Full waveform inversion with unbalanced optimal transport distance

Da Li, Michael P. Lamoureux and Wenyuan Liao

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Optimal transport problem

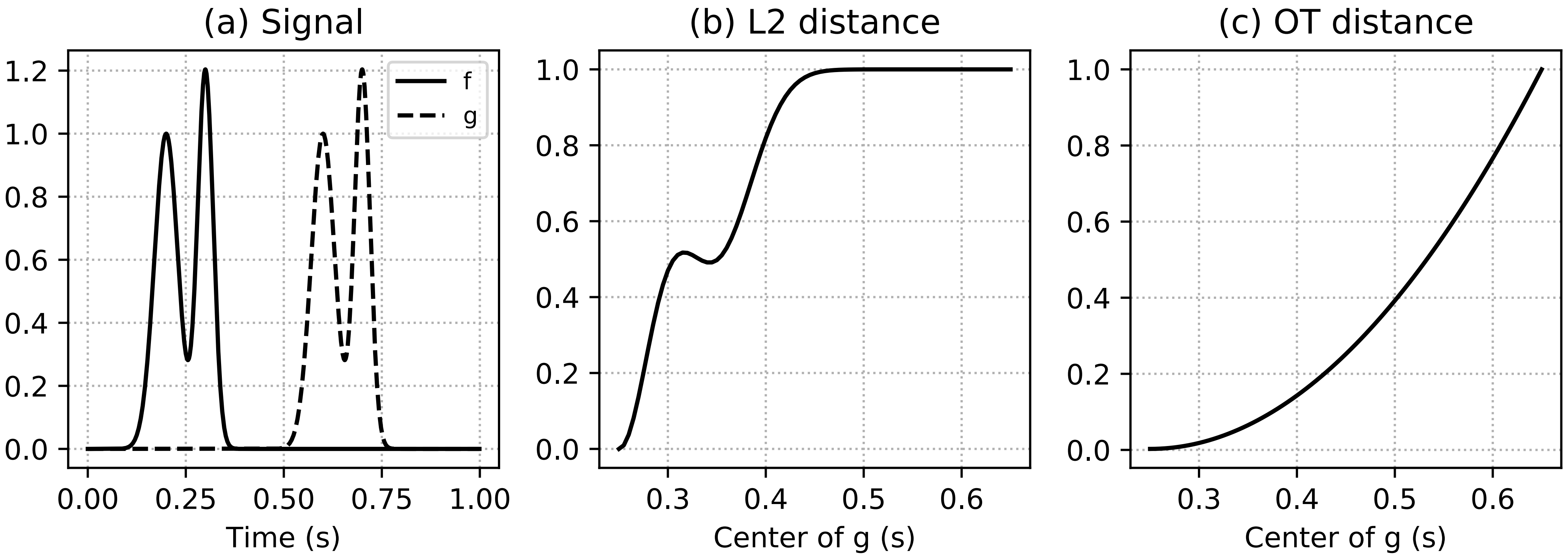
Definition (Optimal transport):
Given $X = Y = \{x_1, x_2, \cdots, x_N\} \subset \mathbb{R}^{\mathrm{d}}$, positive measures $\mu = \sum_i f_i \delta_{x_i}$, $\nu = \sum_i g_i \delta_{x_i}$, with $f_i \geq 0, g_i \geq 0$, and $\sum_i f_i = \sum_i g_i$. Let cost matrix C defined by $C_{ij} = \left|x_i - x_j\right|^2$.
The optimal transport problem between f and g is:

$$\min_{T \in \mathbb{R}^{N\times N}} < T, C > = \sum_{i,j=1}^{N} T_{ij} C_{ij}\,, \qquad s.t.\ T 1_N = f, \qquad T^T 1_N = g.$$

The **optimal transport distance** (2-Wasserstein distance) is given by:

$$W_2^2(f, g) = \min_{T \in \mathbb{R}^{N\times N}} < T, C >, \qquad s.t.\ T 1_N = f, \qquad T^T 1_N = g.$$

