

Framework of the hybrid Bayesian analytical inversion coupled with simulated annealing optimization

Bayesian analysis

Input: Jacobian matrix $\mathbf{K}$, prior error covariance $\mathbf{S}_A$, observational error covariance $\mathbf{S}_O$ (including TROPOMI and existing ground-based observations)

Compute the posterior error covariance
$$\hat{\mathbf{S}} = (\gamma \mathbf{K}^T \mathbf{S}_O^{-1} \mathbf{K} + \mathbf{S}_A^{-1})^{-1}$$

Calculate the degrees of freedom for signal in China as the objective function
$$\text{DOFS} = \text{tr}(\mathbf{I} - \hat{\mathbf{S}} \mathbf{S}_A^{-1})$$

Simulated annealing process

Initialize with a current solution s_0 ,
a starting temperature $T = T_0$

Choose a random neighbor s' of s_k

Evaluate the objective function
difference $\Delta E = \mathcal{C}(s') - \mathcal{C}(s_k)$

If $\Delta E \geq 0$, then replace s_k by s' ;
Otherwise, replace s_k by s' with
probability $\exp(\Delta E / T)$

Replace T by a smaller number
(e.g. $T_{k+1} = \alpha T, \alpha = 0.85$)

No

$T < T_f?$

Yes

Output

Initialize
parameters

Solution
perturbation

Energy
evaluation

Metropolis
acceptance

Cooling
schedule

Check
termination

Output

Optimal ground
monitoring station
locations

Maximized DOFS
values