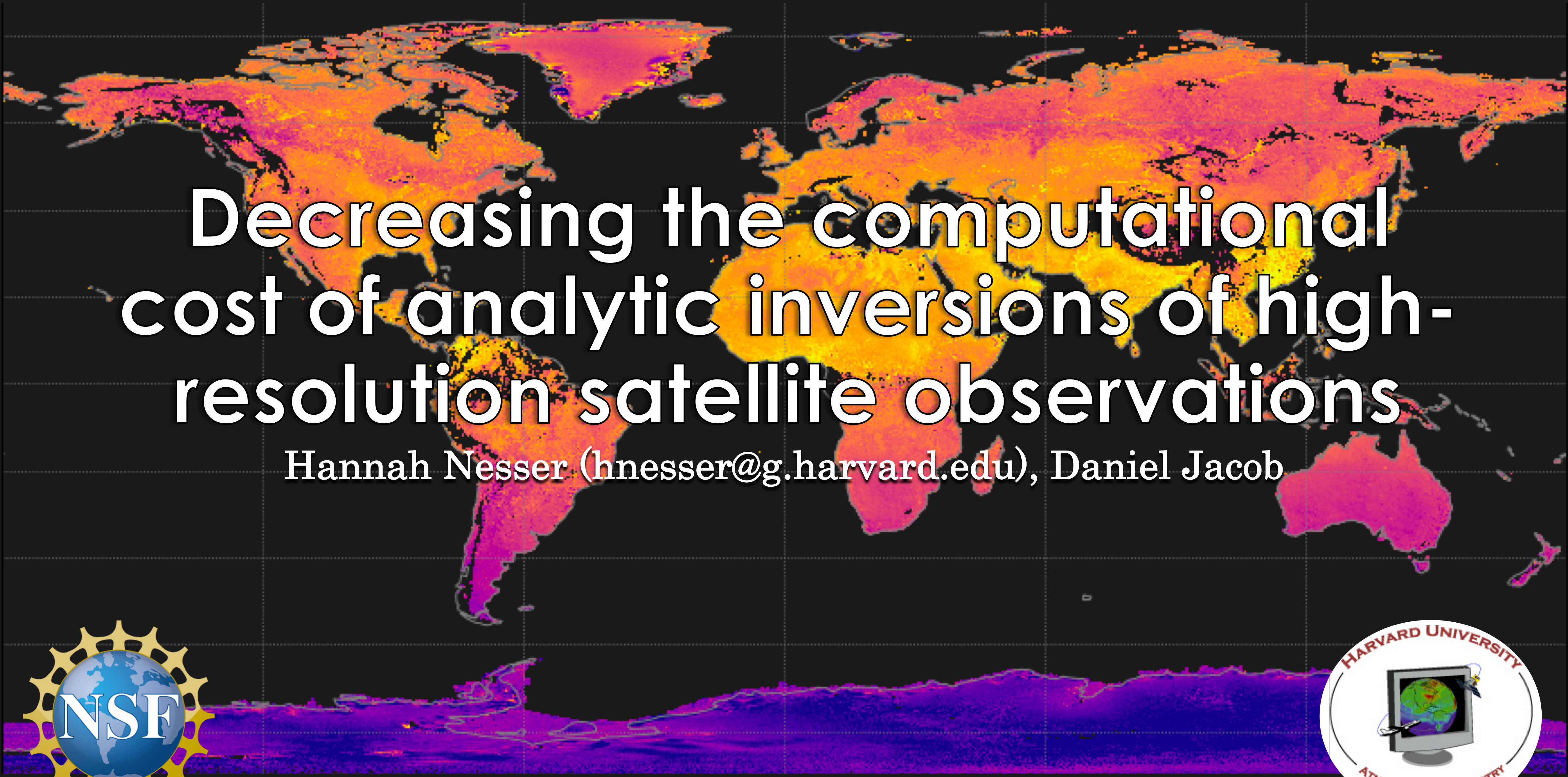


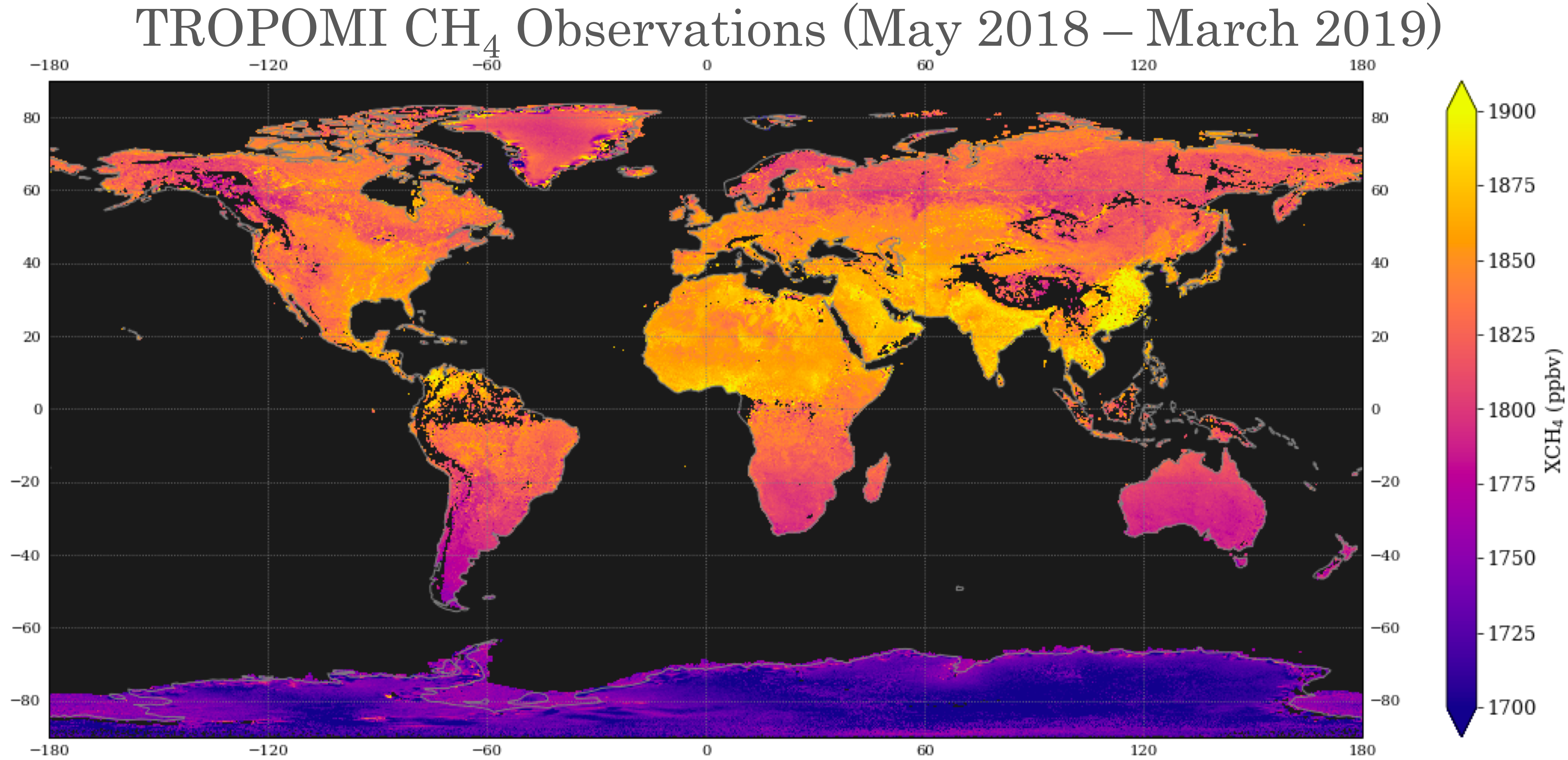
Decreasing the computational cost of analytic inversions of high-resolution satellite observations

Hannah Nesser (hnesser@g.harvard.edu), Daniel Jacob

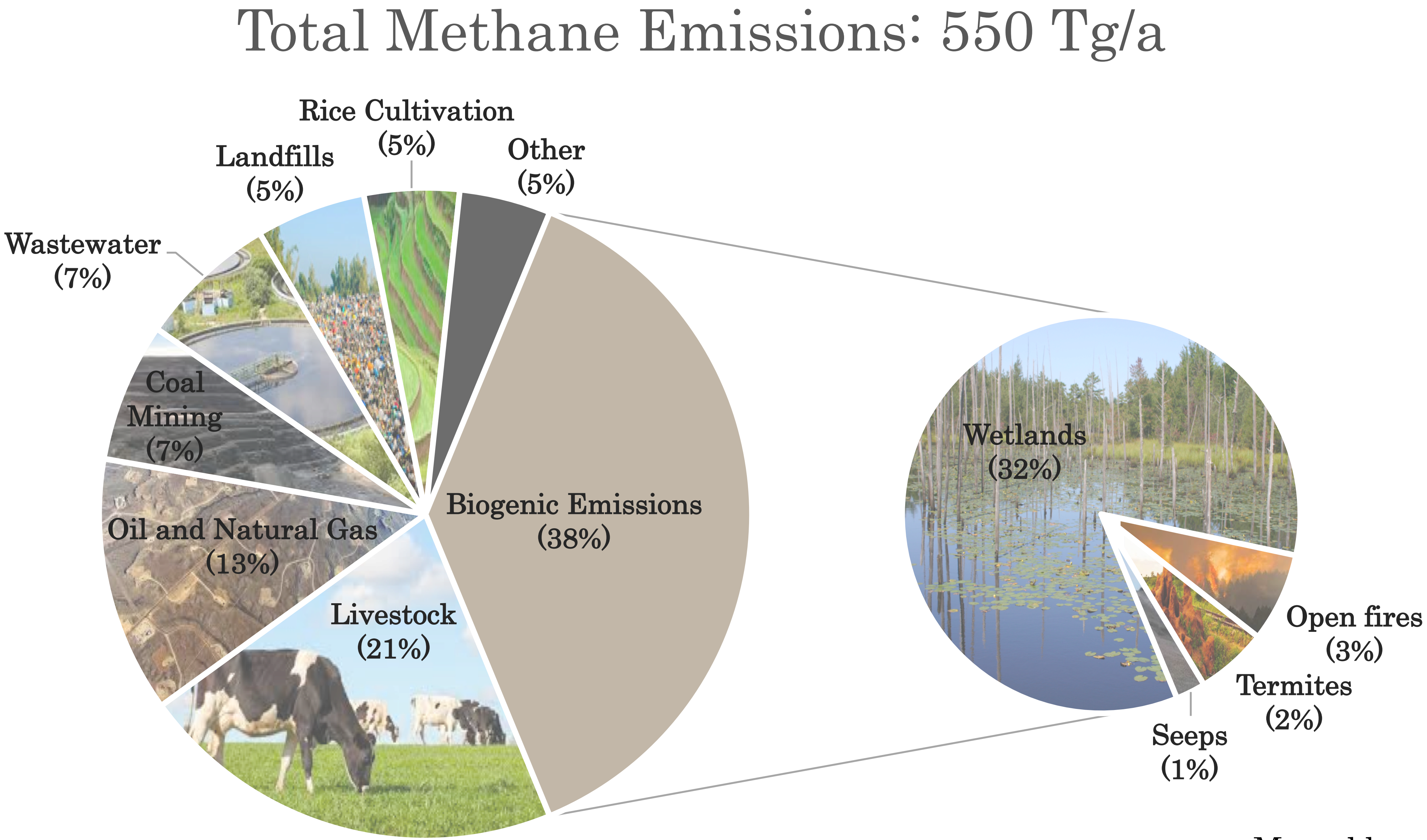
NSF

Harvard University
Atmospheric Chemistry Modeling Group

TROPOMI methane observations provide a unique opportunity to improve constraints on emission estimates