Optimal transport problem



Limitations:

1. Positive measure: $f_i \geq 0, g_i \geq 0$. For signals, normalization methods are needed.

2. Mass equality condition: $\sum_i f_i = \sum_i g_i$. Unbalanced optimal transport.

Unbalanced optimal transport problem

Definition (Unbalanced optimal transport):
Given cost matrix C, regularization coefficients ε and ε_m. The unbalanced optimal transport (UOT) distance between f and g is:

$$W^2_{2,\varepsilon,\varepsilon_m}(f,g) = \min_{T\in\mathbb{R}^{N\times N}} < T, C > -\varepsilon E(T) + \varepsilon_m KL(T 1_N | f) + \varepsilon_m KL(T^T 1_N | g)\,. \quad (1)$$

- Entropy regularization $E(T) = -\sum_{i,j=1}^{N} T_{ij}(\log(T_{ij}) - 1)$, increase the computational efficiency.

- Kullback-Leibler divergence $KL(a|b) = \sum_{i=1}^{N} a_i\left(\log\left(\frac{a_i}{b_i}\right) - 1\right)$ as the mass balancing term.

Unbalanced optimal transport problem

Theorem (Dual Problem):

Let matrix K defined by $K_{ij} = \exp\left(-\frac{C_{ij}}{\varepsilon}\right)$. The dual problem of equation (1) is given by:

$$W_{2,\varepsilon,\varepsilon_m}^2(f,g) = \max_{\phi,\psi\in\mathbb{R}_+^N} \sum_{i,j=1}^{N} -\varepsilon_m f_i\left(\exp\left(-\frac{\phi_i}{\varepsilon_m}\right)\right) - \varepsilon_m g_i\left(\exp\left(-\frac{\psi_j}{\varepsilon_m}\right)\right) - \varepsilon K_{ij}\left(\exp\left(\frac{\phi_i}{\varepsilon}\right)\exp\left(\frac{\psi_j}{\varepsilon}\right) - 1\right). \quad (2)$$

Strong duality holds. There exists a unique T^* for the equation (1). And ϕ^*, ψ^* maximize (2) if and only if

$$T_{ij}^* = \exp\left(\frac{\phi_i^*}{\varepsilon}\right) \mathrm{K_{ij}} \exp\left(\frac{\psi_j^*}{\varepsilon}\right).$$

Unbalanced optimal transport problem

Iterative scaling algorithm:

Starting with an initial value $v^{(0)} = 1_N$, compute iteratively with:

$$u_i^{(n+1)} = \left(\frac{f_i}{\sum_j K_{ij} v_j^{(n)}}\right)^{\frac{\varepsilon_m}{\varepsilon_m+\varepsilon}}, \qquad v_j^{(n+1)} = \left(\frac{g_j}{\sum_i K_{ij} u_i^{(n+1)}}\right)^{\frac{\varepsilon_m}{\varepsilon_m+\varepsilon}},$$

until converge requirement is met. Suppose the algorithm converges with u^*, v^*, then $\phi^* = \varepsilon \log u^*, \psi^* = \varepsilon \log v^*$. The transport matrix T^* is:

$$T_{ij}^* = u_i^* K_{ij} v_j^*.$$

Moreover, the gradient of the unbalanced optimal transport distance is:

$$\nabla_{f_i} W_{2,\varepsilon,\varepsilon_m}^2(f, g) = -\varepsilon_m \left(\exp\left(-\frac{\phi_i^*}{\varepsilon_m}\right) - 1\right).$$

Normalization methods

For discrete signal $f \in \mathbb{R}^N$, define normalization function $h: \mathbb{R}^N \to \mathbb{R}_+^N$.

Two normalization methods are studied:

- Linear normalization: $h_{linear,k}(f) = f + k$.
- Exponential normalization: $h_{exp,k}(f) = \exp(kf)$.

Here k is the normalization coefficient.

