Novel Optimization Schemes for Full Waveform Inversion: Optimal Transport and Inexact Gradient Projection

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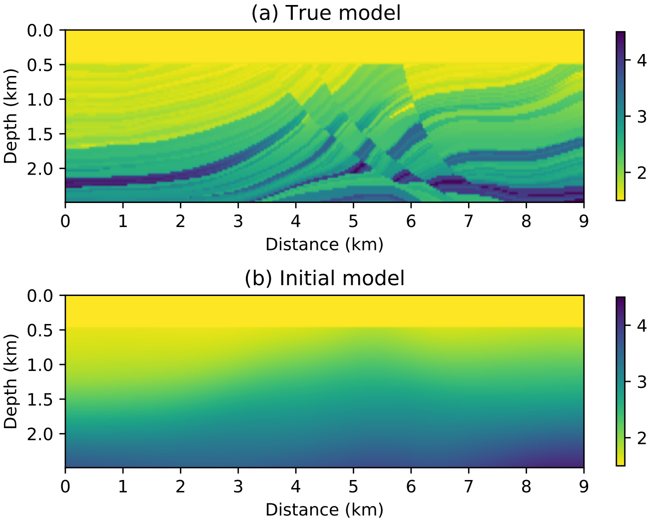
Full waveform inversion problem



Formulation of full waveform inversion problem

Full waveform inversion (FWI) is a PDE constrained optimization problem:

$$\min_{(y,u)\in Y\times U_{\text{ad}}} J(y,u) = \frac{1}{2}\|Qy - y_d\|_Y^2 + \lambda_r \mathcal{R}(u), \quad \text{such that } e(y,u) = 0. \tag{1}$$

The constraint PDE $e(y,u) = 0$ is well-posed, the parameter-to-state map can be defined as $F(u) = y$.

The PDE constrained optimization problem (1) has a reduced form:

$$\min_{u\in U_{\text{ad}}} f(u) = J(F(u), u). \tag{2}$$

The gradient of $f(u)$ can be achieved through the adjoint state method.

Improving the inverse result

The parameter-to-state map $F(u) = y$ is nonlinear, the objective function $f(u)$ is non-convex.

Only local minima can be expected.

We hope the local minimum is close to the global minimum, several methods can be considered:

- Enlarge the search space: wavefield reconstruction inversion (from U to $Y \times U$), etc.
- Change the distance in the objective function: optimal transport based distance (Wasserstein distance), etc.
- Add regularization term to the objective function: total variation regularization, adaptive regularization, etc.
- Solve the constraint optimization problem: box constraint set, etc.

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Optimal transport problem

Define discrete probability measure:

$$\alpha = \sum_{i=1}^{n} a_i \delta_{x_i}, \quad \beta = \sum_{i=1}^{m} b_i \delta_{y_i},$$

where $a_i > 0$, $b_i > 0$, $\sum_i a_i = \sum_i b_i = 1$.

Optimal transport distance

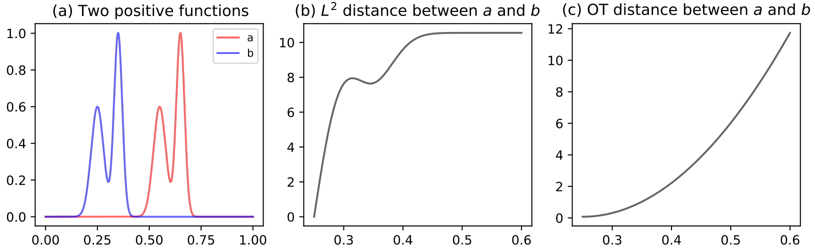
$$W_2^2(\alpha, \beta) = \min_{P \in \Pi_d(\alpha,\beta)} \langle P, C \rangle = \min_{P \in \Pi_d(\alpha,\beta)} \sum_{i,j} C_{i,j} P_{i,j},$$

where the cost matrix $C_{i,j} = |x_i - y_j|^2$, the set of discrete transport plan is

$$\Pi_d(\alpha, \beta) = \left\{ P \in \mathbb{R}_+^{n \times m} \;\middle|\; P\mathbf{1}_m = a \text{ and } P^{'}\mathbf{1}_n = b \right\}.$$

Initial idea and limitations

Convexity with respect to shift of 2-Wasserstein distance:



Limitations of OT distance:

- Mass equality condition ($\sum_i a_i = \sum_i b_i = 1$): unbalanced optimal transport distance, mixed L^1/Wasserstein distance;
- Positive vectors are needed ($a_i > 0$, $b_i > 0$): normalization methods.