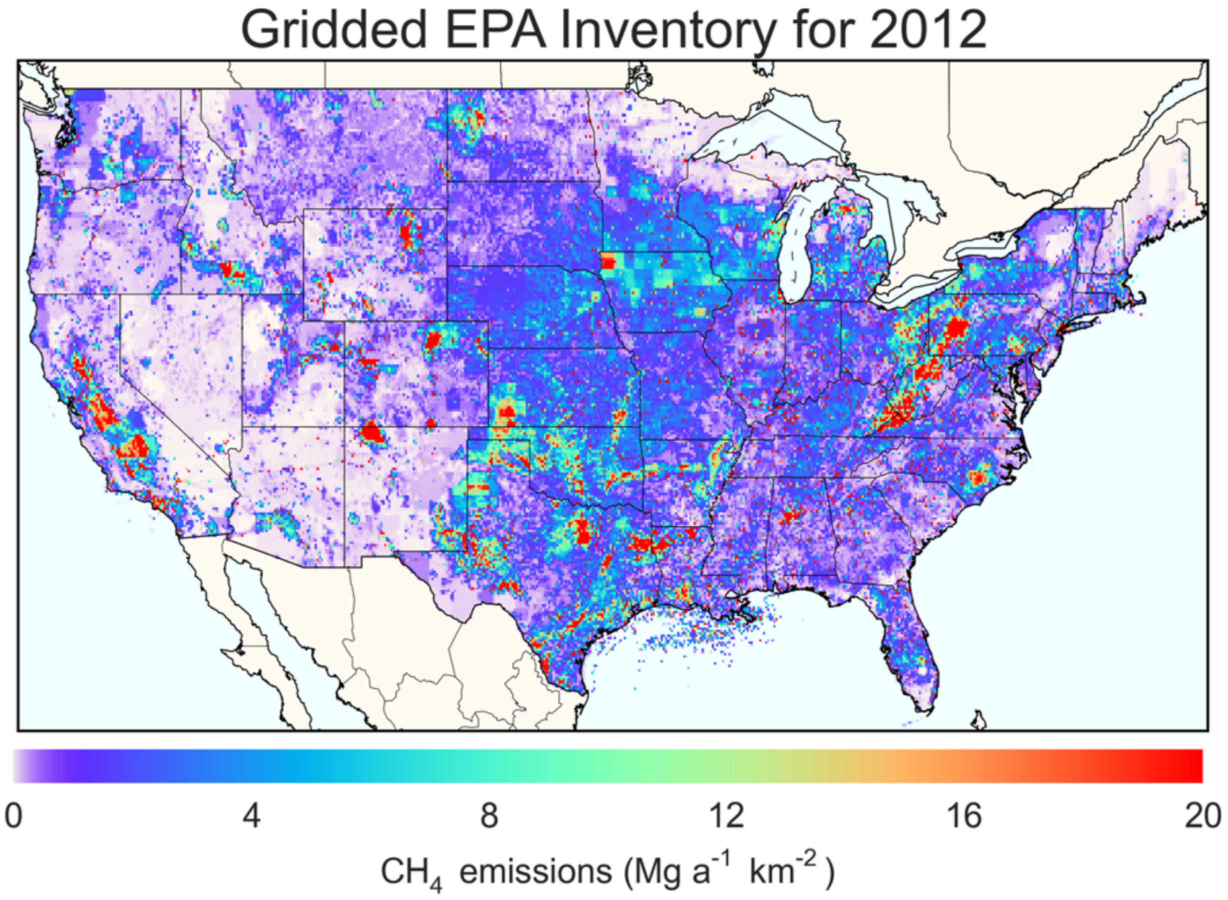


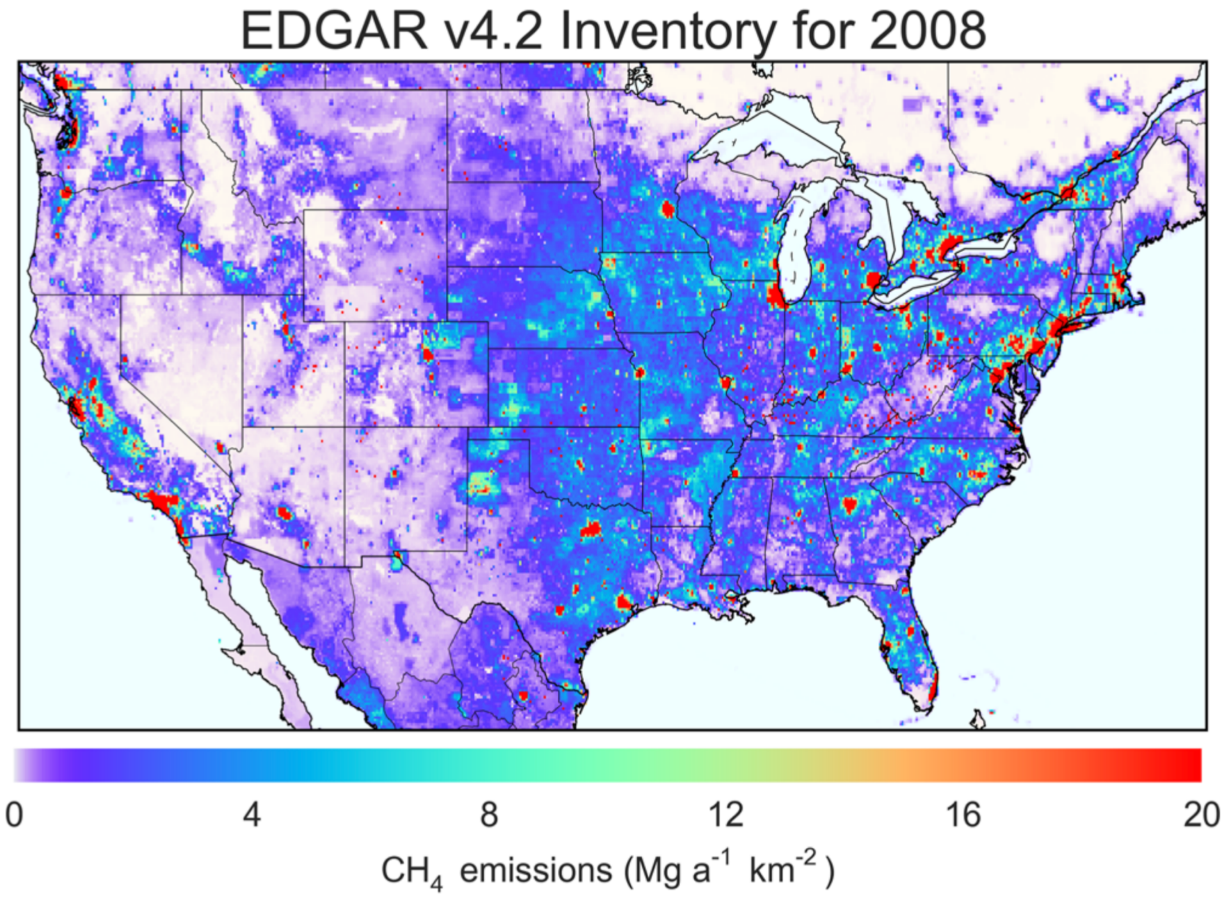
The spatial and temporal distribution of methane emissions is uncertain



Maasakkers et al. (2019)

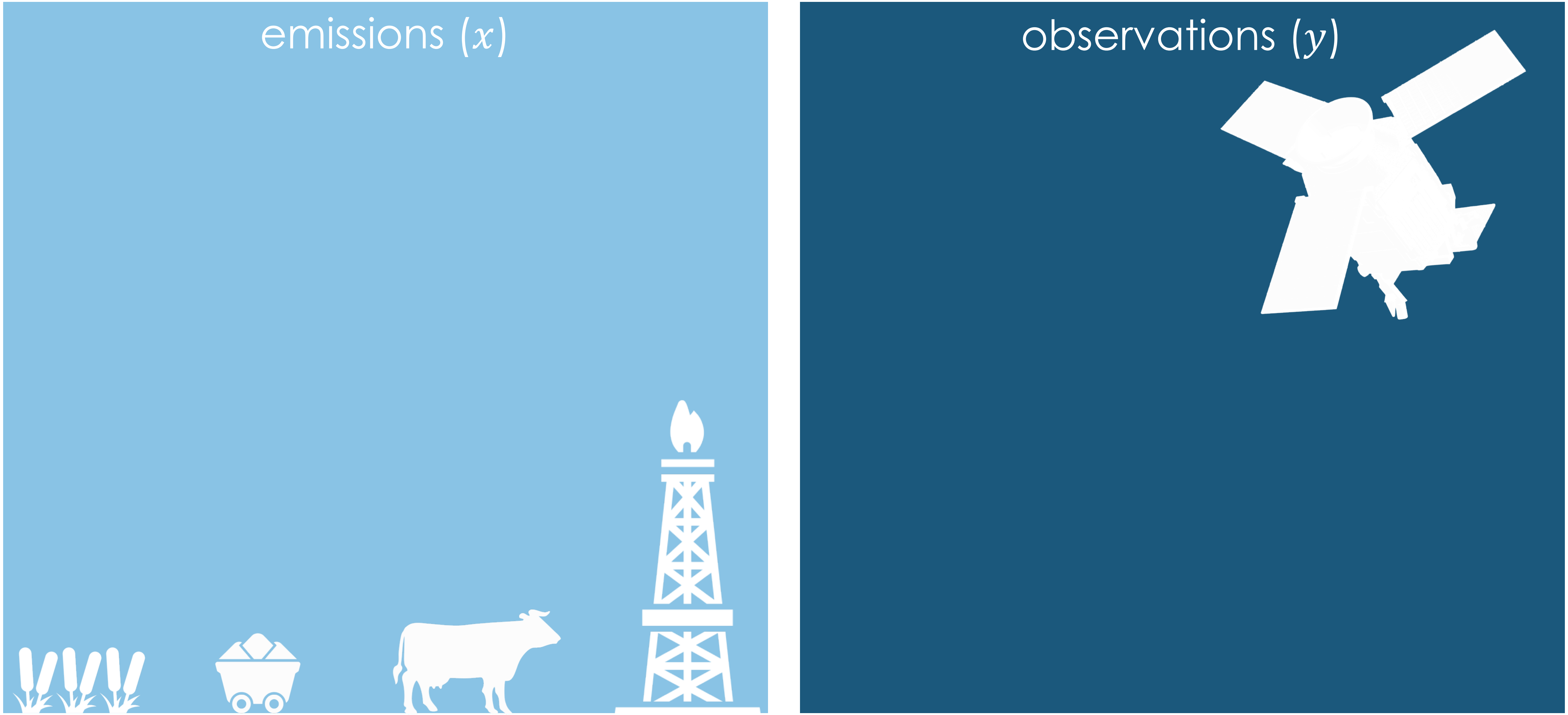
Significant errors exist in prior emission inventories



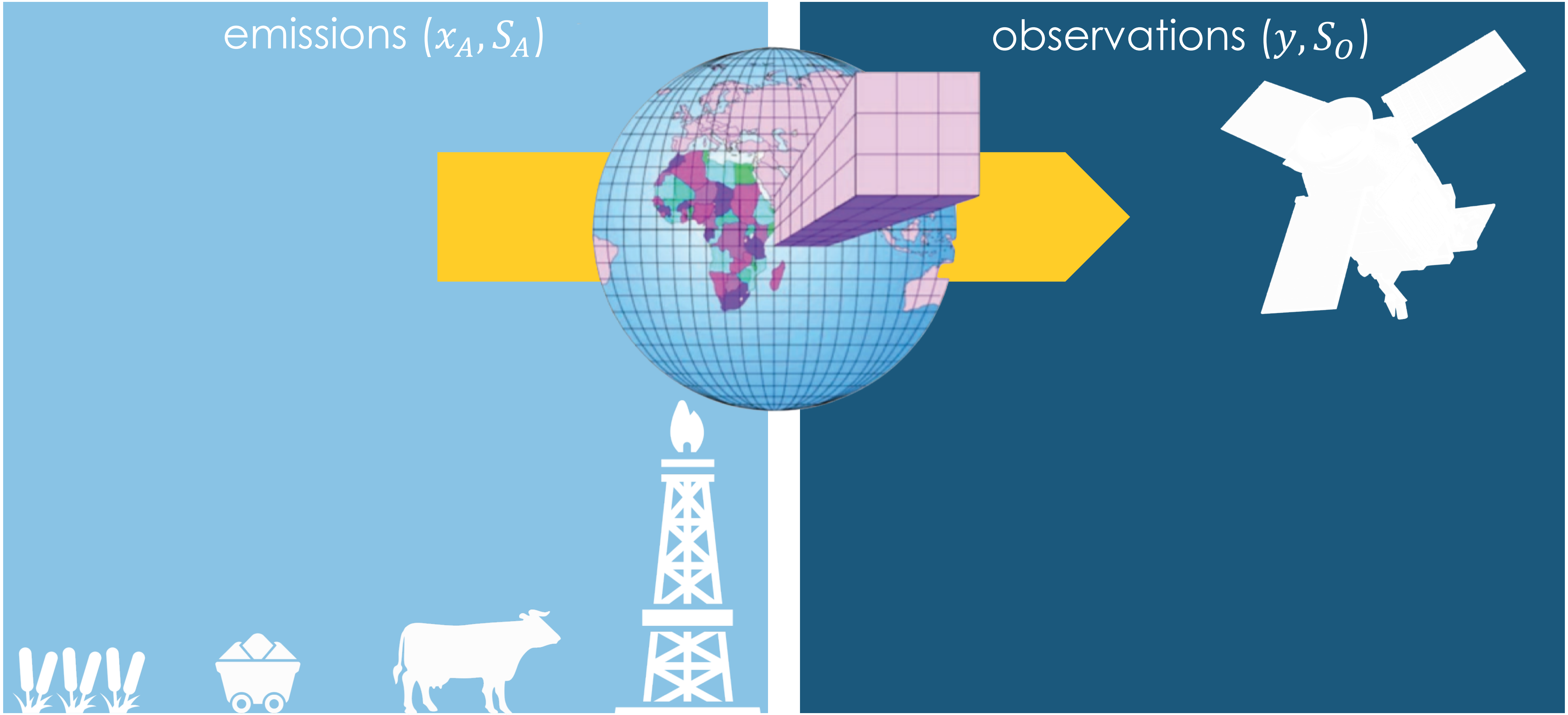


Maasakkers et al. (2016)

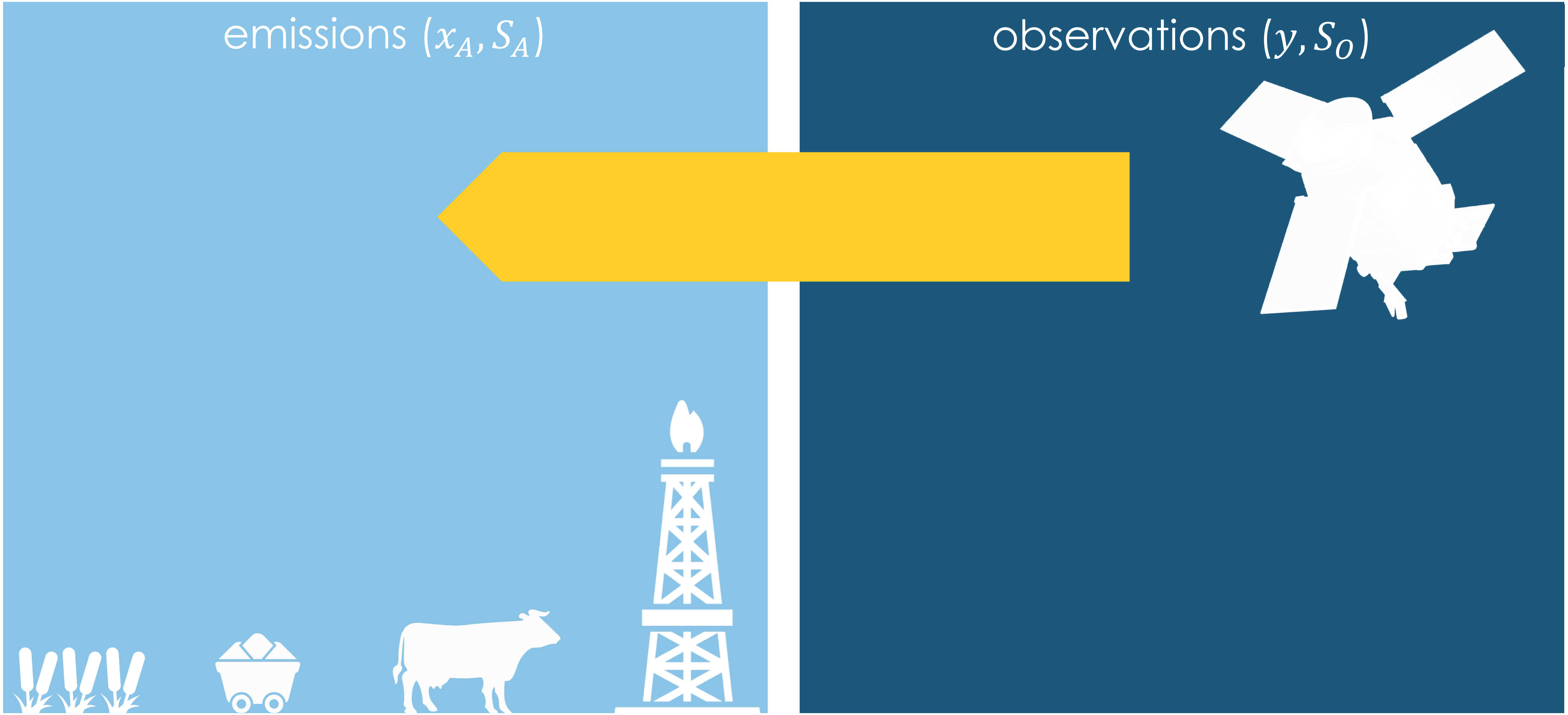
Observations of methane reflect emissions, atmospheric transport, and atmospheric chemistry



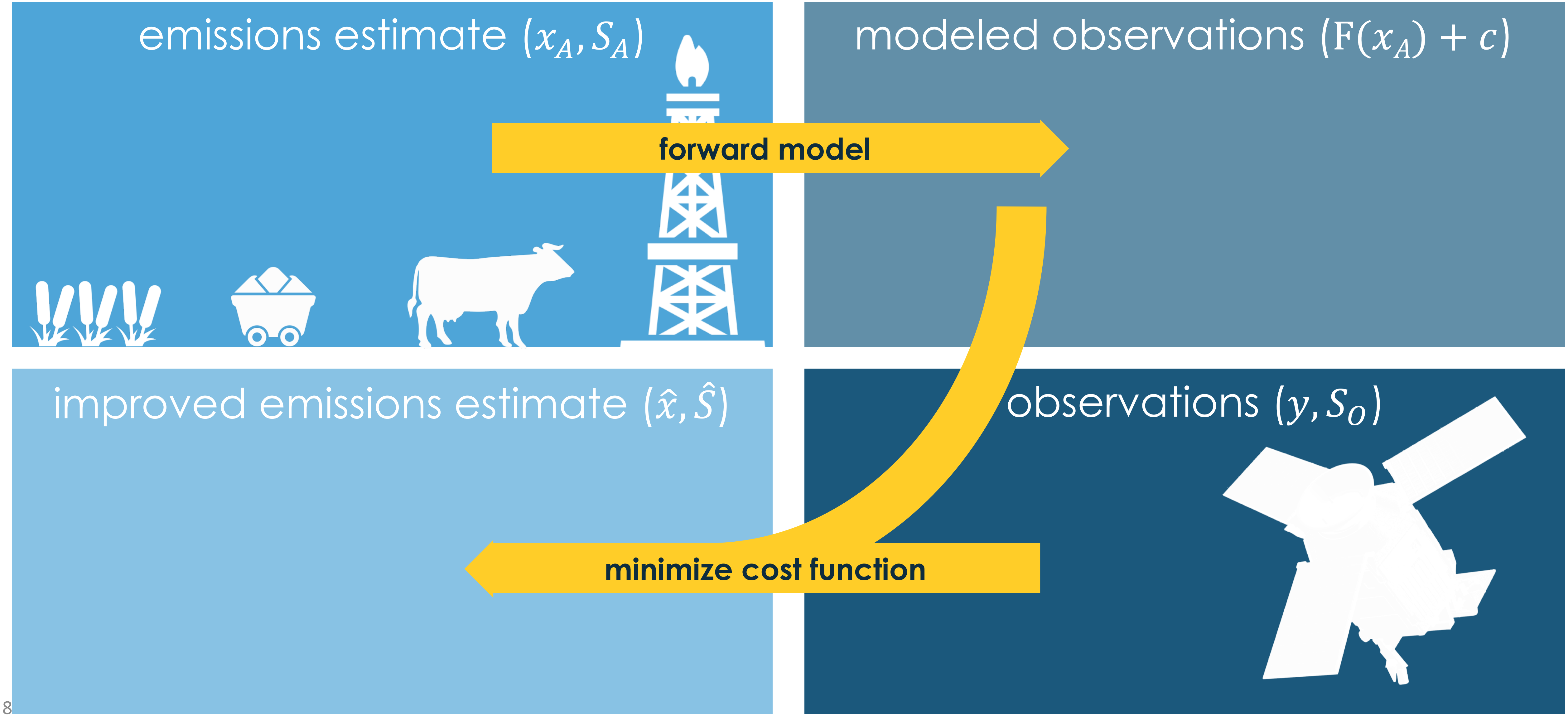
Forward models replicate transport and chemistry to describe the dependence of observations on estimated emissions



