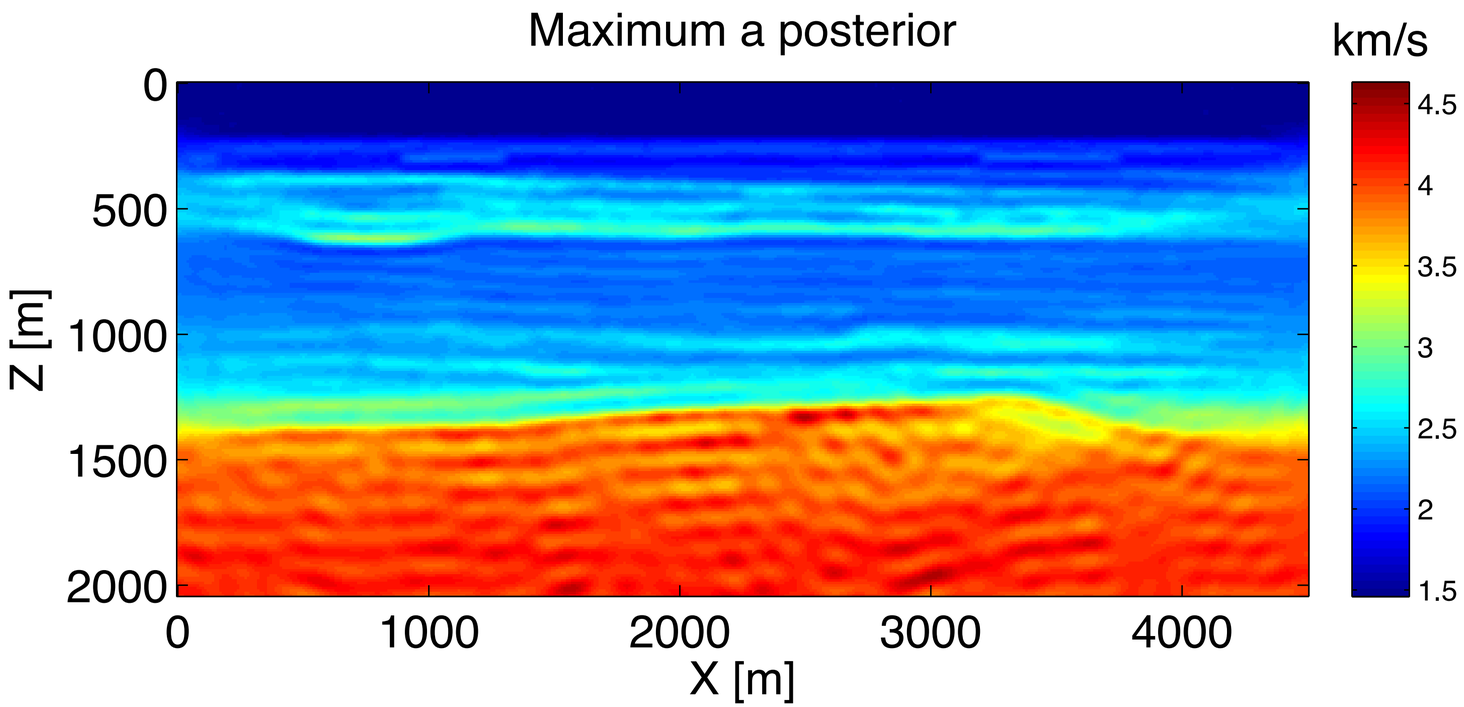
91 shots

451 receivers

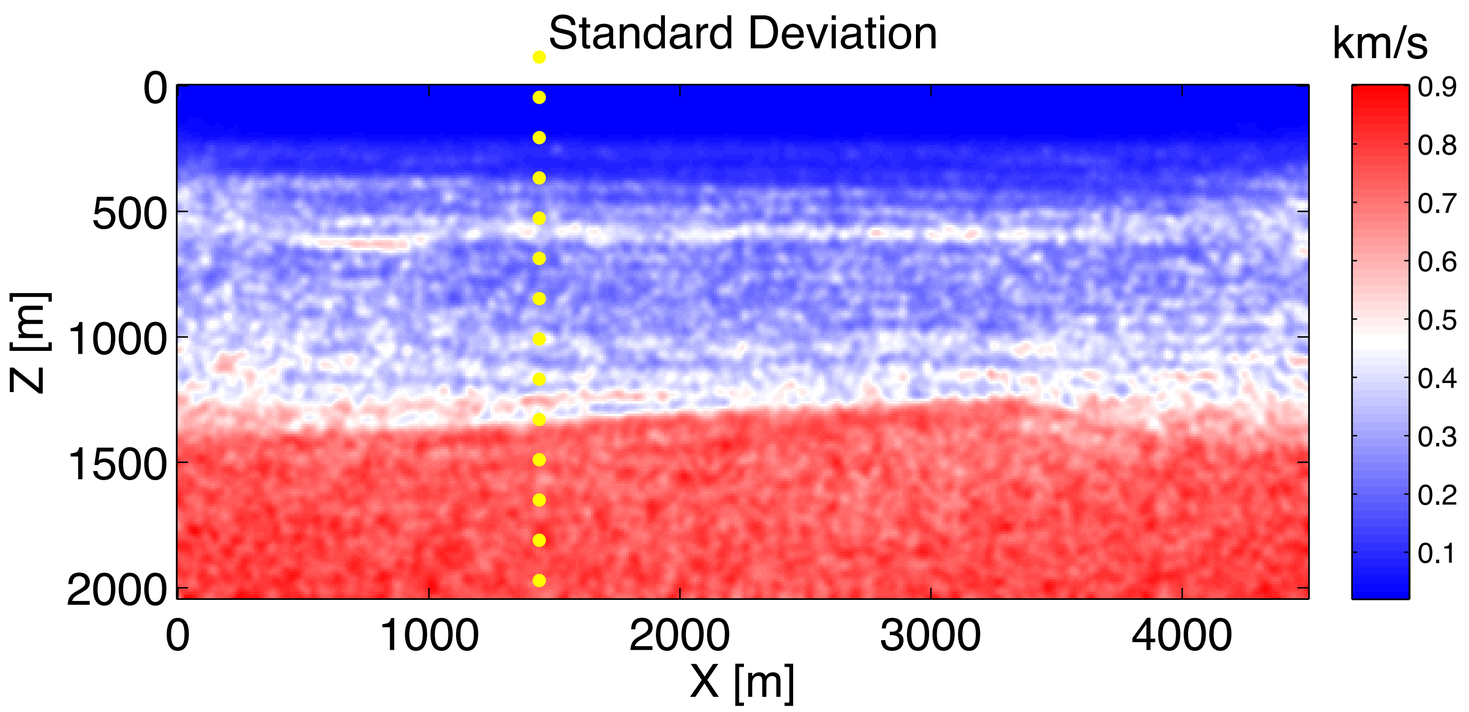
15 frequencies from 3Hz to 17Hz



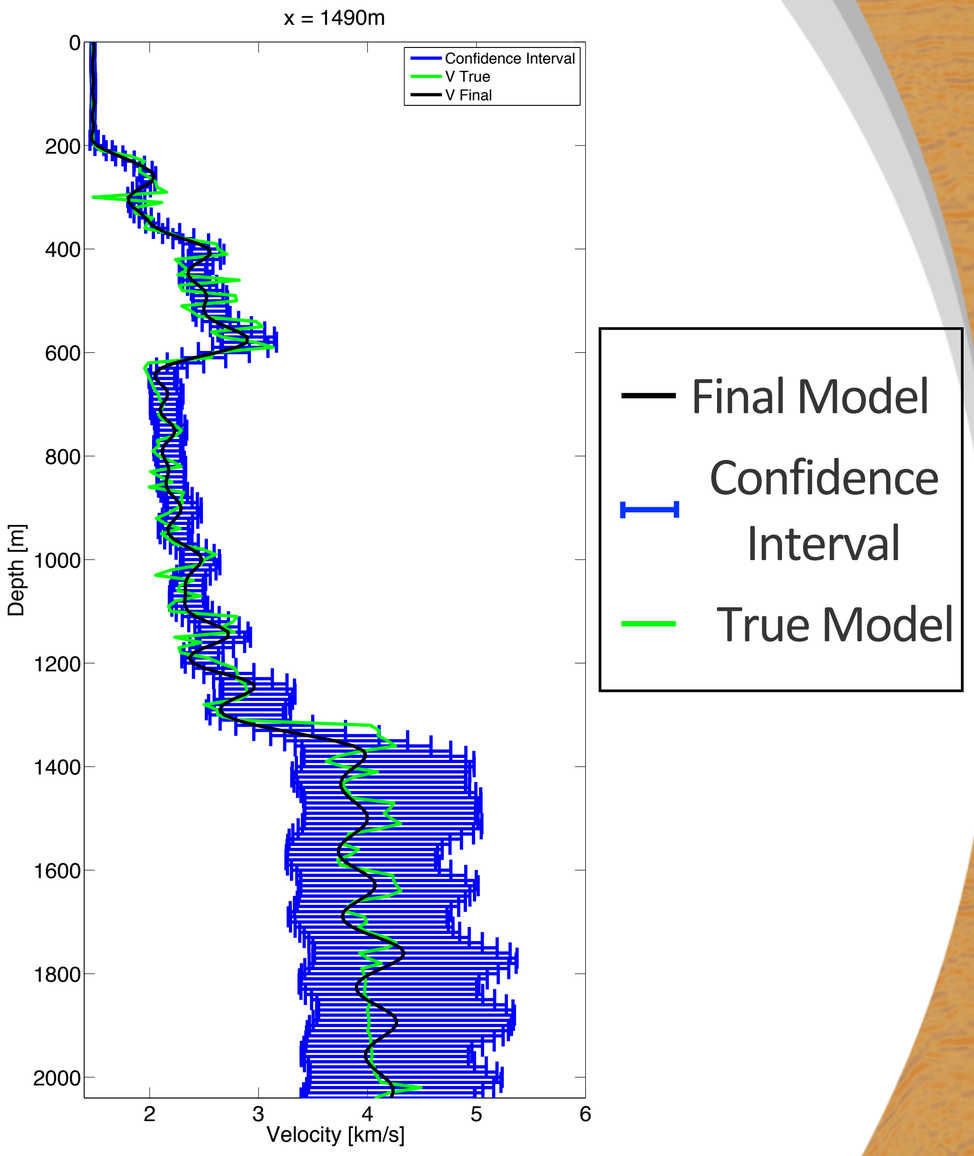