Overcome the mass equality condition

Unbalanced optimal transport distance [Chizat et al., 2018]

When the mass equality condition is not satisfied ($\sum_i a_i \neq \sum_i b_i$):

$$W^2_{2,\varepsilon_u}(\alpha,\beta) = \min_{P \in \mathbb{R}_+^{n\times m}} \langle P, C\rangle + \varepsilon_u KL(P\mathbf{1}_m|a) + \varepsilon_u KL(P^{'}\mathbf{1}_n|b),$$

where the Kullback–Leibler (KL) divergence is defined by

$$KL(a|b) = \sum_{i=1}^{n} a_i \log\left(\frac{a_i}{b_i}\right).$$

Mixed L^1/Wasserstein distance

Normalized discrete measure $\hat{\alpha} = \frac{1}{\|a\|_1}\sum_{i=1}^{n} a_i \delta_{x_i}$ and $\hat{\beta} = \frac{1}{\|b\|_1}\sum_{i=1}^{m} b_i \delta_{y_i}$,

$$\bar{W}_2(\alpha,\beta) = W_2(\hat{\alpha},\hat{\beta}) + \left|\|a\|_1 - \|b\|_1\right|. \quad (3)$$

Overcome the mass equality condition

Proposition 1

The mixed L^1/Wasserstein distance defined in equation (3) is a distance over the set of positive discrete measures.

Since,

$$\bar{W}_2^2(\alpha, \beta) = \left(W_2(\hat{\alpha}, \hat{\beta}) + \left| \|a\|_1 - \|b\|_1 \right| \right)^2 \leq 2 \left(W_2^2(\hat{\alpha}, \hat{\beta}) + \left(\|a\|_1 - \|b\|_1 \right)^2 \right),$$

define,

$$J(\alpha; \beta) = W_2^2(\hat{\alpha}, \hat{\beta}) + \left(\|a\|_1 - \|b\|_1 \right)^2.$$

Proposition 2

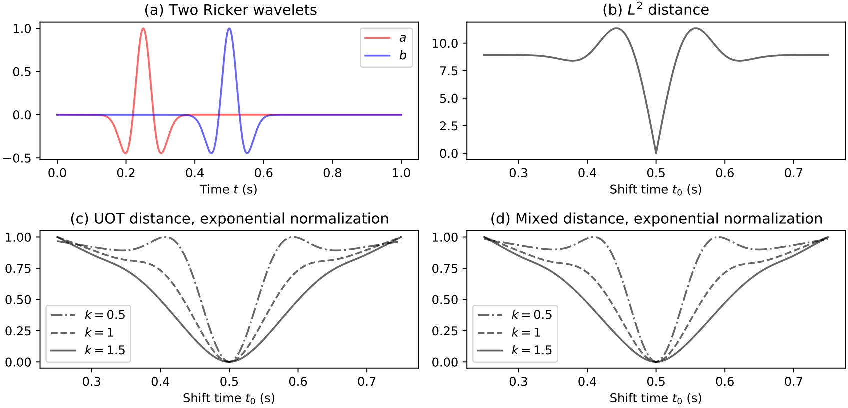
The objective function $J(\alpha; \beta)$ is convex with respect to the shift, dilation, and mass change of α.

Normalization methods

Normalization methods are needed for signals:

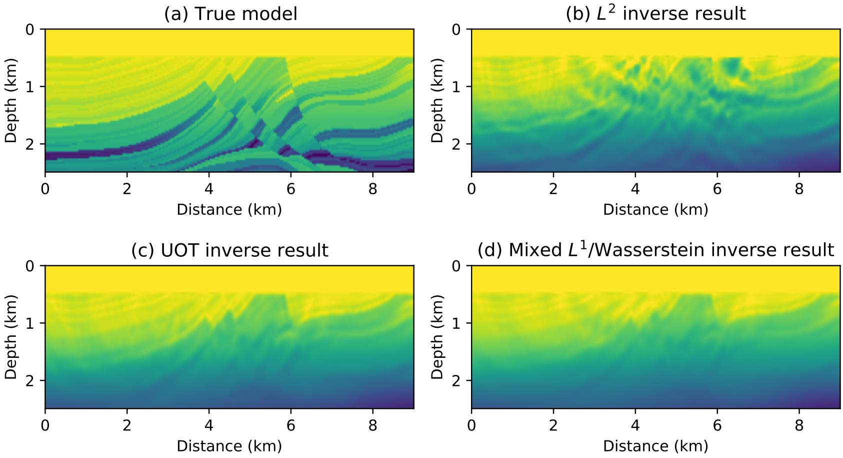
$$h_{\mathsf{l}}(a,k)(t) = a(t) + k, \quad h_{\mathsf{e}}(a,k)(t) = e^{ka(t)}.$$