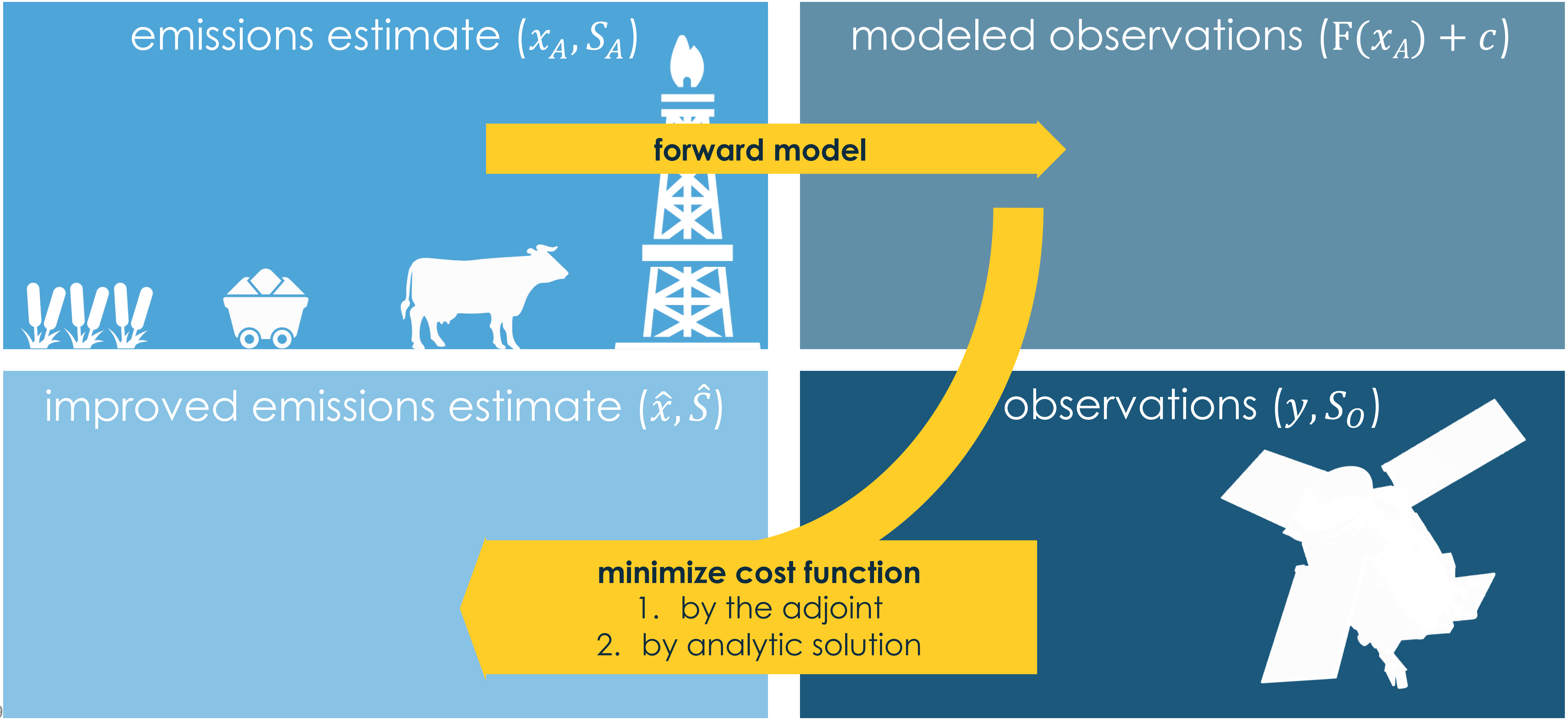
Inversions describe the dependence of emissions on observations



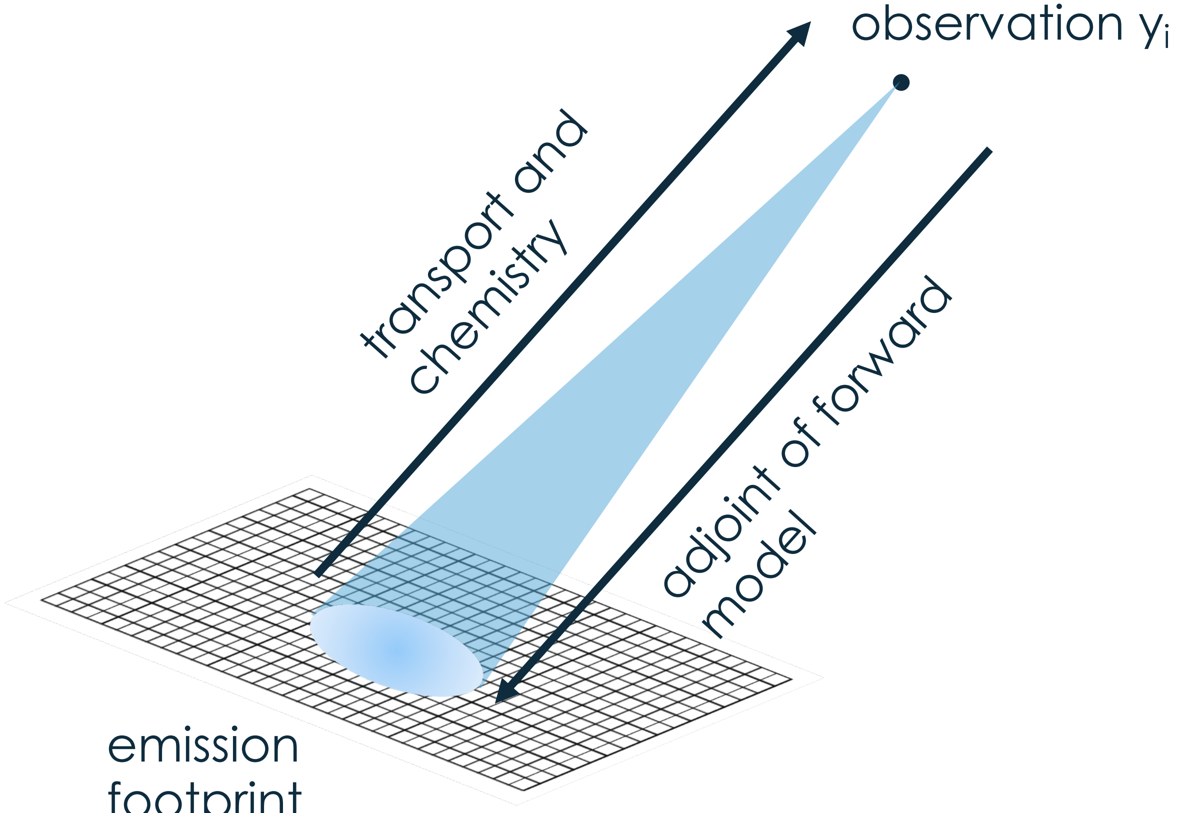
A Bayesian inversion accounts for these errors by maximizing the probability of the emissions given the observations



A Bayesian inversion accounts for these errors by maximizing the probability of the emissions given the observations



While the adjoint efficiently computes the derivative, it does not support analytic solution of errors or extensive sensitivity testing



adjoint solutions do not:

- find the true minimum of the cost function
- provide analytic posterior error
- support extensive sensitivity testing
- reduce adjoint development costs

Source: Brasseur and Jacob

An analytic solution to the cost function minimum exists when the forward model is linear

emissions estimate (x_A, S_A)

forward model

modeled observations $(\mathrm{K}x_A + c)$

observations (y, S_o)

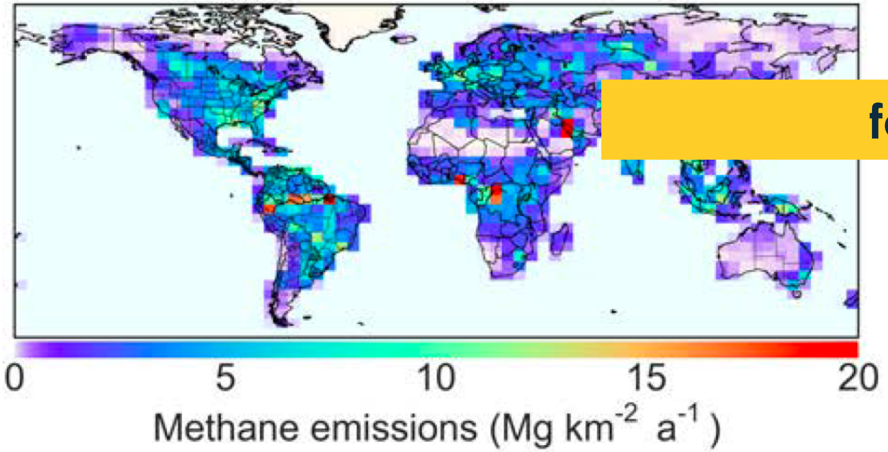
minimize cost function

improved emissions estimate $(\hat{x}, \hat{S})$

- improved emission estimate
  $\hat{x} = x_A + \hat{S}K^T S_O^{-1}(y - (Kx_A + c))$
- improved error estimate
  $\hat{S} = \left(S_A^{-1} + K^T S_O^{-1} K\right)^{-1}$
- information content
  $A = \hat{S}K^T S_O^{-1} K$

Past inversions optimized emissions on a coarse grid, but denser satellite observations support higher resolution inversions

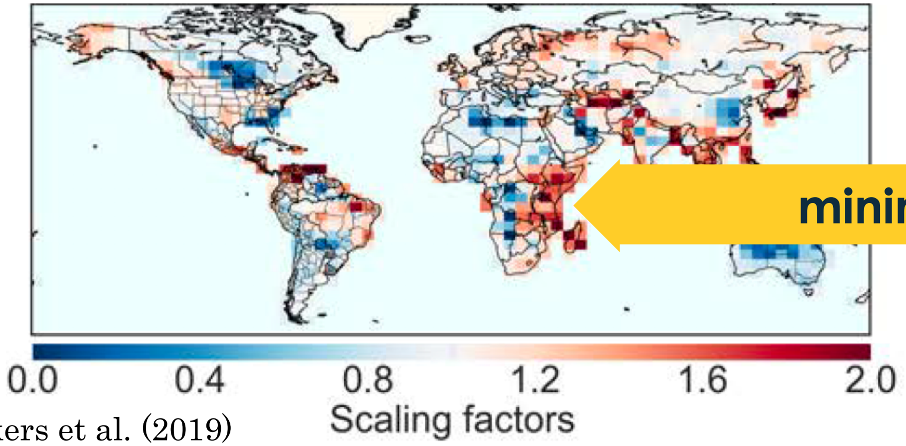
emissions estimate (x_A, S_A)



modeled observations $(\mathrm{K}x_A + c)$

forward model

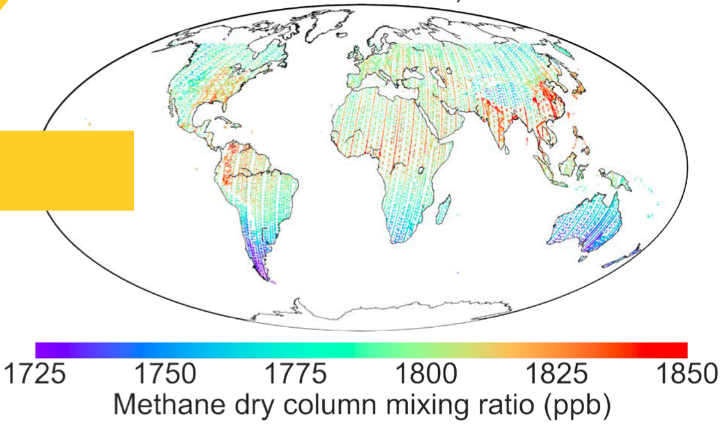
improved emissions estimate $(\hat{x}, \hat{S})$



minimize cost function

observations (y, S_O)

Mean GOSAT methane, 2010-2015



 Maasakkers et al. (2019)

Increasing inversion resolution increases computational cost, which is limited by the number of grid boxes optimized

emissions estimate (x_A, S_A)

forward model

modeled observations $(\boxed{K}x_A + c)$

n+1 model runs

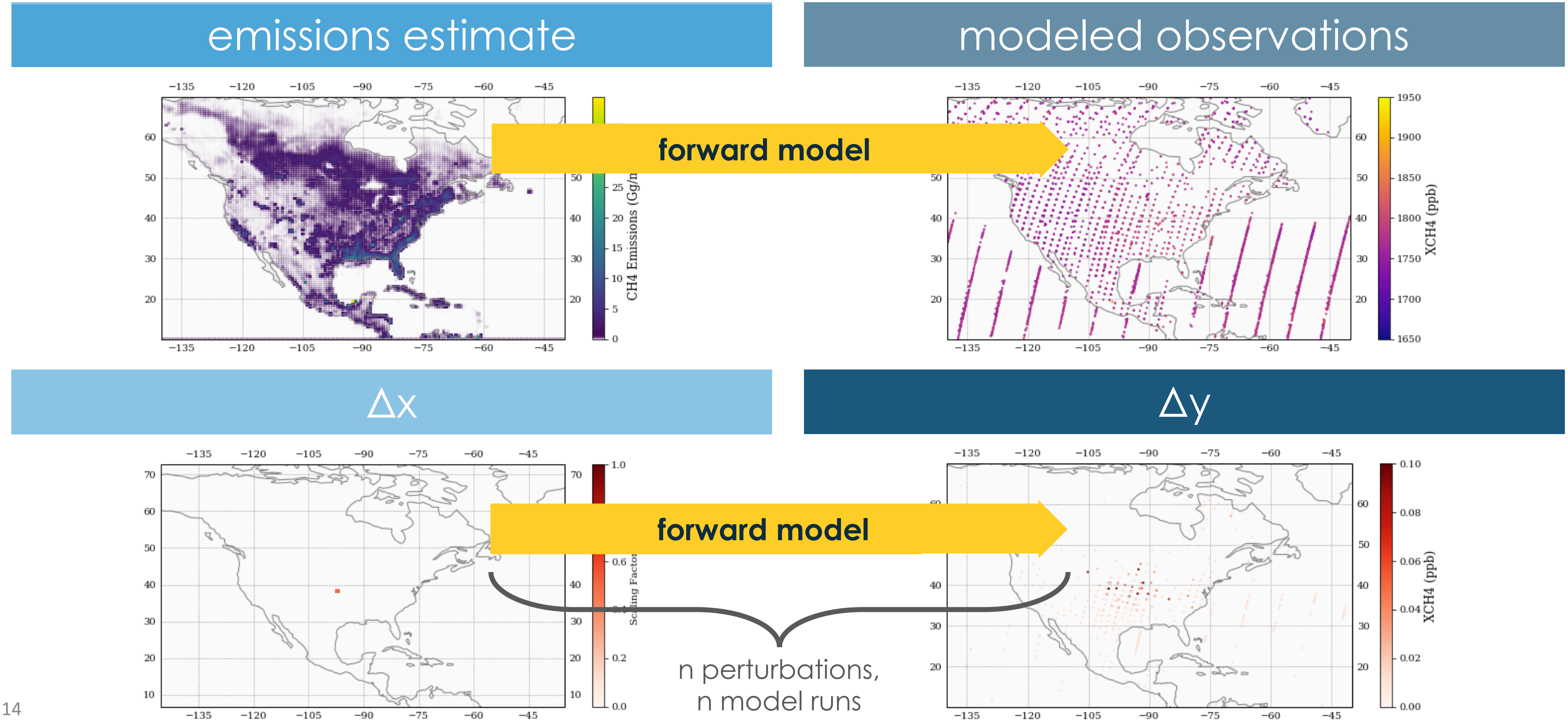
observations (y, S_O)

minimize cost function

optimal emissions estimate $(\hat{x}, \hat{S})$

- optimal emission estimate
  $\hat{x} = x_A + \hat{S}K^T S_O^{-1}(y - (Kx_A + c))$
- optimal error estimate
  $\hat{S} = (S_A^{-1} + K^T S_O^{-1} K)^{-1}$
- information content
  $A = \hat{S}K^T S_O^{-1} K$