Formulation of full waveform inversion

Let the spatial domain Ω large enough. The full waveform inversion is a PDE constrained optimization problem. We use the acoustic wave equation with certain boundary condition as the constraint. Suppose there are N_s sources and N_r receivers in the model.

$$\min_c J[c] = \sum_{s=1}^{N_s} \sum_{r=1}^{N_r} W_{2,\varepsilon,\varepsilon_m}^2 \left(h_k\left(d_{s,r}\right), h_k\left(d_{obs,s,r}\right)\right).$$

$$s.t. \ \frac{1}{c^2(x)} \frac{\partial^2}{\partial t^2} u_s(x,t) - \Delta u_s(x,t) = f_s(x,t).$$

$$d_{s,r}(t) = P_r u_s(x,t) = u_s(x_r,t).$$

The gradient is given by the adjoint state method:

$$\nabla J[c](x) = \sum_{s=1}^{N_s} -\frac{2}{c^3(x)} \left(\frac{\partial^2}{\partial t^2} u_s(x,t)\right) v_s(x,t).$$

Here v_s is the adjoint wavefield.

Formulation of full waveform inversion

Adjoint equation:

$$\frac{1}{c^2(x)}\frac{\partial^2}{\partial t^2}v_s(x,t) - \Delta v_s(x,t) = \widetilde{f}_s(x,t).$$

Where $\widetilde{f}_s$ is the adjoint source:

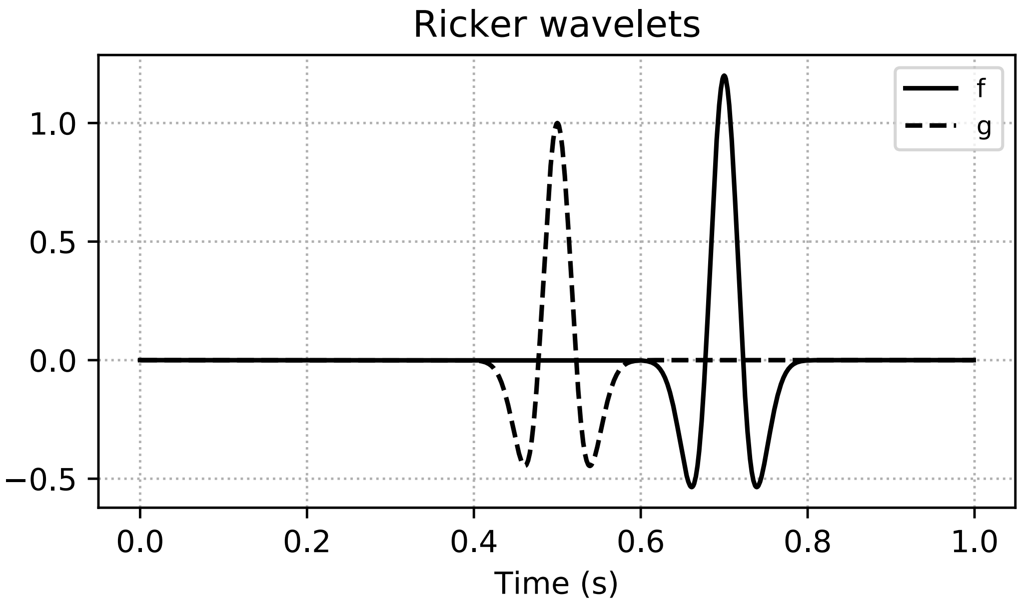
- Linear normalization

$$\widetilde{f}_s = -\sum_{r=1}^{N_r} P_r^T \, \nabla W_{2,\varepsilon,\varepsilon_m}^2 \left(h_k(d_{s,r}), h_k(d_{obs,s,r})\right).$$

- Exponential normalization:

$$\widetilde{f}_s = -\sum_{r=1}^{N_r} P_r^T \left(k e^{k d_{s,r}}\right)^T \nabla W_{2,\varepsilon,\varepsilon_m}^2 \left(h_k(d_{s,r}), h_k(d_{obs,s,r})\right).$$