Normalization methods only partially solve the problem.
Shift signal a from left to right:



OT based distance for the FWI problem

Marmousi model inverse results:



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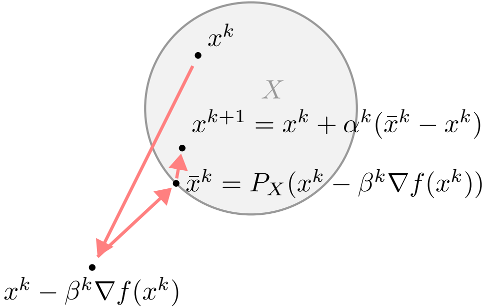
Initial idea

Objective function f is smooth and nonlinear, X is convex, consider the constrained optimization problem:

$$\min_x f(x), \quad \text{such that } x \in X.$$

Gradient projection method at the k-th iteration:

$$\begin{aligned} \bar{x}^k &= P_X(x^k - \beta^k \nabla f(x^k)), \\ x^{k+1} &= x^k + \alpha^k(\bar{x}^k - x^k). \end{aligned}$$



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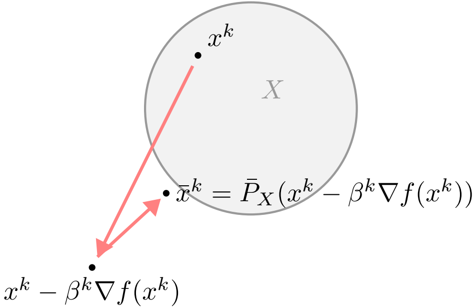


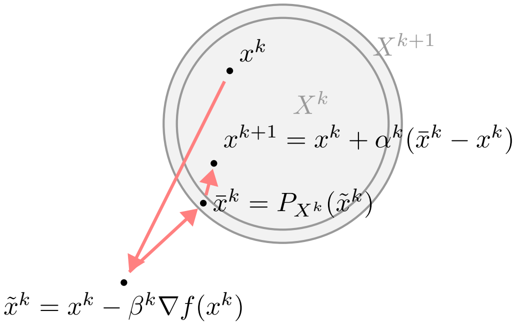
Set expanding strategy

Definition

Given a feasible set X is nonempty, closed, and convex, construct an expanding set sequence $\{X^k\}$ such that

$$X = \lim_{k \to \infty} X^k, \quad X^k \subset X^{k+1}, \quad X^k \neq X^{k+1}, \tag{4}$$

where X^k is nonempty, closed, and convex for each $k \in \mathbb{N}$.



Gradient projection method with inexact projection

Algorithm 1: Gradient projection method with inexact projection

Initialization: Given feasible set X, construct set sequence $\{X^k\}$ satisfies (4). Given the initial point $x^0 \in X^0$.

while *not convergent* **do**

Step 1: Compute $\tilde{x}^k = x^k - \beta\nabla f(x^k)$;

Step 2: Project $\tilde{x}^k$ to X^k, until equation $\bar{P}_{X^k}(\tilde{x}^k) \in X^{k+1}$, $\left\langle \tilde{x}^k - \bar{P}_{X^k}(\tilde{x}^k), x^k - \bar{P}_{X^k}(\tilde{x}^k) \right\rangle \leq 0$ are satisfied.

Step 3: Evaluate the line search stepsize with Armijo rule or Wolfe conditions, update with $x^{k+1} = x^k + \alpha^k(\bar{x}^k - x^k)$;

Step 4: Enlarge the feasible set $X^k = X^{k+1}$, let $k = k + 1$.

end

Theorem 1

Under proper assumptions, let $\{x^k\}$ be the sequence generated by Algorithm 1. Then every limit point of $\{x^k\}$ is stationary.