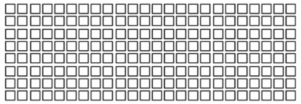
The Jacobian $\mathbf{K}$ represents the sensitivity of observations to emissions: $\mathbf{y} = \mathbf{K}\mathbf{x} + \mathbf{c}$ with $\mathbf{K} = \frac{\partial \mathbf{y}}{\partial \mathbf{x}}$



The computational cost of an analytic Bayesian inversion is limited by the resolution

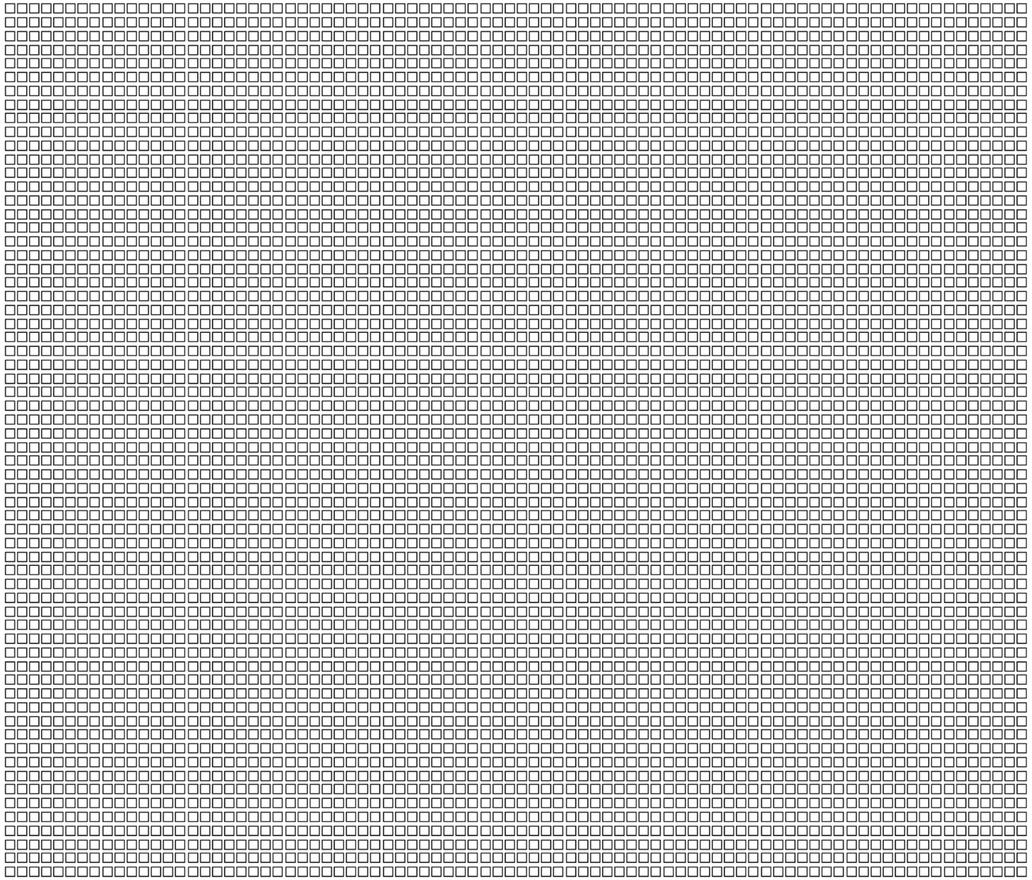
4° x 5 ° : ~16,000 core-hours

1,000 grid cells, 8 cores, 2 hours per simulation-year



2° x 2.5 ° : ~3,000,000 core-hours

4,000 grid cells, 32 cores, 24 hours per simulation-year



1° x 1.25 ° : ~86,000,000 core-hours

16,000 grid cells, 32 cores, 7 days per simulation-year

How can analytic inversions:

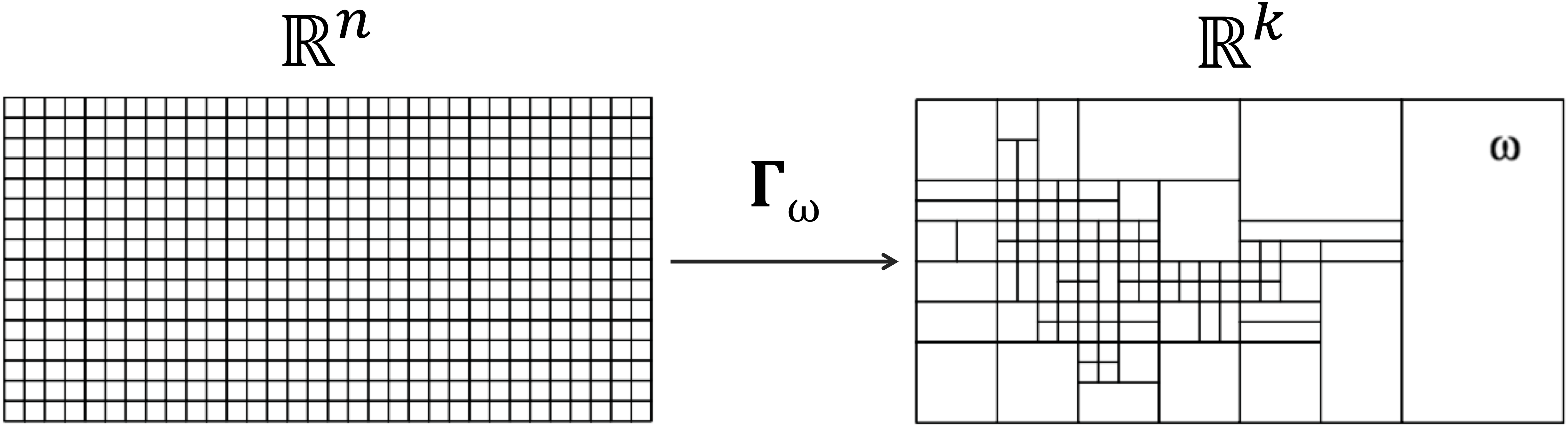
i. increase resolution;
ii. minimize computational cost;
iii. and maintain information content?

Reduced-Rank Jacobian Construction

I. Reduced-rank inversions
(Bousserez et al. 2018)

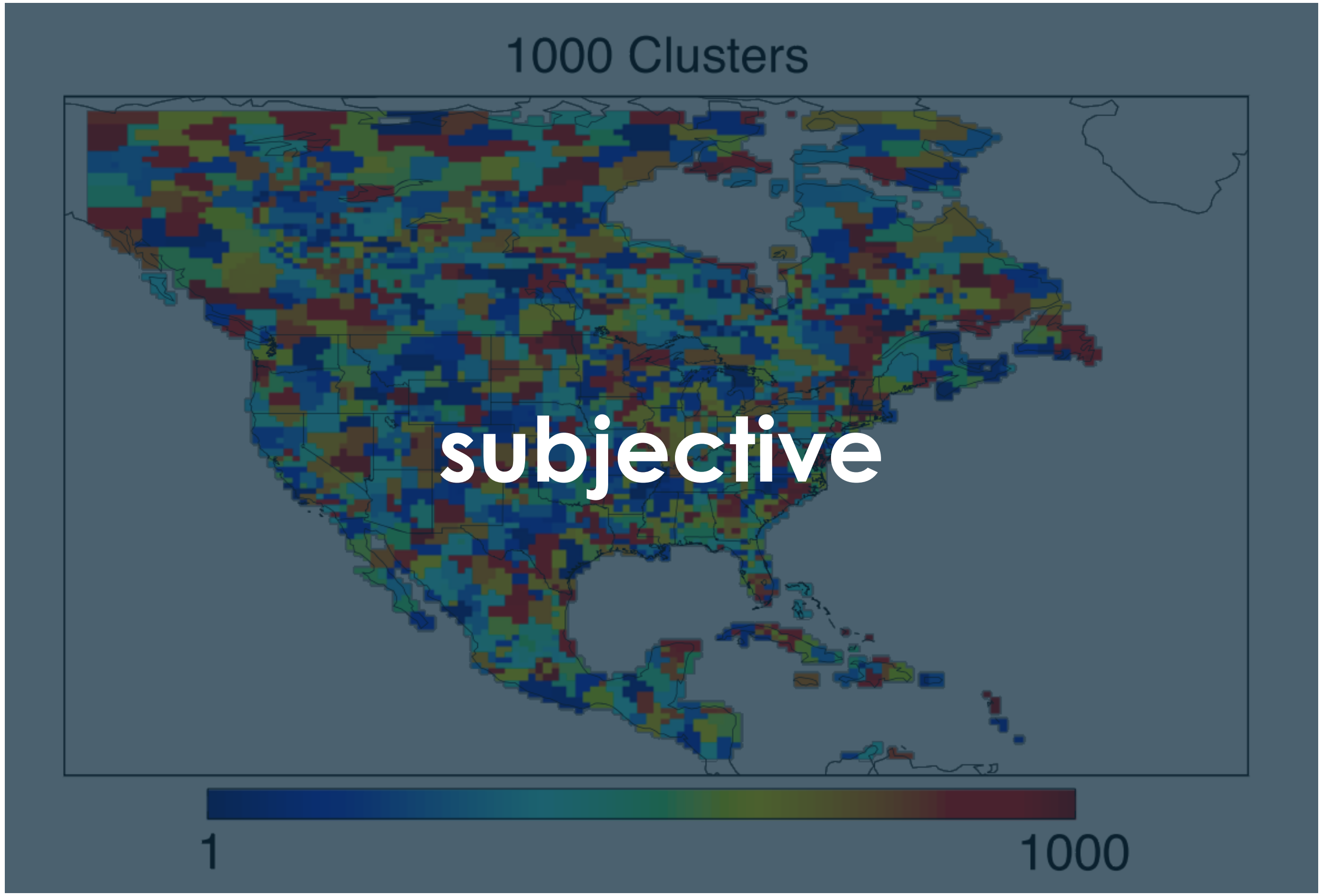
II. Reduced-rank Jacobians

Reducing the dimension of the state space from n to p << n can reduce the computational cost of an analytic inversion



Bocquet et al. (2011)

There are multiple methods of discretely clustering grid cells to reduce the state space dimension

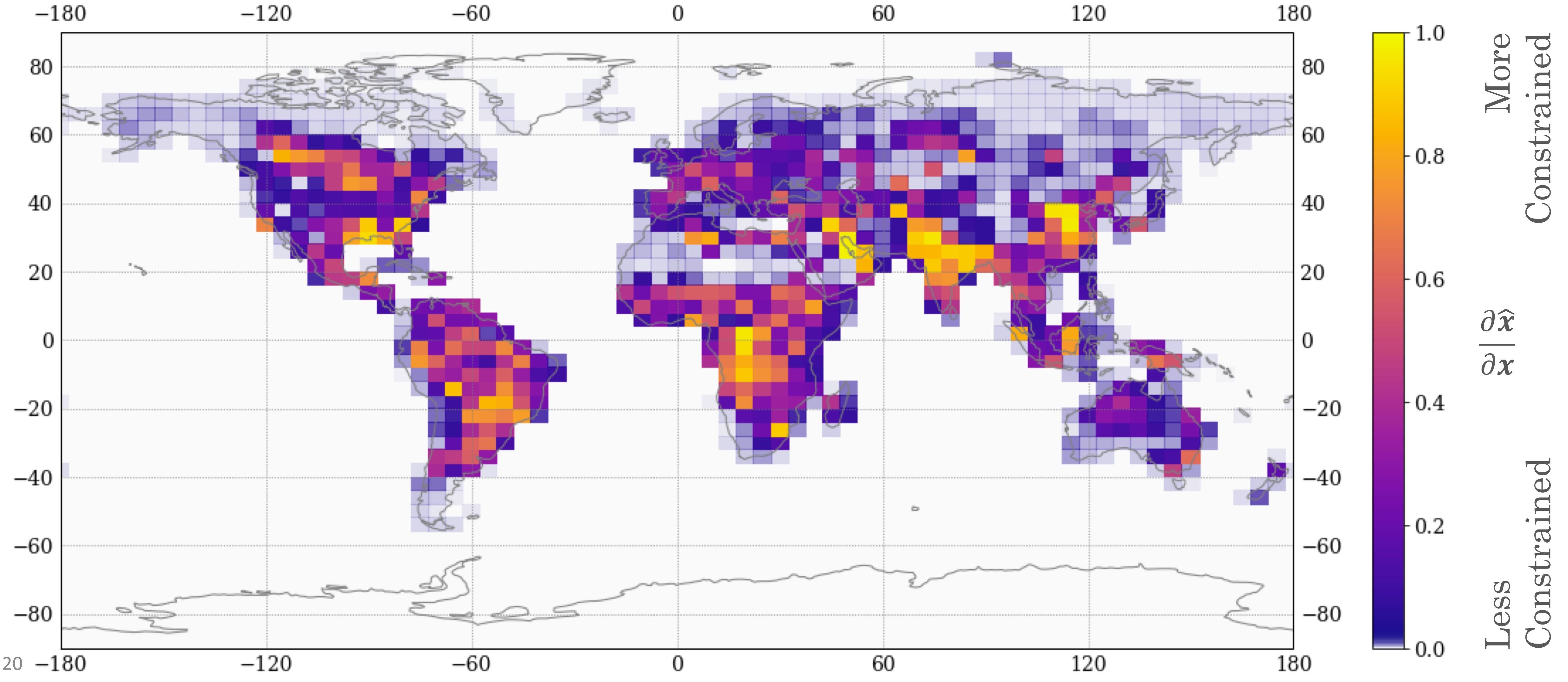


Wecht et al. (2014)