Numerical example 1

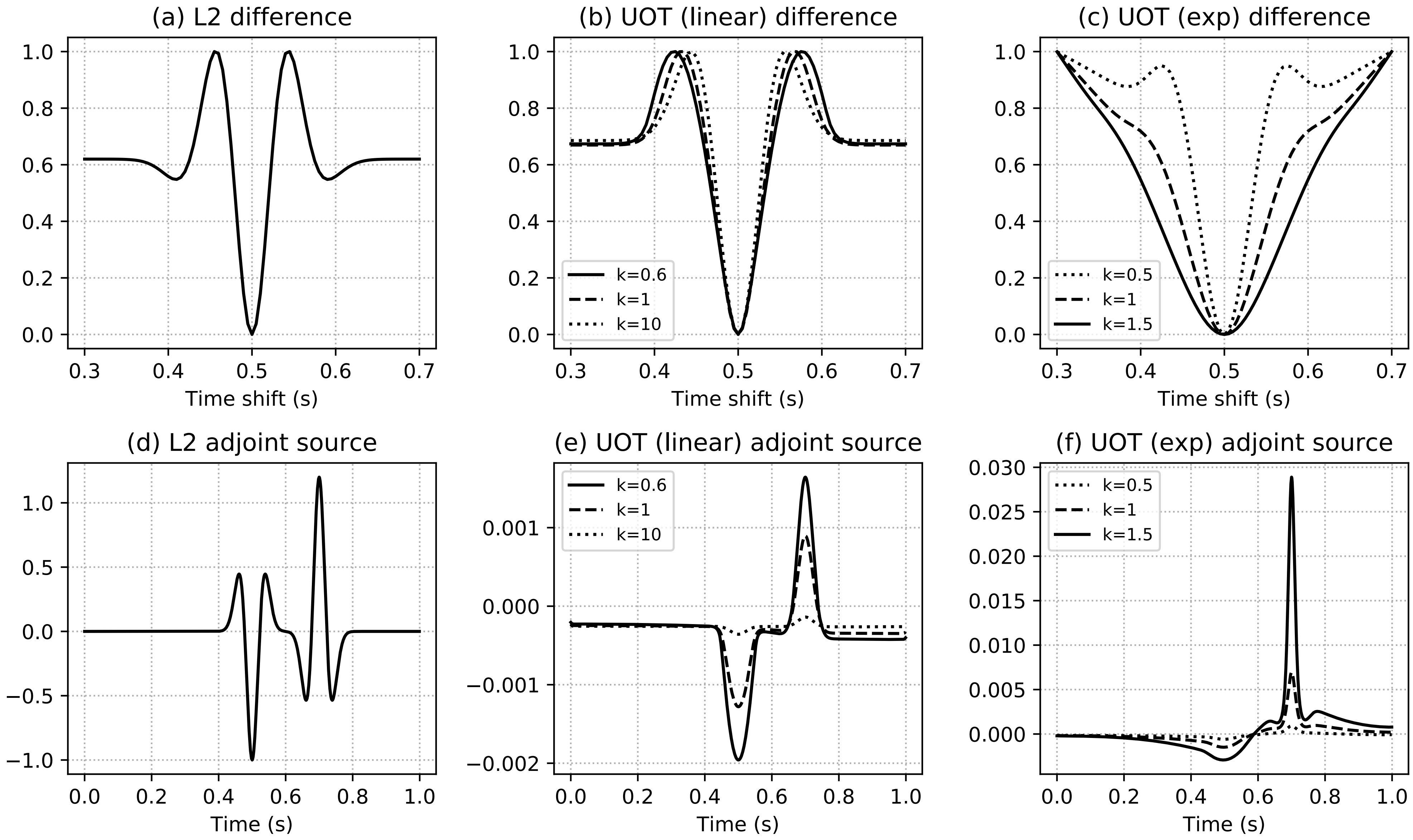


- Two 10 Hz Ricker wavelets f and g. The amplitude of f is 1.2 times of g.
- Define the misfit function:

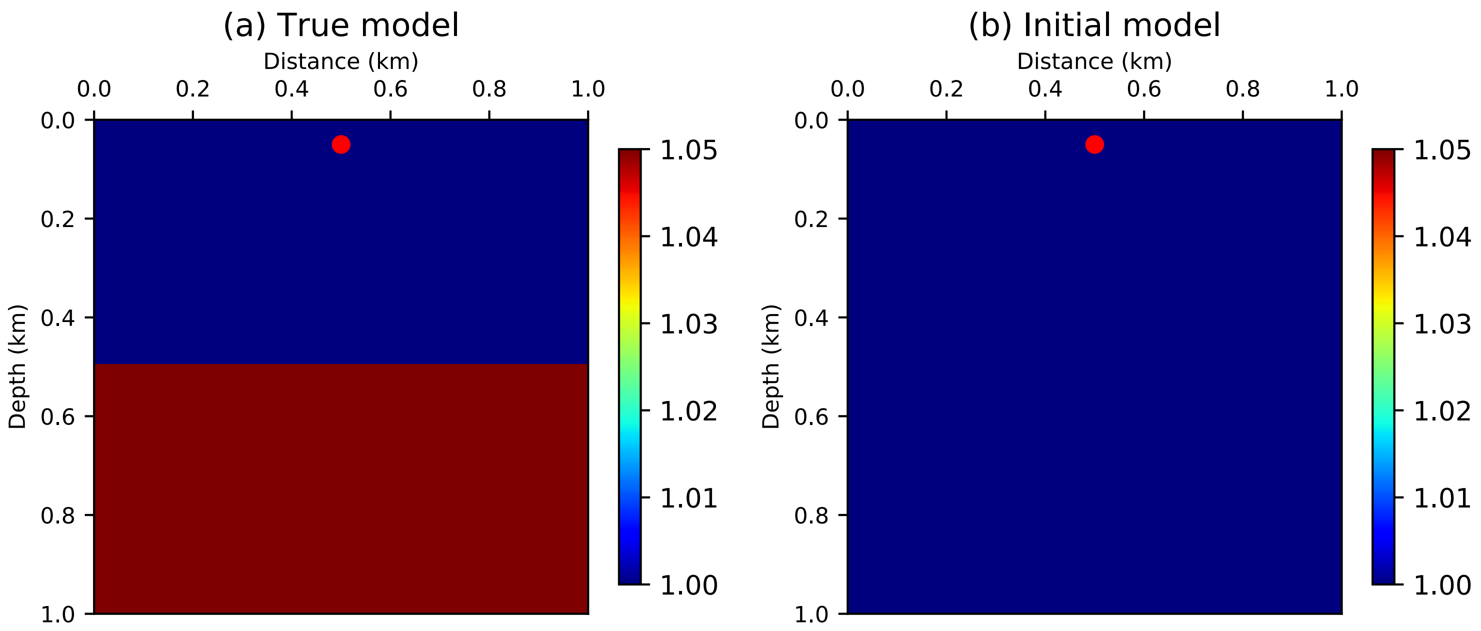
$$J(s) = \mathrm{d}\big(f(t-s), g(t-0.5)\big),$$

Here d is L2 distance, UOT distance with linear and exponential normalization.