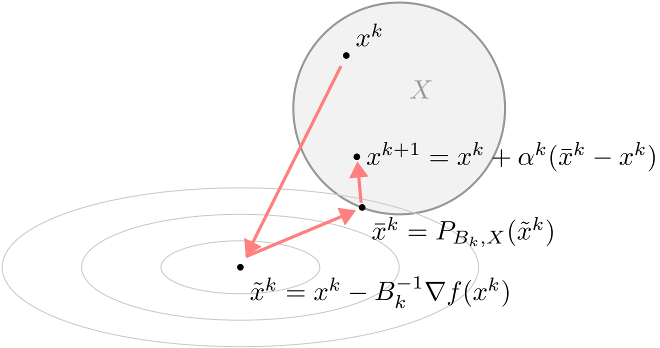
Scaled gradient projection method

The scaled gradient projection method is given by:

$$\bar{x}^k = \arg\min_{x \in X} \left\langle \nabla f(x^k), x - x^k \right\rangle + \frac{1}{2} \left\langle B_k(x - x^k), x - x^k \right\rangle,$$
$$x^{k+1} = x^k + \alpha^k(\bar{x}^k - x^k).$$

The first equation equivalents to

$$\tilde{x}^k = x^k - B_k^{-1} \nabla f(x^k), \quad \bar{x}^k = P_{B_k, X}(\tilde{x}^k).$$



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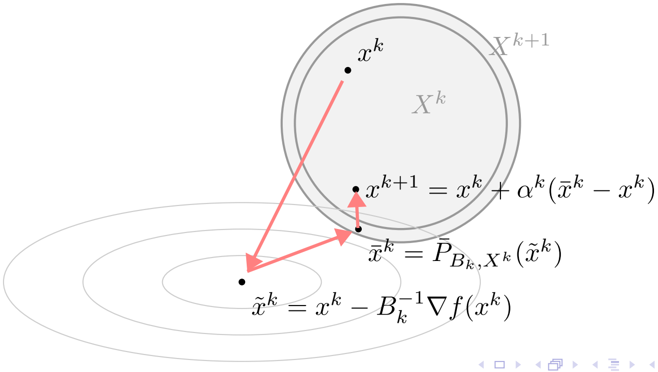

Scaled gradient projection method with inexact projection

Algorithm 2: Scaled gradient projection method with inexact projection

Initialization: Given feasible set X, construct set sequence $\{X^k\}$ satisfies (4). Given the initial point $x^0 \in X^0$.

while *not convergent* **do**

Step 1: Find a scaling matrix B_k, compute $\tilde{x}^k = x^k - B_k^{-1}\nabla f(x^k)$;

Step 2: Project $\tilde{x}^k$ towards X^k, until equation $\bar{P}_{B_k,X^k}(\tilde{x}^k) \in X^{k+1}$ and $\left\langle \tilde{x}^k - \bar{P}_{B_k,X^k}(\tilde{x}^k), x^k - \bar{P}_{B_k,X^k}(\tilde{x}^k) \right\rangle_{B_k} \leq 0$ are satisfied.

Step 3: Evaluate the line search stepsize with Armijo rule or Wolfe conditions, update with $x^{k+1} = x^k + \alpha^k(\bar{x}^k - x^k)$;

Step 4: Enlarge $X^k = X^{k+1}$, let $k = k+1$.

end

Theorem 2

Under certain assumptions, let $\{x^k\}$ be the sequence generated by Algorithm 2. Then every limit point of $\{x^k\}$ is stationary.

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Initial idea

Consider the constrained optimization problem with multiple constraints:

$$\min_u f(u), \quad \text{such that } u \in U_{\text{ad}} = \cap_i U_i,$$

where U_i is nonempty, closed, and convex, U_{ad} is nonempty.

A priori information can be described by constraint sets.

Two kinds of constraint sets:

- Constraint set with closed-form projection function: box constraint, hyperplane constraint, etc.
- Constraint set with subgradient projection: total variation constraint, l_1 constraint.

Proposed algorithm is a combination of scaled gradient projection method with inexact projection, L-BFGS Hessian approximation, an iterative projection method [Combettes, 2003].

Main algorithm

Algorithm 3: Scaled gradient projection method with multiple constraints

Given: the objective function f and initial value u^0; a family of nonempty, closed, convex constraint sets U_i.

For each U_i construct the set sequence $\{U_i^j\}_{j\in\mathbb{N}}$; set $U_{\text{ad}}^k = \cap_{i\in I} U_i^k$ for all k.

while *Not converge* **do**

Step 1: Compute $\nabla f(u^k)$.

Step 2: Update the L-BFGS coefficients s_k, y_k, S_k, Y_k, R_k, D_k, U_k.

Step 3: Compute $\tilde{u}^k = u^k - H_k \nabla f(u^k)$.