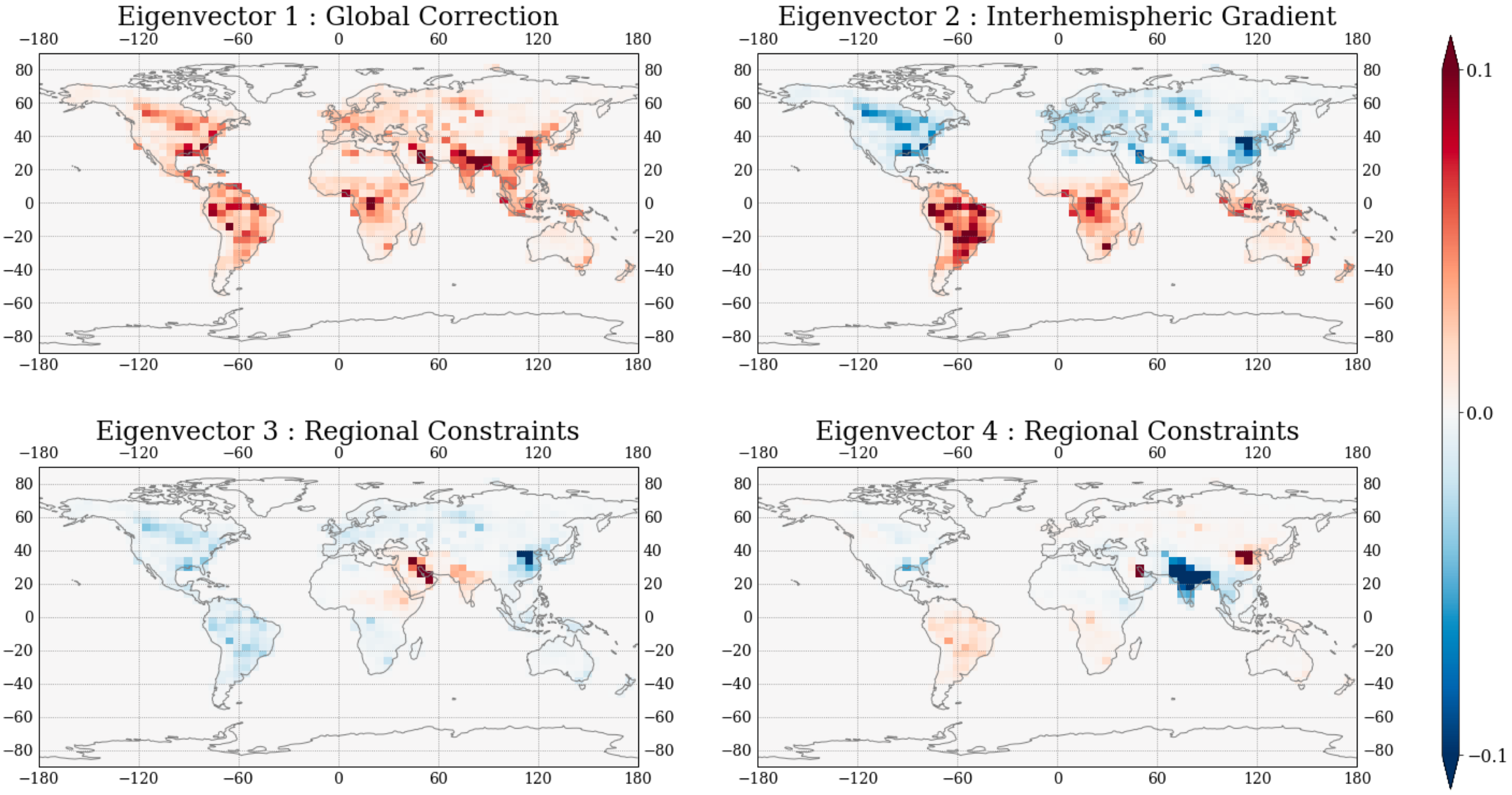
Bocquet et al. (2011)

Known information about the emission-observation system can be used to find an optimal clustering analytically

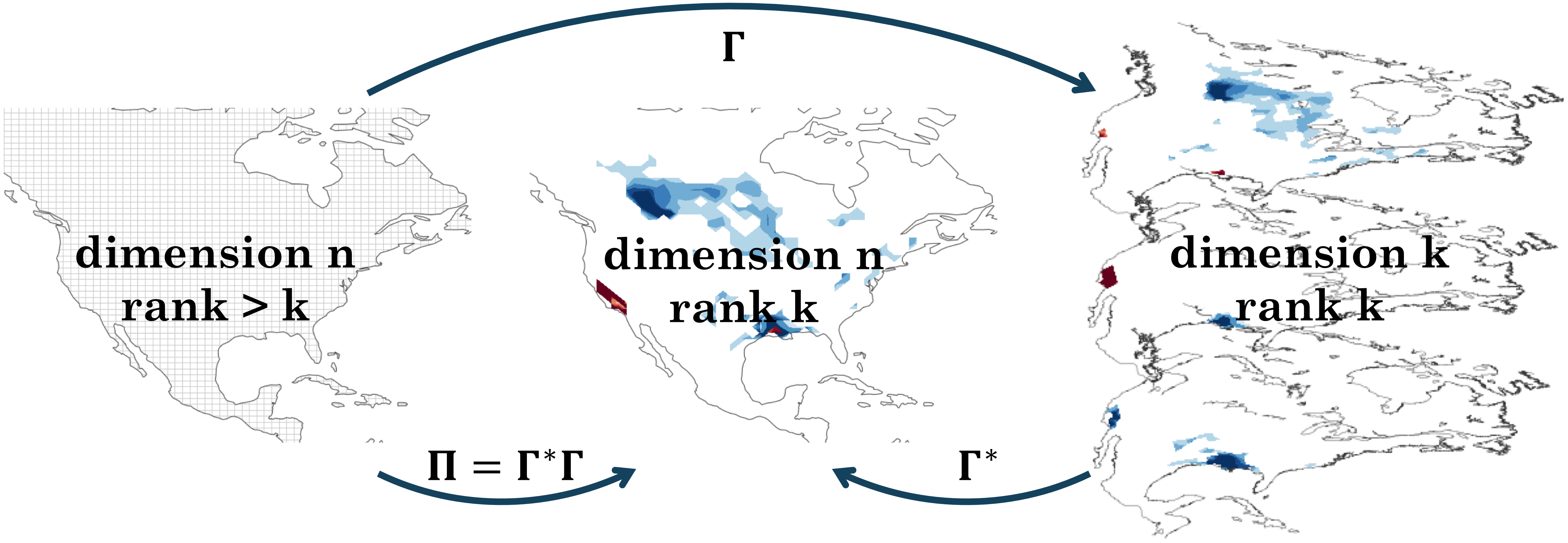
$$\text{Averaging Kernel}: \mathbf{A} = \frac{\partial \hat{\boldsymbol{x}}}{\partial \boldsymbol{x}} = f(\mathbf{S_A}, \mathbf{S_O}, \mathbf{K})$$



An eigendecomposition of $\cancel{A\ Q_{DOF}}\ H_P$ gives the patterns of information in the emission-observation system

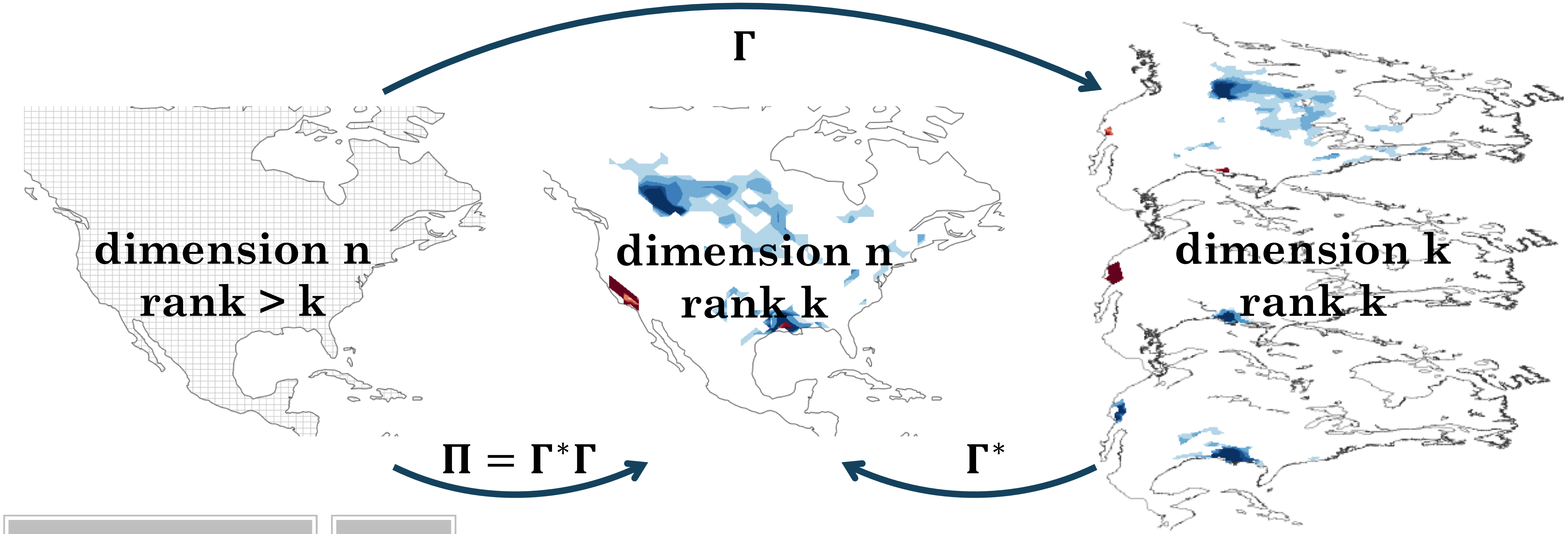


The inversion can be solved in the directions given by the eigenvectors in a reduced-dimension or reduced-rank space



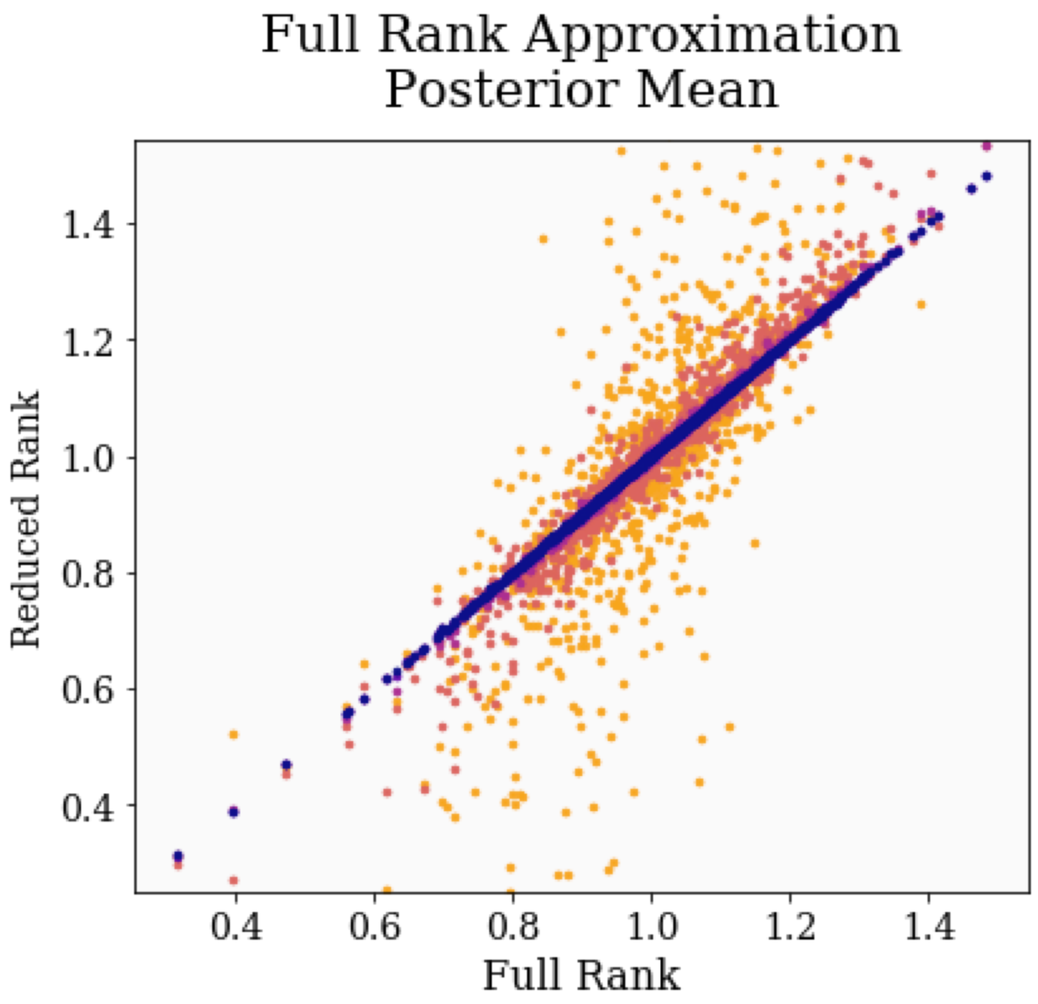
The inversion can be solved in the directions given by the eigenvectors in a reduced-dimension or reduced-rank space

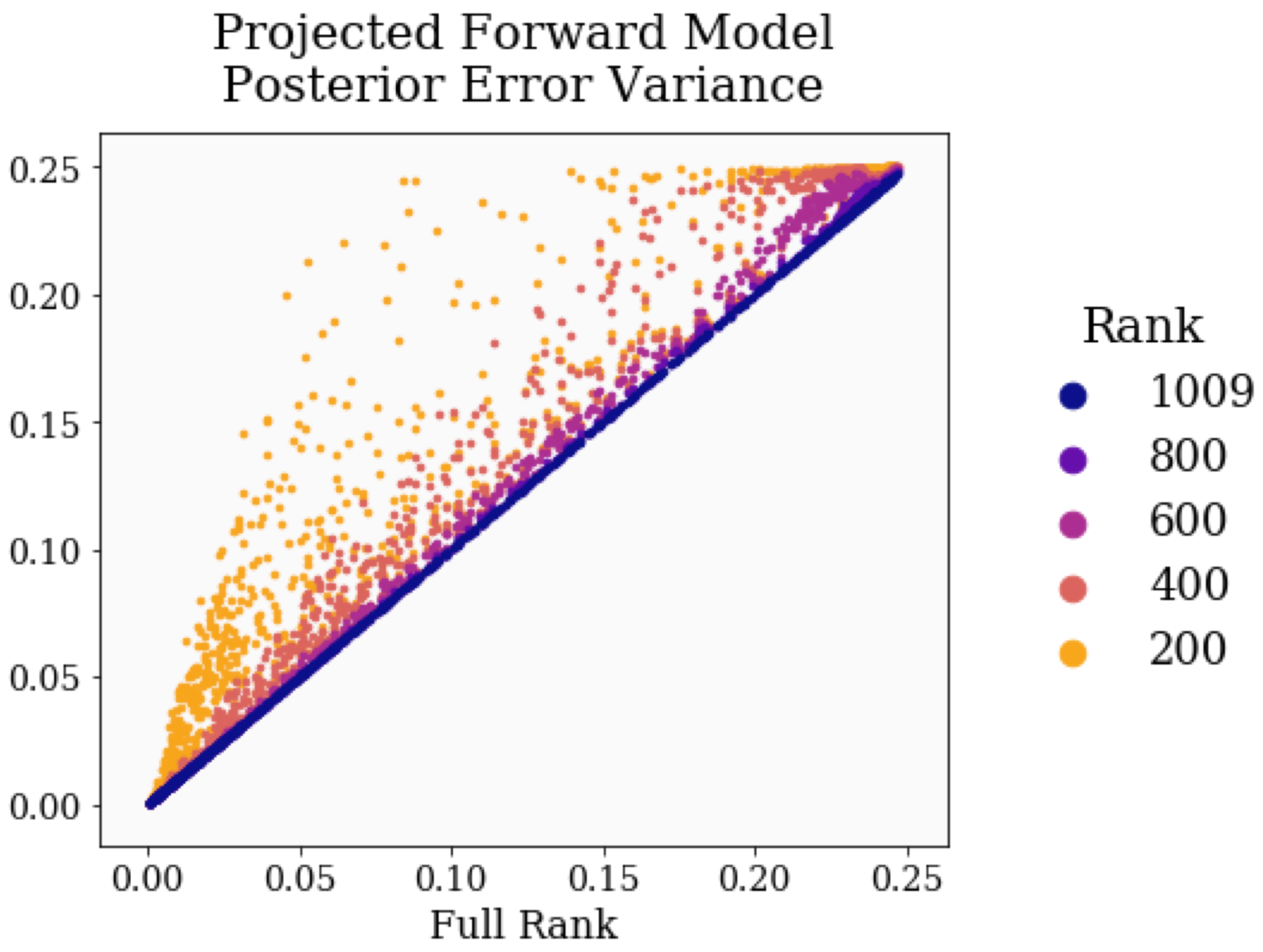
$\hat{\mathbf{x}}, \hat{\mathbf{S}}, \mathbf{A}$ | $\widehat{\mathbf{x}_\Pi}, \widehat{\mathbf{S}_\Pi}, \mathbf{A}_\Pi$ | $\widehat{\mathbf{x}_\omega}, \widehat{\mathbf{S}_\omega}, \mathbf{A}_\omega$