Numerical example 1



Numerical example 2

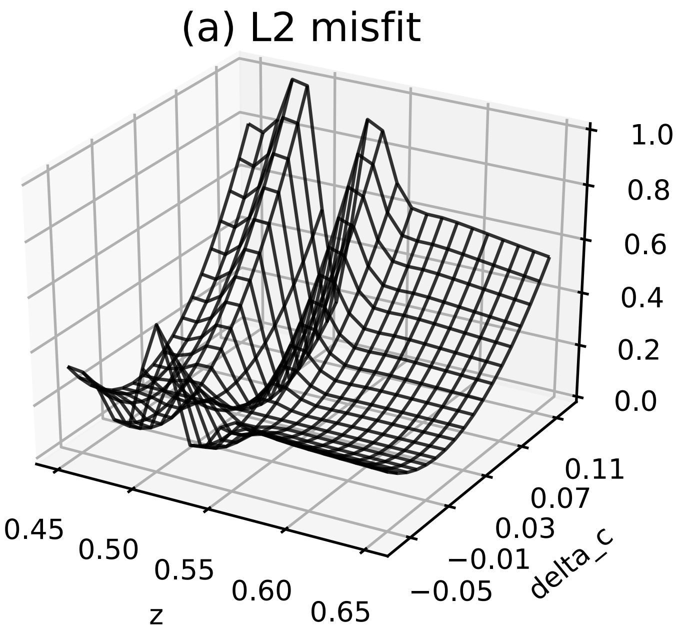


- Velocity model: $c(\delta c, z) = c_0(x, z) + \delta c H(z)$. Here $H(z)$ is the step function. The true model is $c(0.05, 0.51)$ as shown in figure (a).
- Source position are shown as the red spot. There are 51 receivers on the top of the model.
- With homogeneous initial model (b), we compute the misfit function:

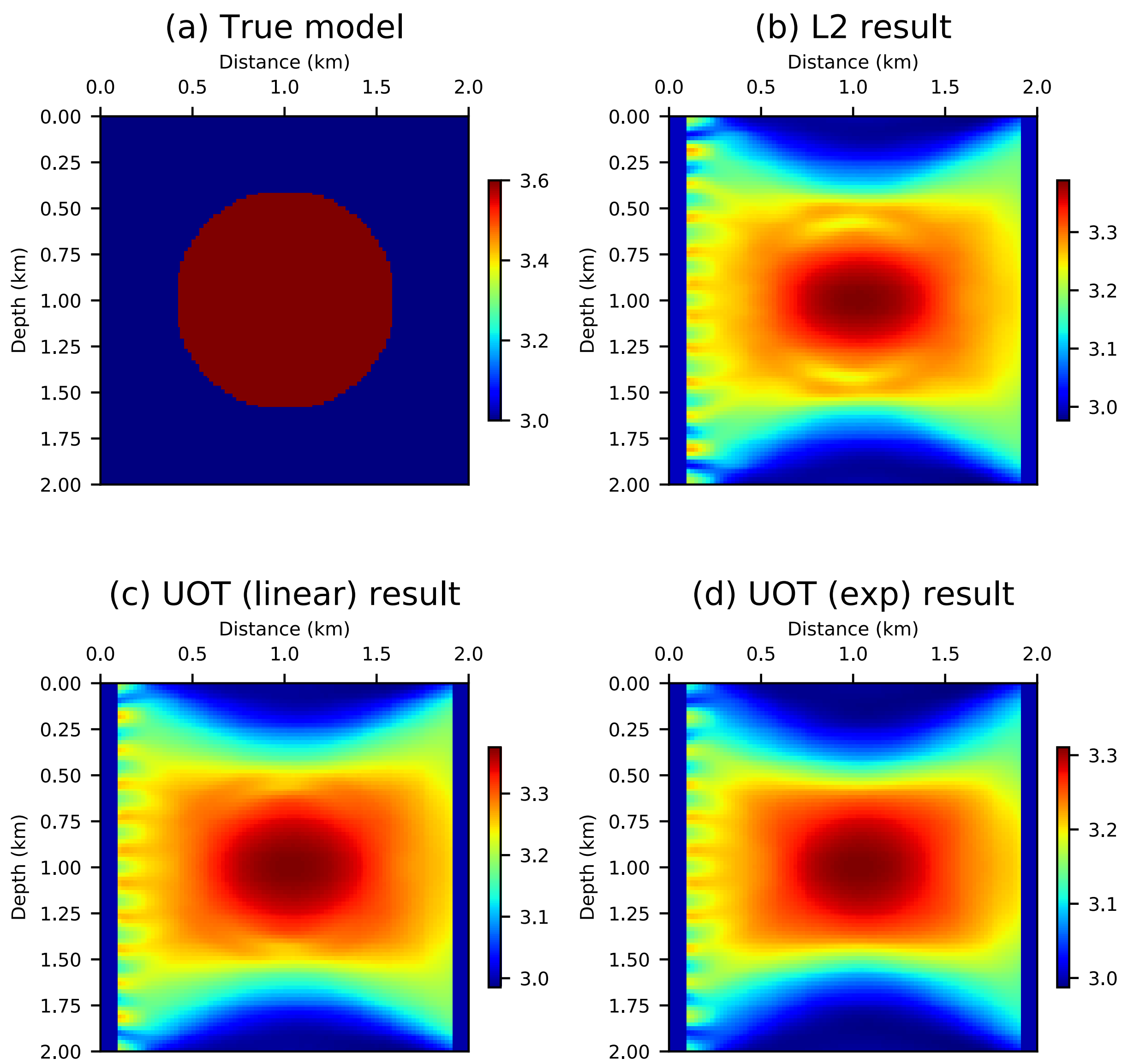
$$\hat{J}(\delta c, z) = J[c(\delta c, z)],$$