Step 4: Compute $\bar{u}^k = \bar{P}_{B_k, U_{\text{ad}}^k}(\tilde{u}^k)$, i.e., project $\tilde{u}^k$ to U_{ad}^k in $\mathcal{H}_{B_k}$ with the inexact projection algorithm [Combettes, 2003], until the following equations are satisfied:

$$\bar{u}^k \in U_{\text{ad}}^{k+1},$$

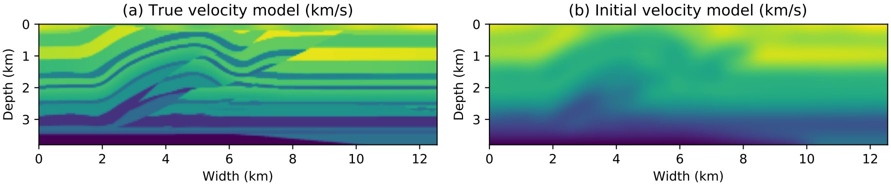
$$\left\langle \tilde{u}^k - \bar{u}^k, u^k - \bar{u}^k \right\rangle_{B_k} \leq 0.$$

Step 5: Update $u^{k+1} = u^k + \alpha^k(\bar{u}^k - u^k)$, here α^k is the linesearch parameter.

Step 6: Set $k = k+1$.

end

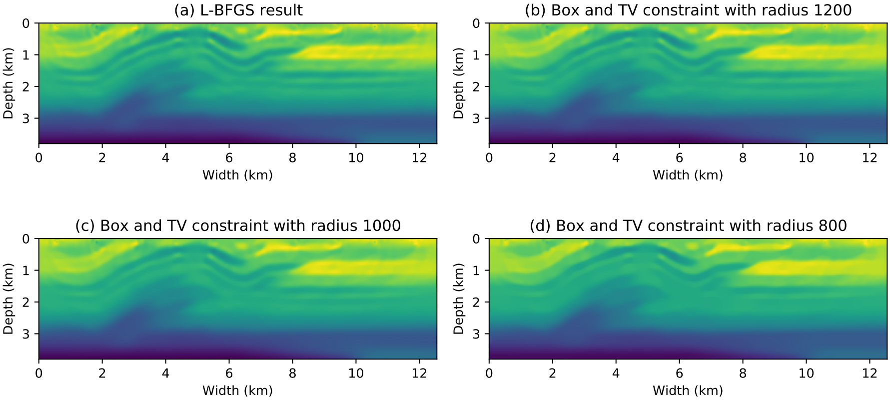
Numerical example



Settings of the sequences of constraint sets:

- $U_1^h = \{u \in \mathbb{R}^n \mid 2.5588 - \theta_1(h) \leq u_i \leq 6 + \theta_1(h),\ i = 1, \cdots, n\}$, where $\theta_1(h) = \sum_{i=1}^{h} 0.02 \times 0.9^i$.
- $U_2^h = \{u \in \mathbb{R}^n \mid f_{\mathsf{TV}}(u) \leq 800 + \theta_2(h)\}$, where $\theta_2(h) = \sum_{i=1}^{h} 40 \times 0.9^i$.
- $U_3^h = \{u \in \mathbb{R}^n \mid f_{\mathsf{TV}}(u) \leq 1000 + \theta_3(h)\}$, where $\theta_3(h) = \sum_{i=1}^{h} 50 \times 0.9^i$.
- $U_4^h = \{u \in \mathbb{R}^n \mid f_{\mathsf{TV}}(u) \leq 1200 + \theta_4(h)\}$, where $\theta_4(h) = \sum_{i=1}^{h} 60 \times 0.9^i$.

Numerical example



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Contributions

This thesis studies the novel optimization methods for the FWI problem:

- Introduce the UOT distance to the FWI problem.
- Construct a mixed L^1/Wasserstein distance and introduced to the FWI problem.
- A set expanding strategy is developed for the gradient projection methods when the inexact projection algorithm is used.
- The convergence results for the gradient projection methods with inexact projection are proved under proper assumptions.
- A new optimization scheme: scaled gradient projection method with multiple constraints. This optimization scheme is applied to the FWI problem.
- All computing programs were written by the author in Julia and are available on Github.

Future studies

- The application of UOT and mixed L^1/Wasserstein distance to the variational problem based on the positive quantities.
- A new optimization scheme can be designed with the combination of the spectral projected gradient method and the set expanding strategy.
- Incorporate the well-log data to the FWI problem with the proposed optimization scheme in Chapter 6.
- Find new constraints for the multi-parameter FWI problem to decrease the cross-talk issue.
- The set expanding strategy developed in Chapter 5 provides a method to analyze the following constrained optimization problem:

$$\min_x f(x), \quad \text{such that } x \in X^k.$$

This might be a new way to analysis the optimization problem with adaptive constraint (regularization).

Acknowledgment

Thank You!

References

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