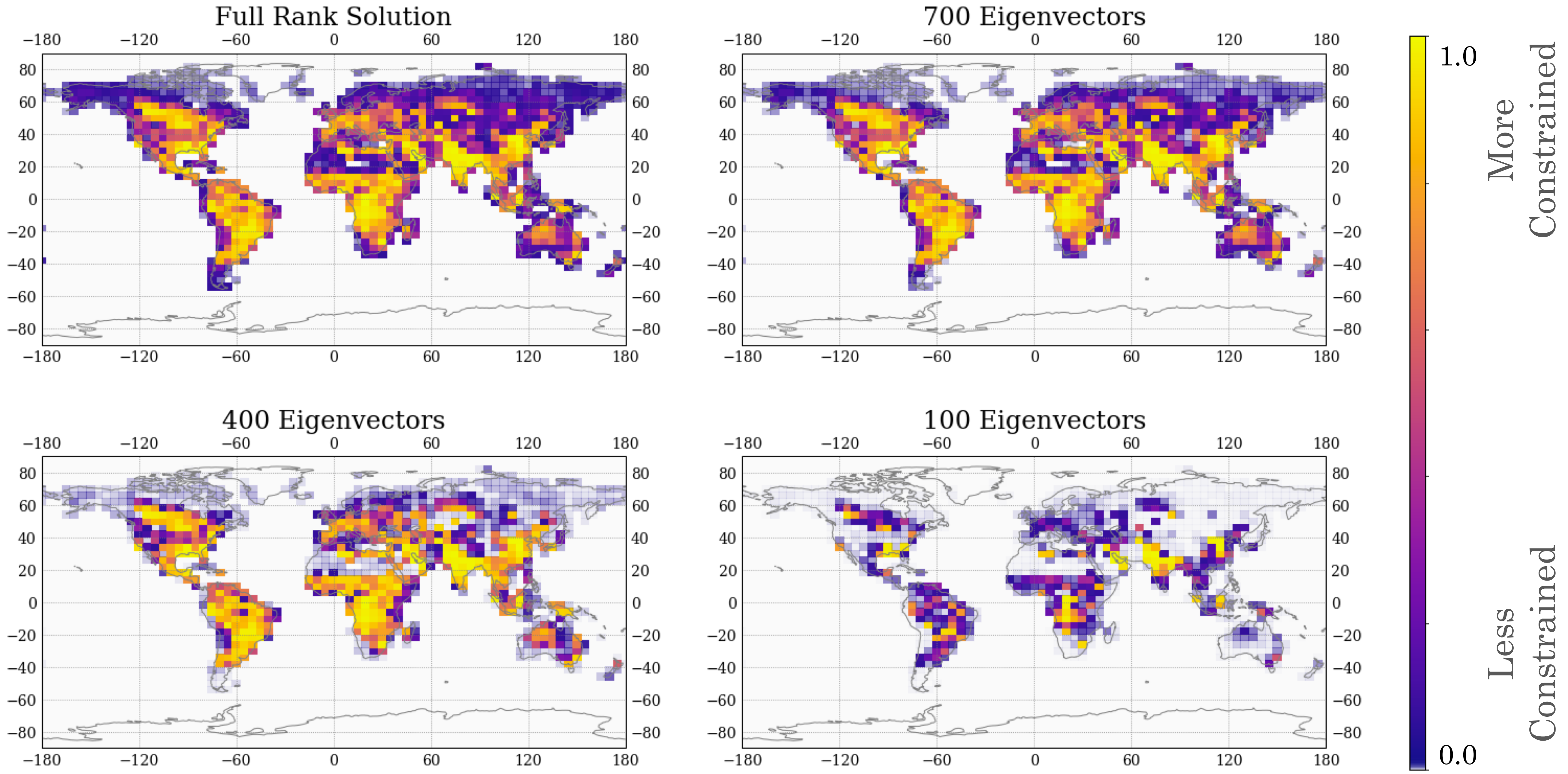
$\widehat{\mathbf{x}_{K_\Pi}}, \widehat{\mathbf{S}_{K_\Pi}}, \mathbf{A}_{K_\Pi}$ | $\widehat{\mathbf{x}_{FR}}$

The full rank approximation reproduces the full rank solution and converges to the true solution as k → n





The "reduced-rank inversion" maximizes the information content of the posterior solution



Reduced-Rank Jacobian Construction

Reduced-rank inversions decrease computational cost without significant loss of information content in the posterior solution.

Increasing inversion resolution increases computational cost, which is limited by the number of grid boxes optimized

emissions estimate (x_A, S_A)

forward model

modeled observations $(\boxed{K}x_A + c)$

n+1 model runs

minimize cost function

optimal emissions estimate $(\hat{x}, \hat{S})$

- optimal emission estimate
  $\hat{x} = x_A + \hat{S}K^T S_O^{-1}(y - (Kx_A + c))$
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- information content
  $A = \hat{S}K^T S_O^{-1} K$

observations (y, S_o)

Reduced-Rank Jacobian Construction

Reduced-rank inversions decrease computational cost without significant loss of information content in the posterior solution.

Next steps:

I. Reduce the computational cost of constructing Jacobians for analytic Bayesian inversions.

Reduced-Rank Jacobian Construction

I. Reduced-rank inversions

(Bousserez et al. 2018)

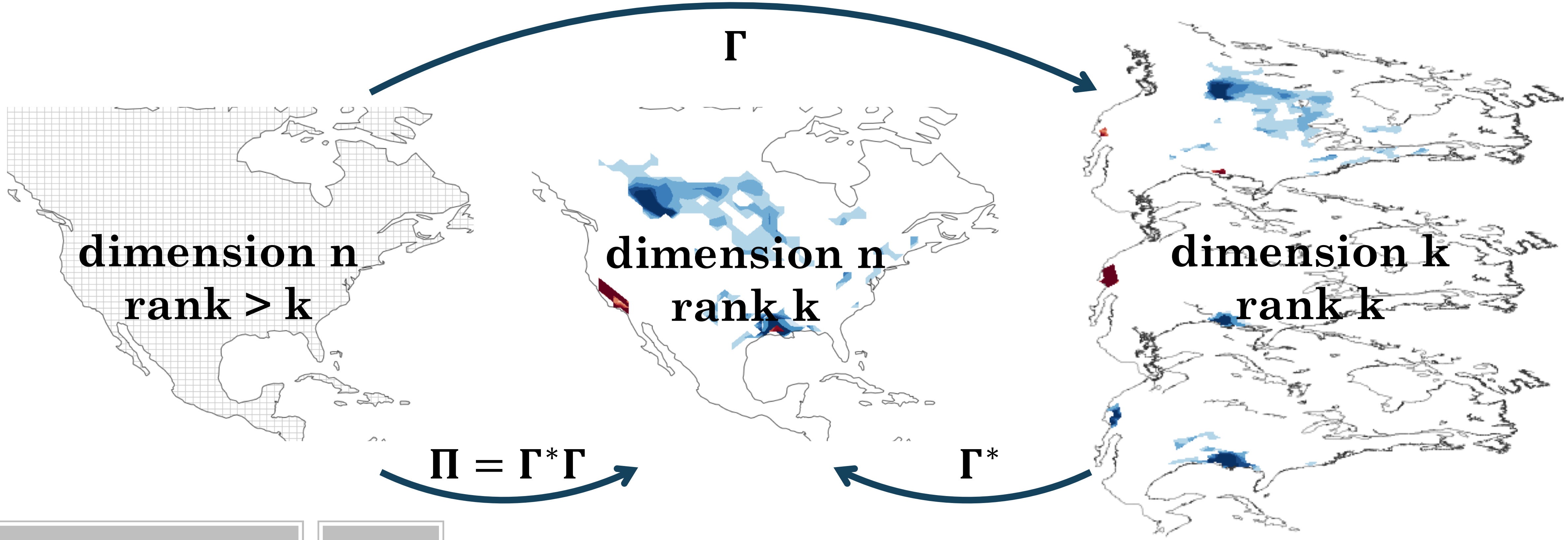
II. Reduced-rank Jacobians

The approximated posterior implicitly uses a reduced-rank Jacobian

$\hat{\mathbf{x}}, \hat{\mathbf{S}}, \mathbf{A}$

$\widehat{\mathbf{x}_\Pi}, \widehat{\mathbf{S}_\Pi}, \mathbf{A}_\Pi$

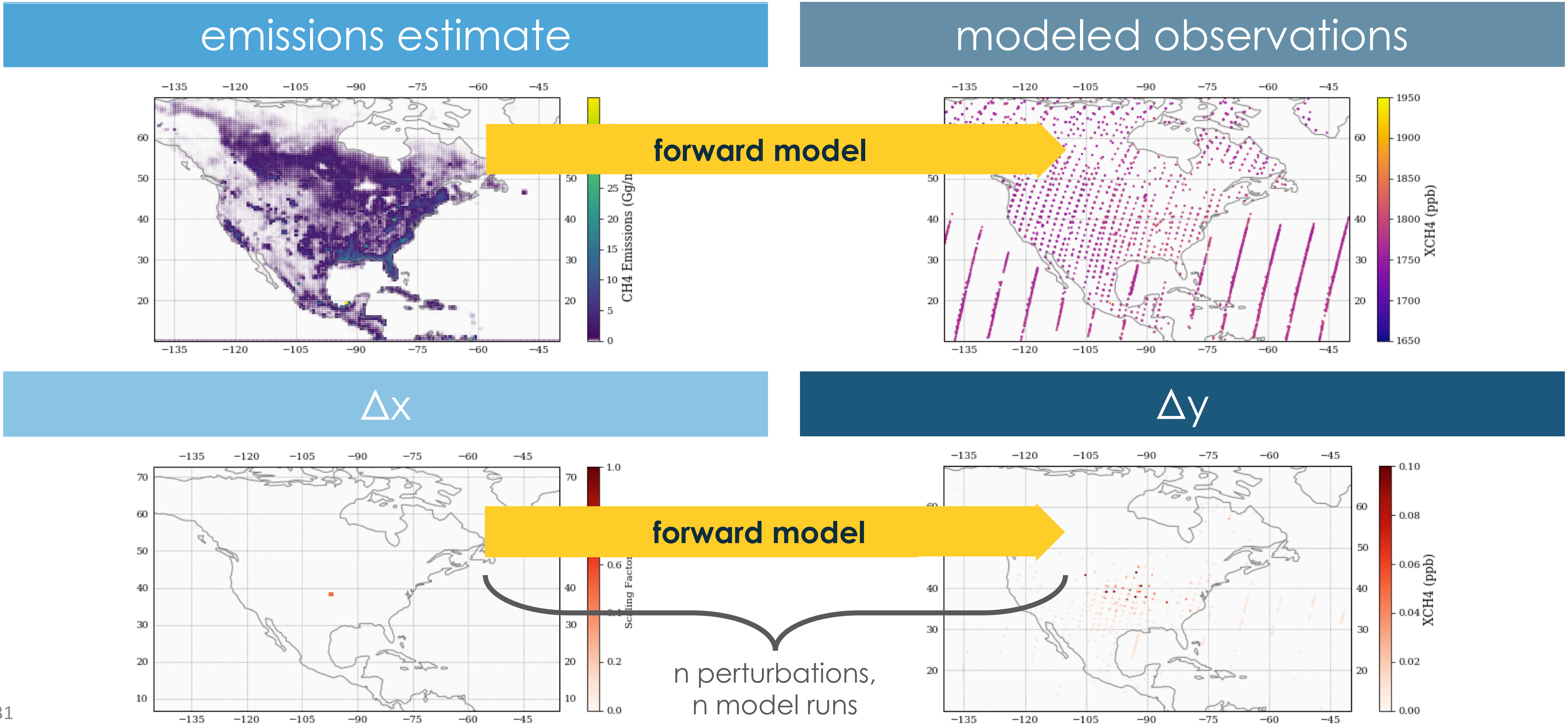
$\widehat{\mathbf{x}_\omega}, \widehat{\mathbf{S}_\omega}, \mathbf{A}_\omega$



$\widehat{\mathbf{x}_{K_\Pi}}, \widehat{\mathbf{S}_{K_\Pi}}, \mathbf{A}_{K_\Pi}$

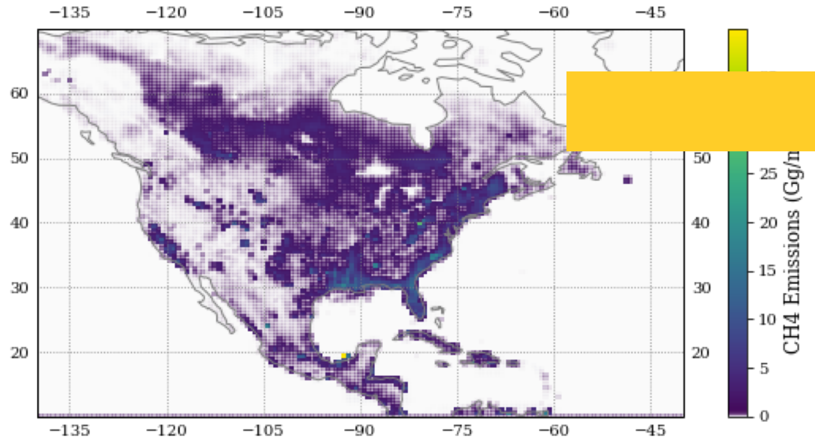
$\widehat{\mathbf{x}_{FR}}$

The Jacobian $\mathbf{K}$ represents the sensitivity of observations to emissions: $\mathbf{y} = \mathbf{Kx} + \mathbf{c}$ with $\mathbf{K} = \frac{\partial \mathbf{y}}{\partial \mathbf{x}}$

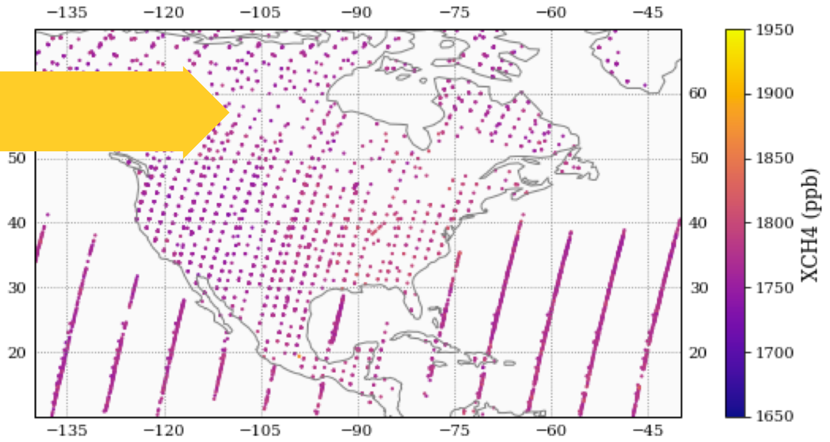


Perturbing eigenvectors would require k < n model runs and yield a reduced-rank Jacobian