Initial model



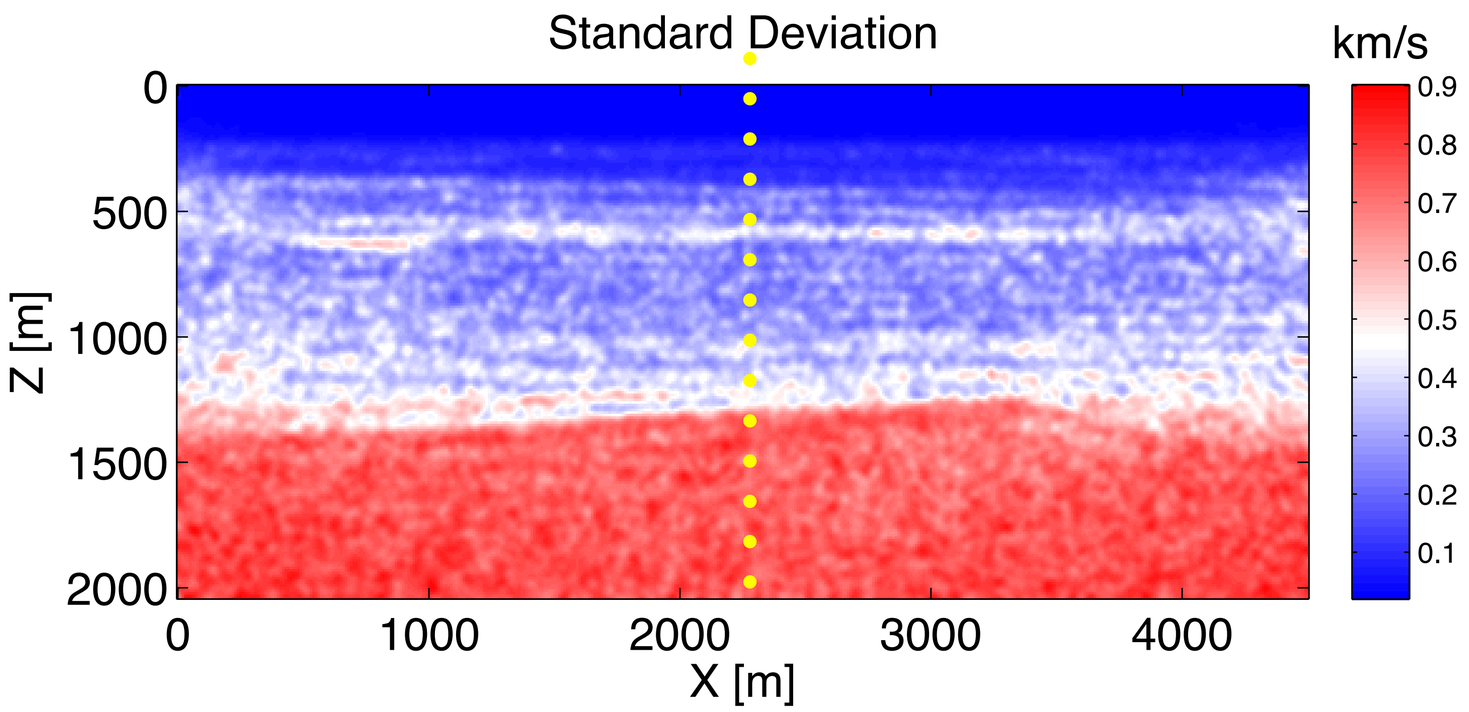
MAP



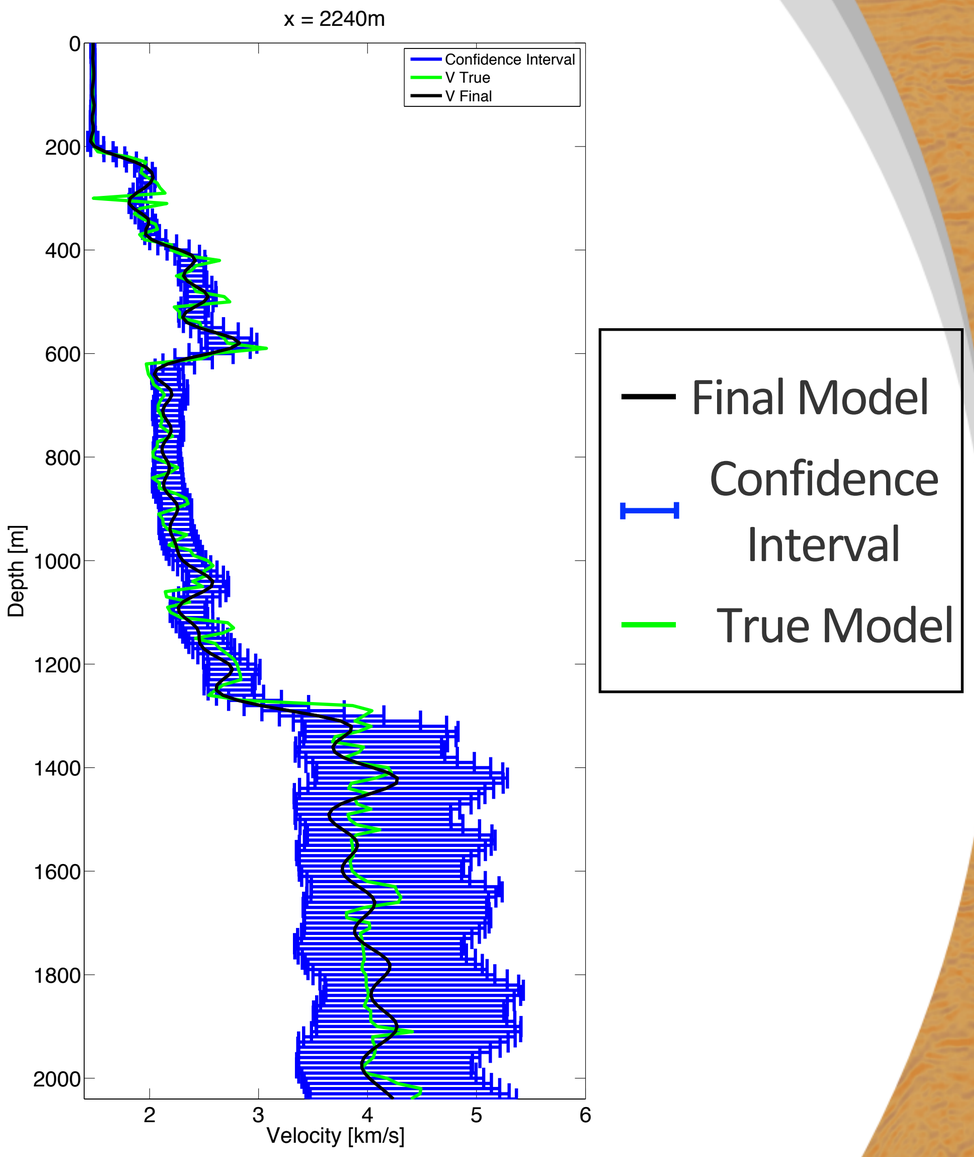
Standard deviation



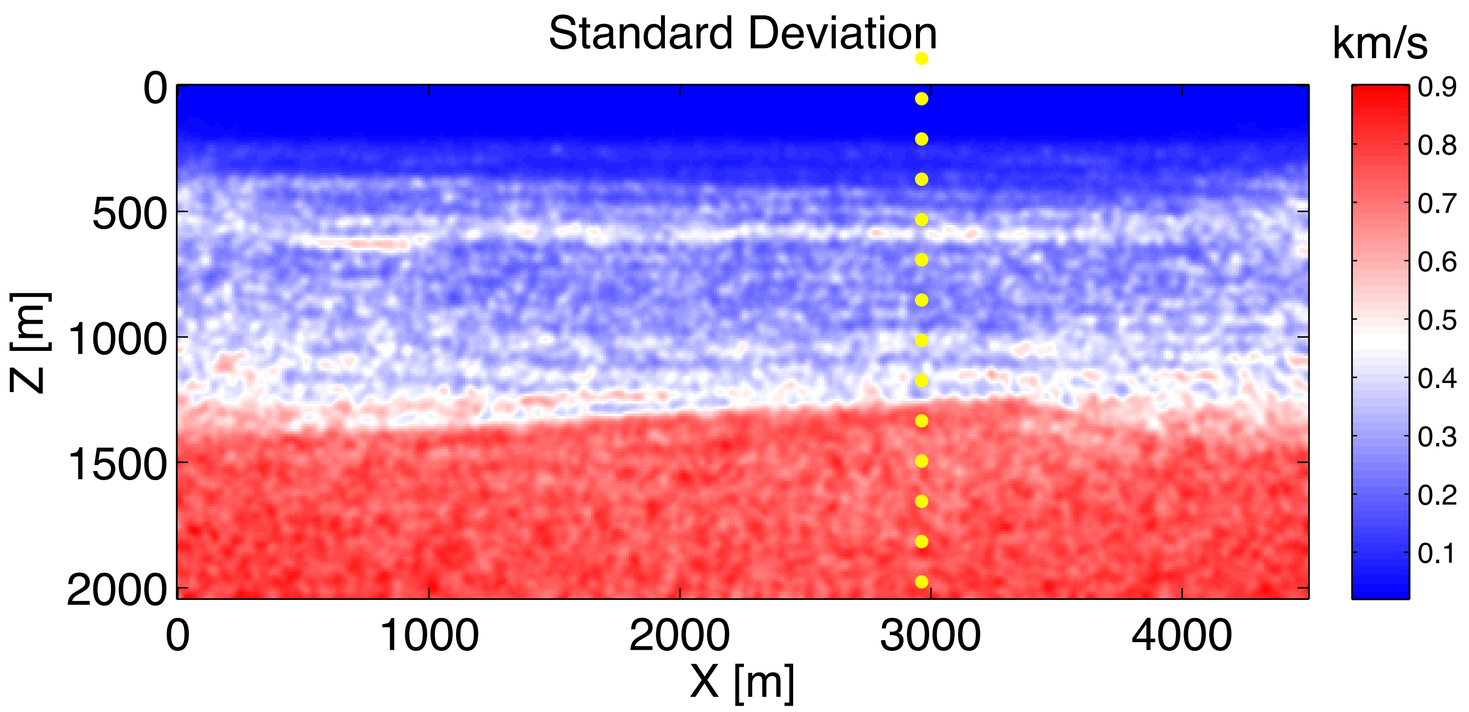