where J is the misfit function of FWI problem with L2 distance or UOT distance.

Numerical example 2

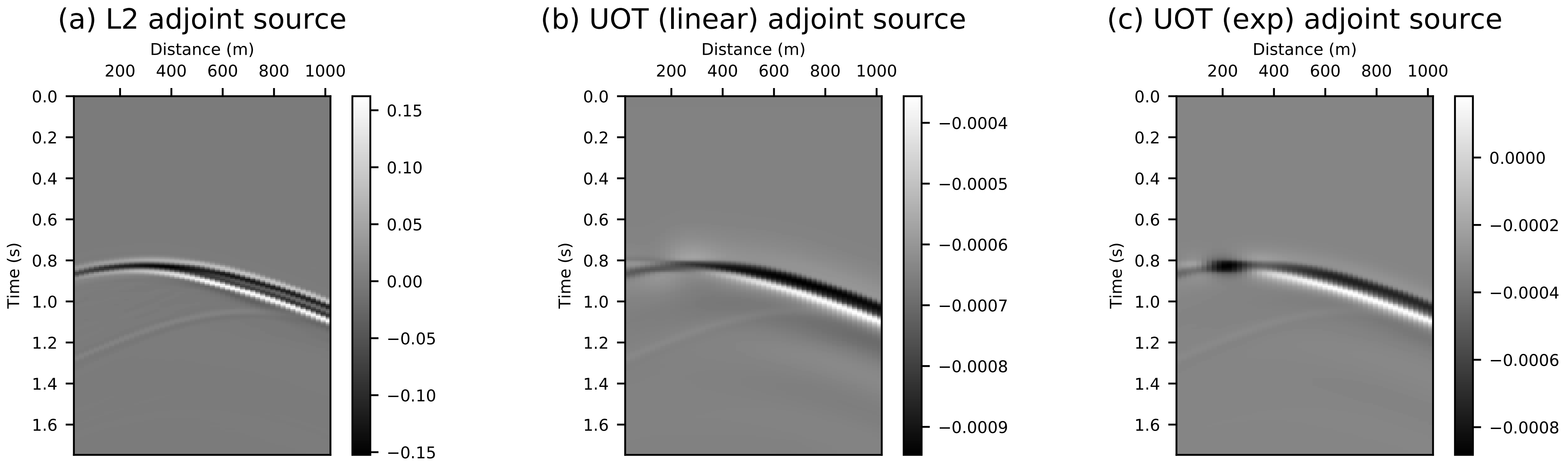


Numerical example 3



- 11 sources with 10 Hz Ricker wavelet on the left-hand side and 101 receivers on the right-hand side.
- Gradient descent method after 5 iterations.

Numerical example 3



Conclusions and future works

Conclusions:
- Comparing to L2 distance, optimal transport distance has better result with respect to time shift.
- The optimal transport distance provides smooth gradient comparing to L2 distance.

Future works:
- How to choose the parameters of optimal transport efficiently.
- Mathematical results on how the optimal transport distance mitigate the cycle-skipping issue.
- More realistic numerical experiments are needed such as Marmousi 2 model or SEG 2014 benchmark data.

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Main references

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