emissions estimate

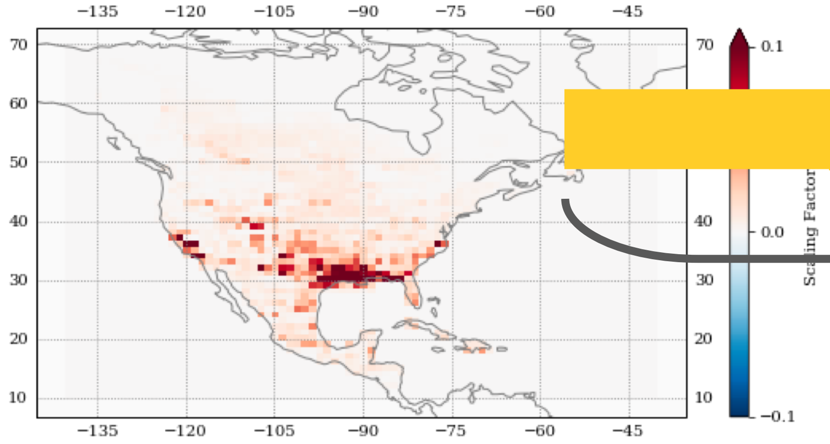


modeled observations

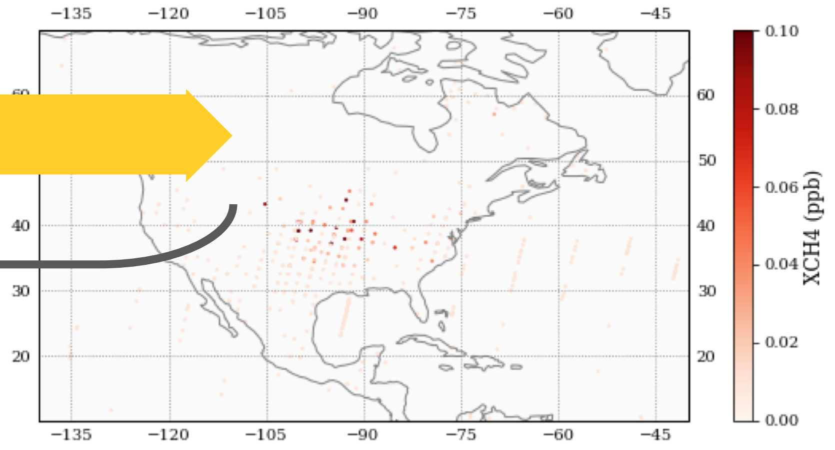


forward model

Δx



Δy



forward model

k perturbations,
k model runs

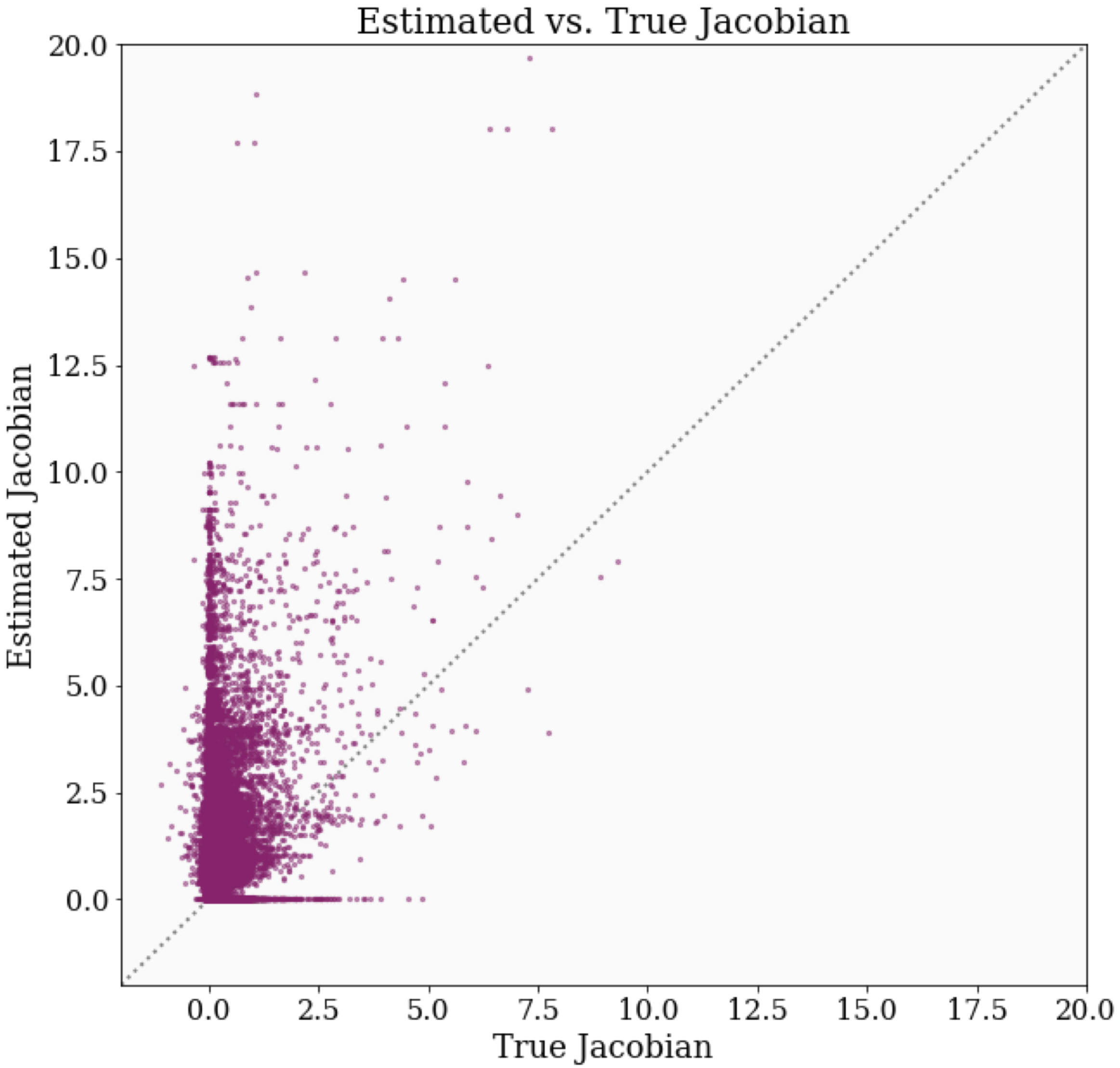
Because the eigenvectors include a contribution from the model, constructing the Jacobian is an iterative process

I. Initialize the Jacobian K_0 [m x n]

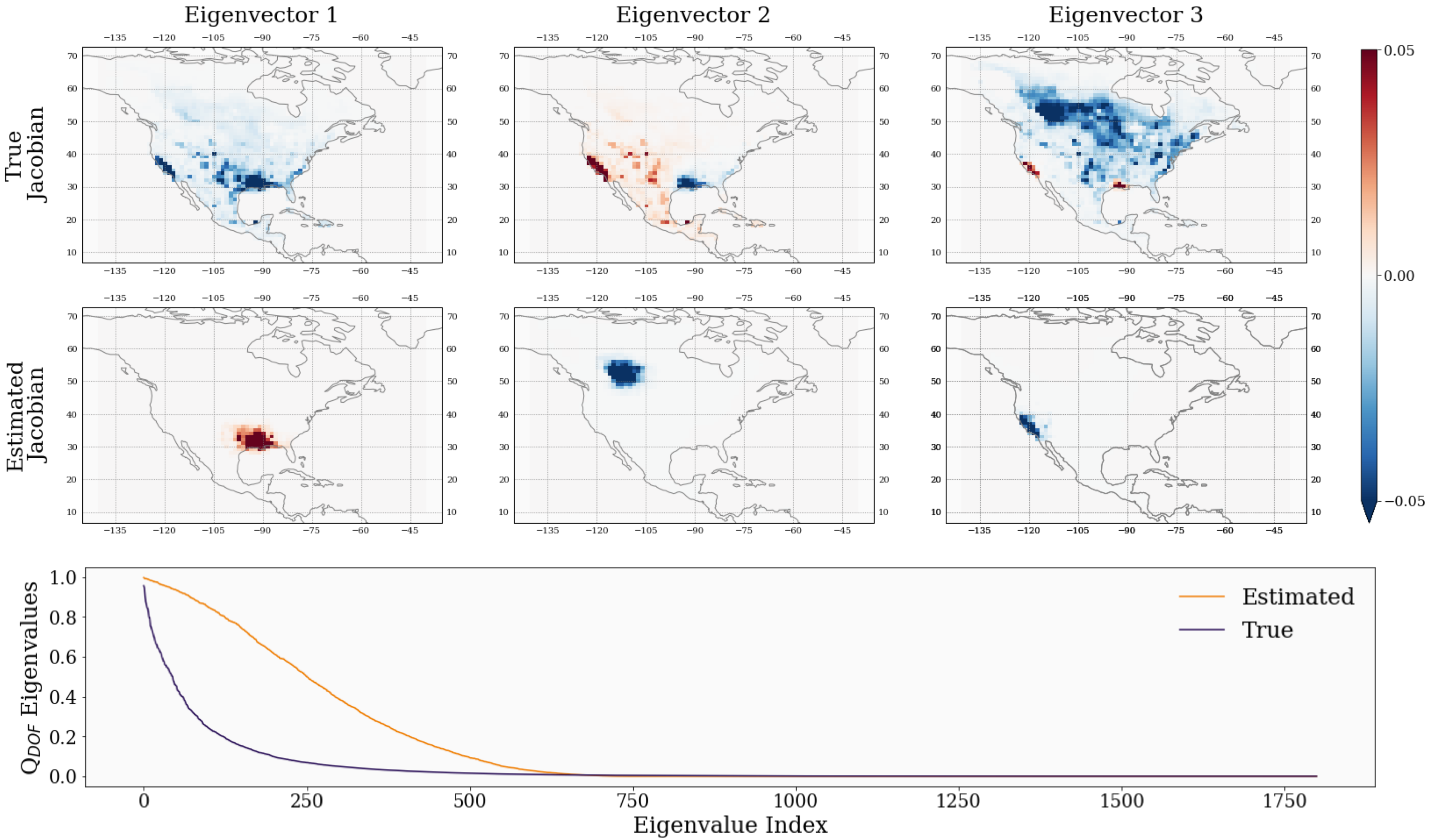
II. Perturb *k* eigenvectors and find the reduced dimension Jacobian K_ω [m x k]

III. Calculate the full dimension Jacobian K_1 [m x n]

The Jacobian can be initialized using a mass-balance approach



The initial estimate produces sufficiently similar eigenpairs



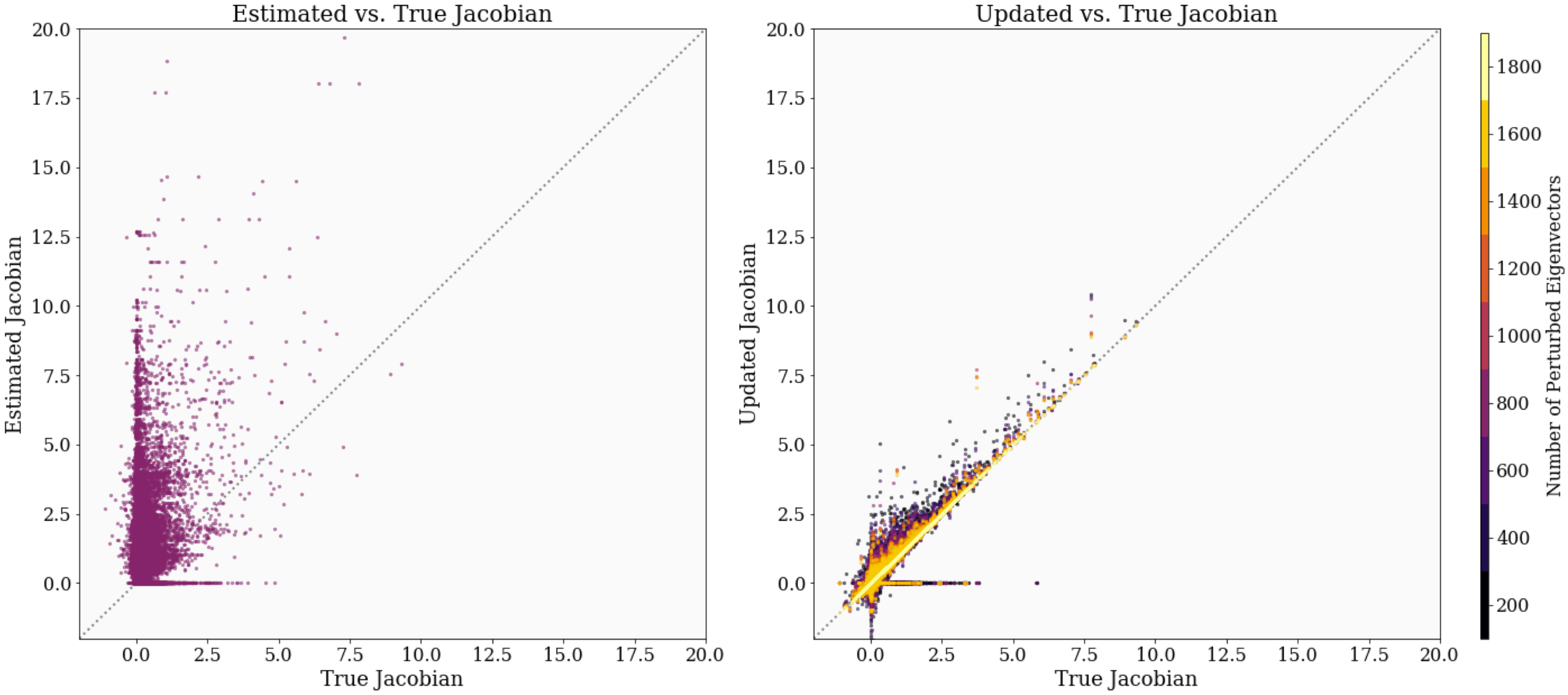
Because the eigenvectors include a contribution from the model, constructing the Jacobian is an iterative process

I. Initialize the Jacobian K_0 [m x n]

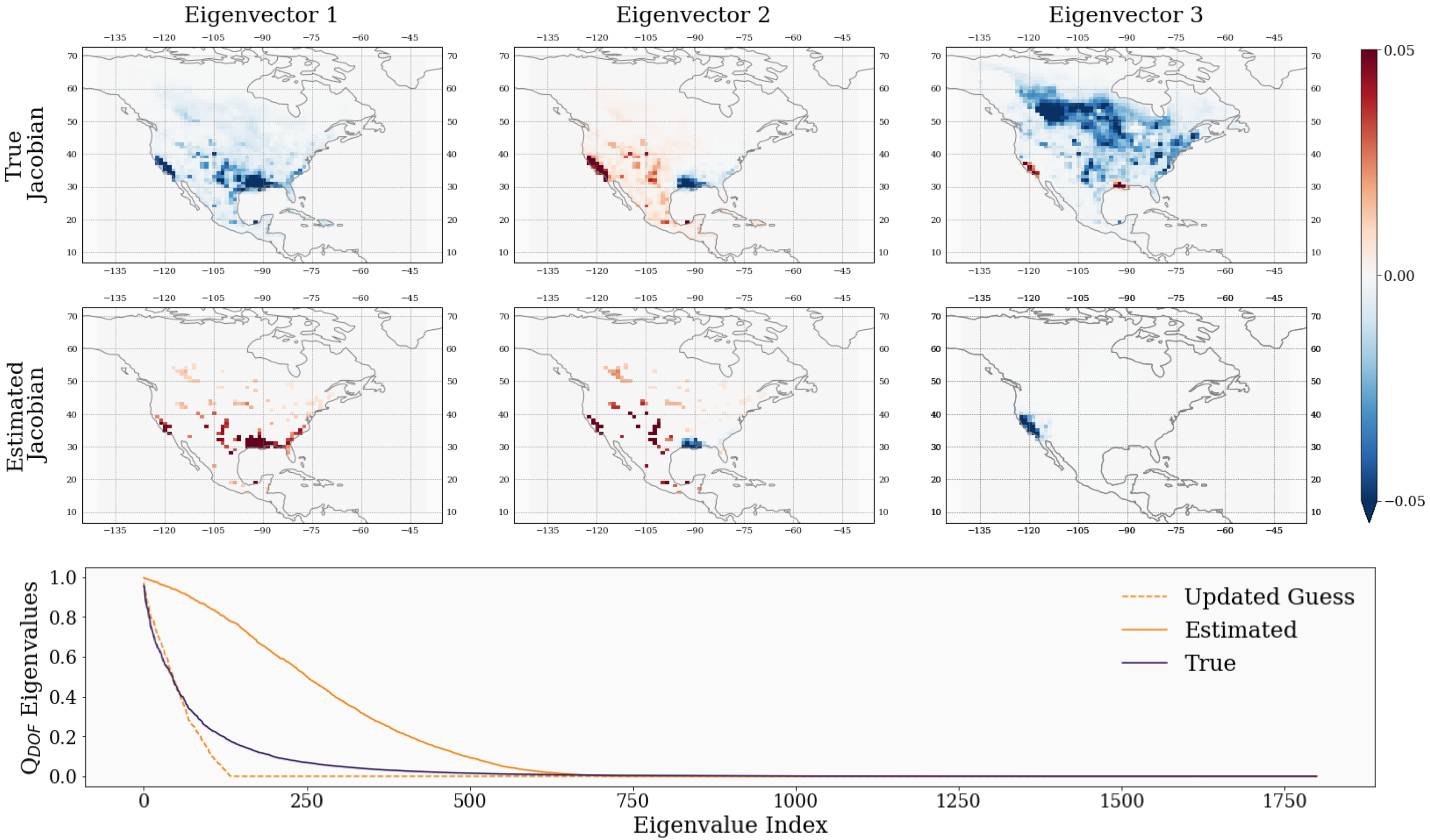
II. Perturb k eigenvectors and find the reduced dimension Jacobian K_ω [m x k]