x = 1490m



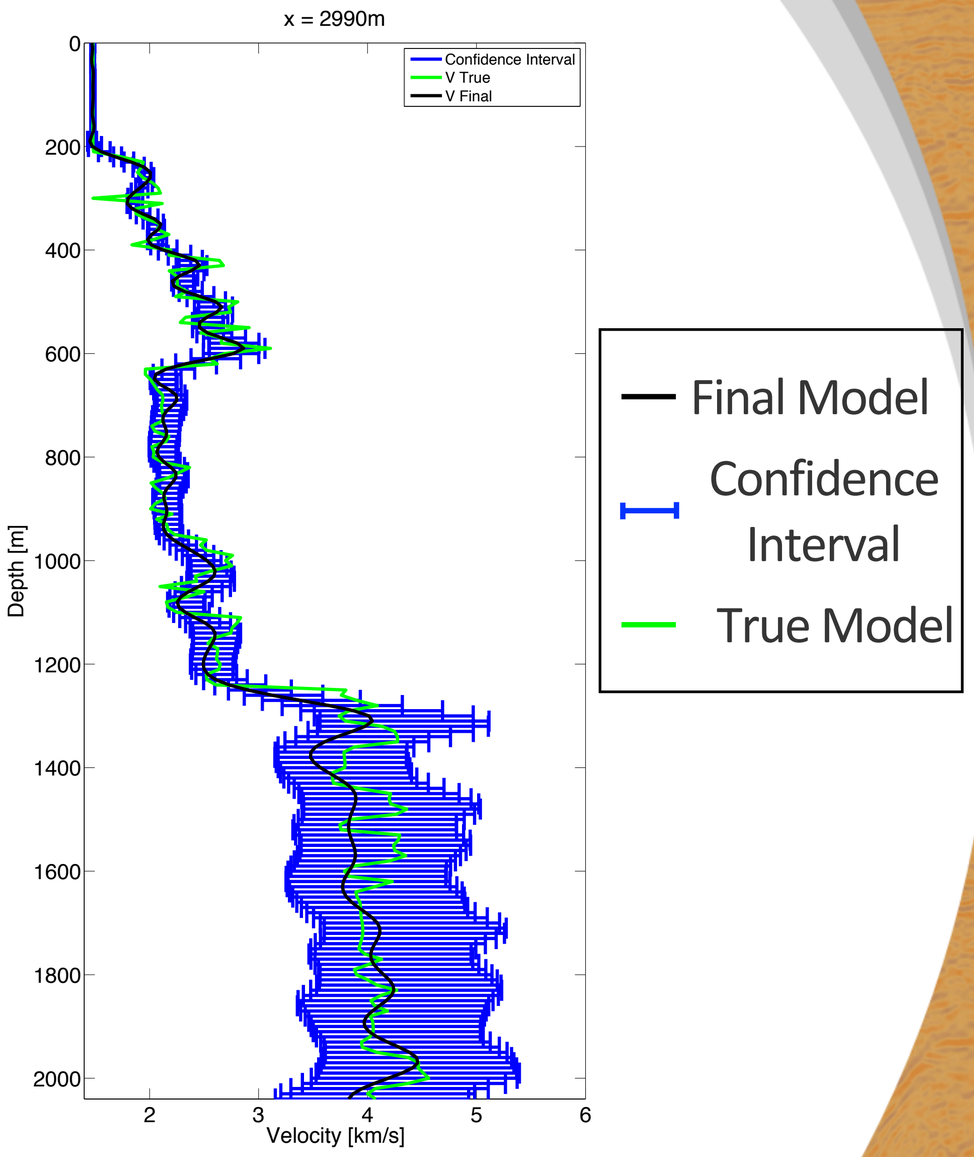
Standard deviation



x = 2240m



Standard deviation



x = 2990m

Conclusions

- Using the L-BFGS Hessian, we reduce the computational cost of estimating the Hessian.
- Using the randomized source sub-sampling method, we decrease the computational cost of the McMC.

Future Work

- Use penalty method frame work to reset up the probability distribution function.
- Use different sampling method to analyze the posterior distribution.
- Uncertainty quantification for 3D FWI.

Acknowledgements

Thank you for your attention !

https://www.slim.eos.ubc.ca/

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