III. Calculate the full dimension Jacobian K_1 [m x n]

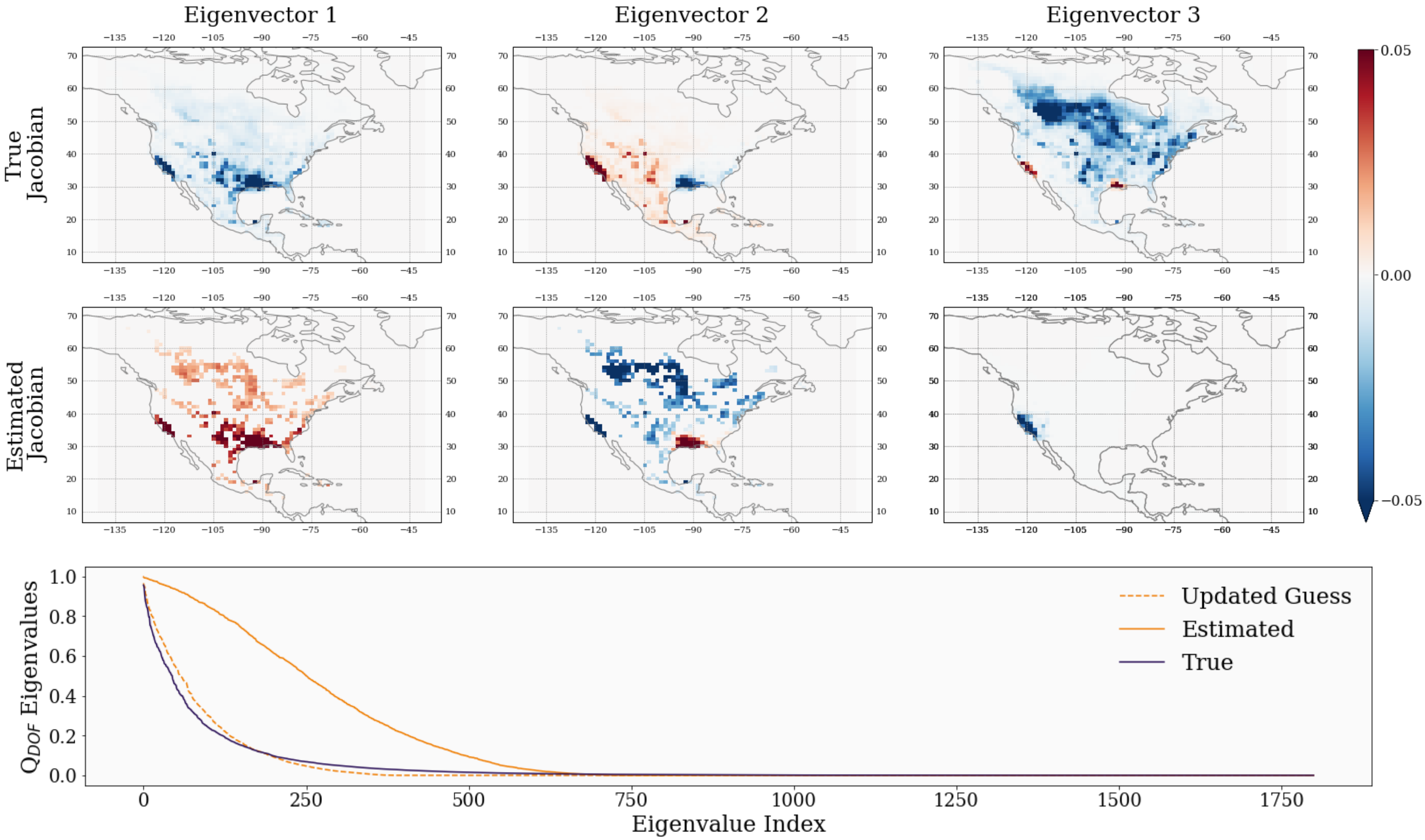
A single iteration significantly improves the estimated Jacobian



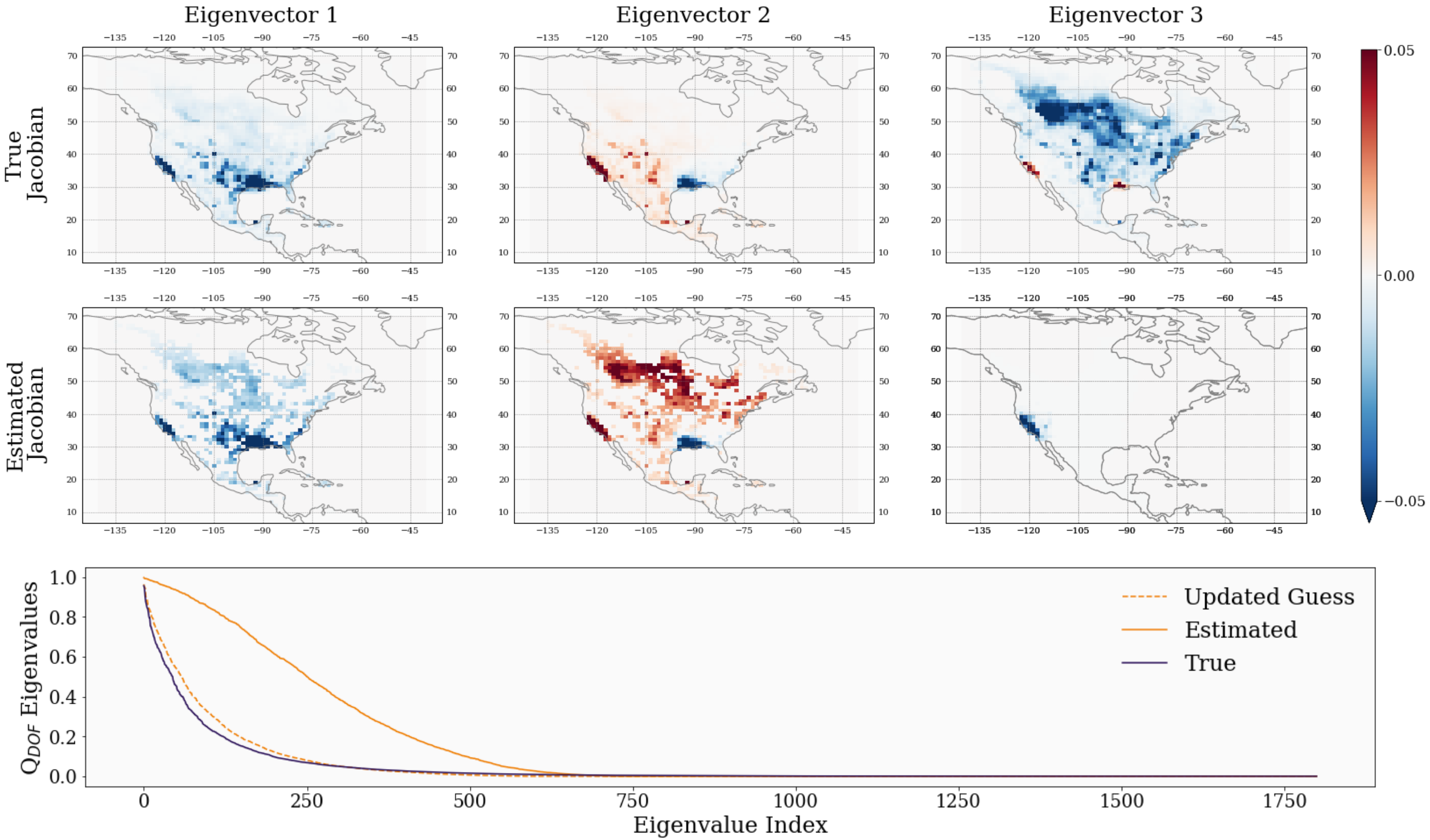
A single iteration with 200 perturbations improves the eigenpairs



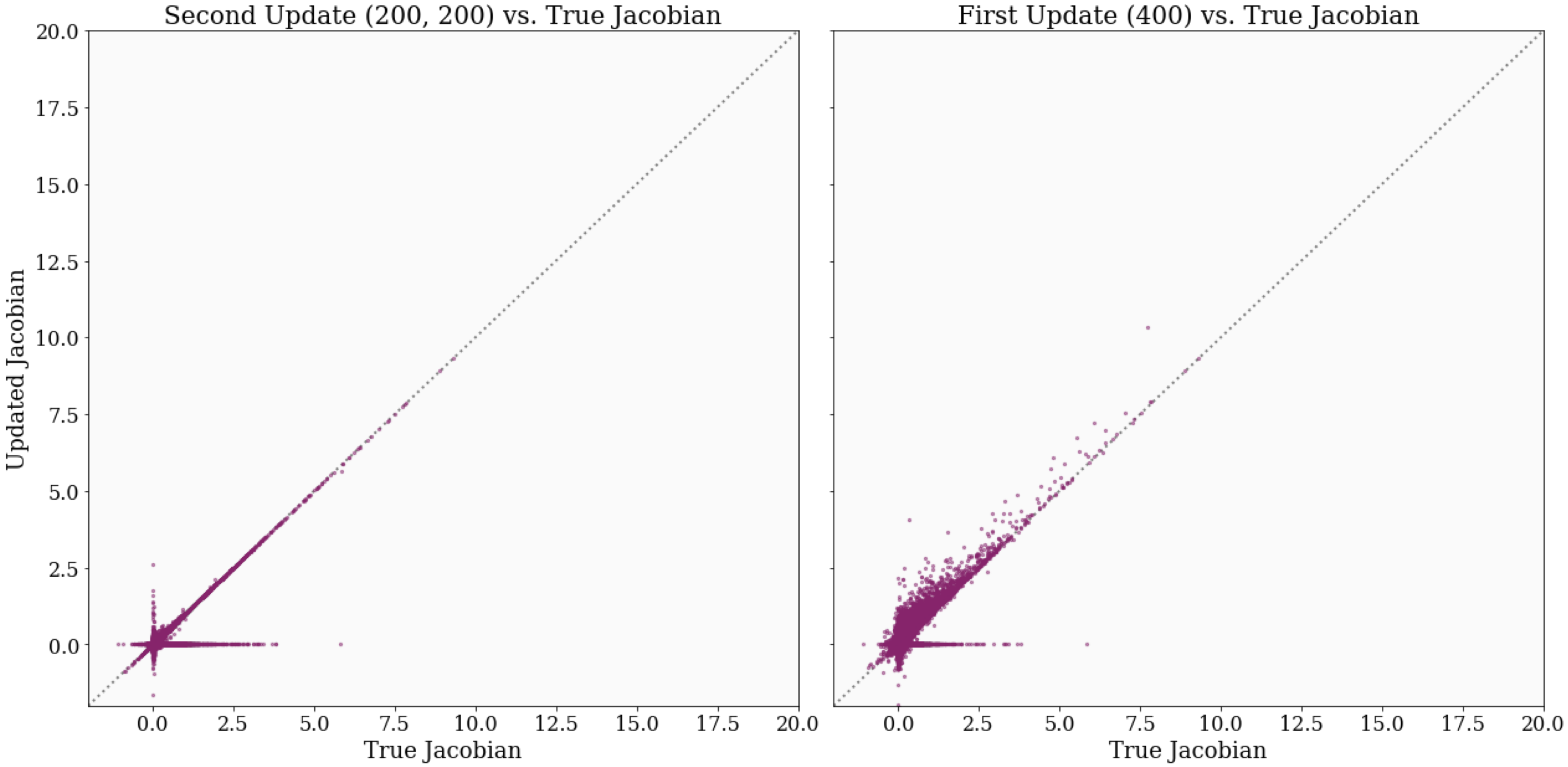
A single iteration with 400 perturbations improves the eigenpairs



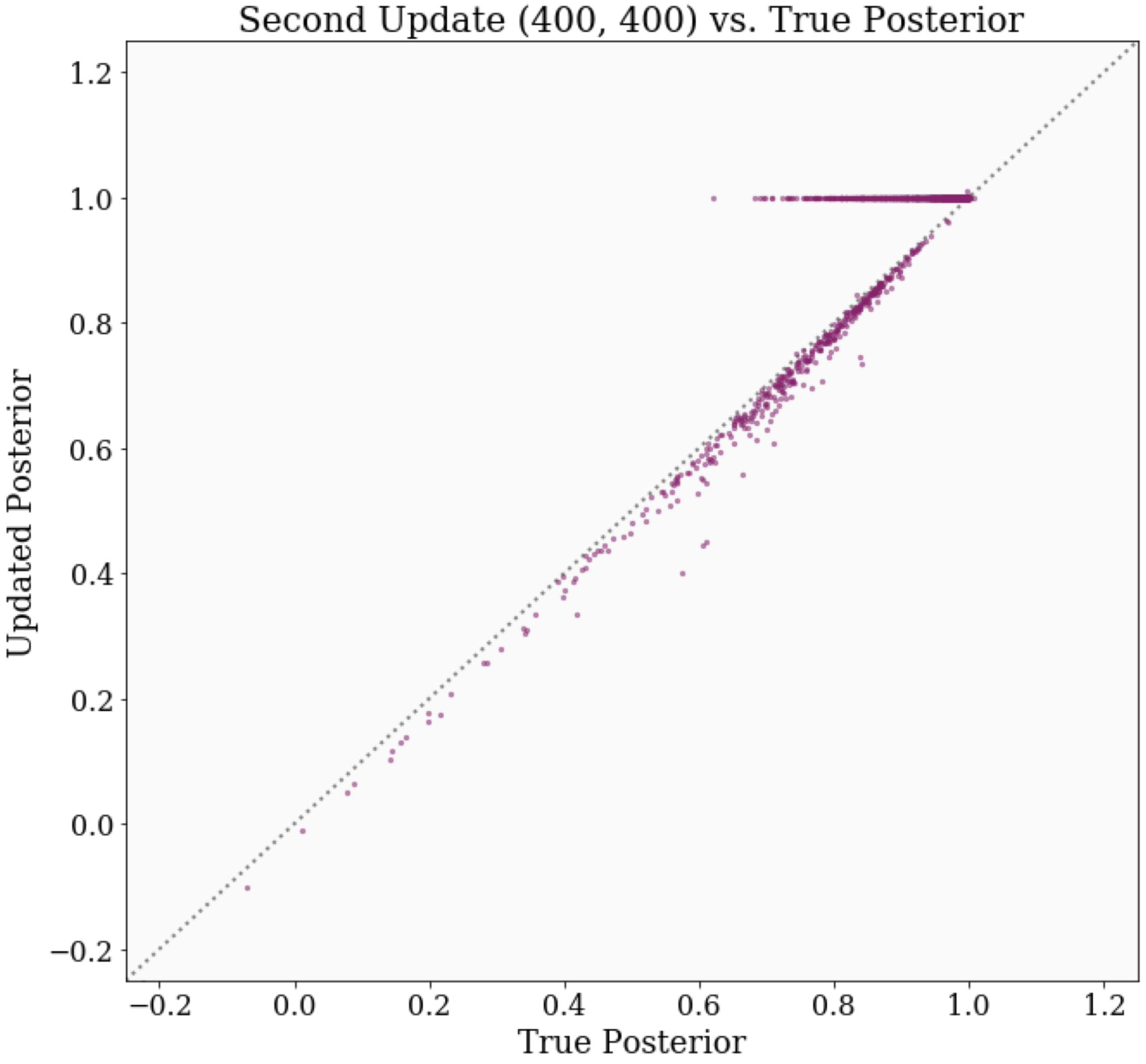
A single iteration with 600 perturbations improves the eigenpairs



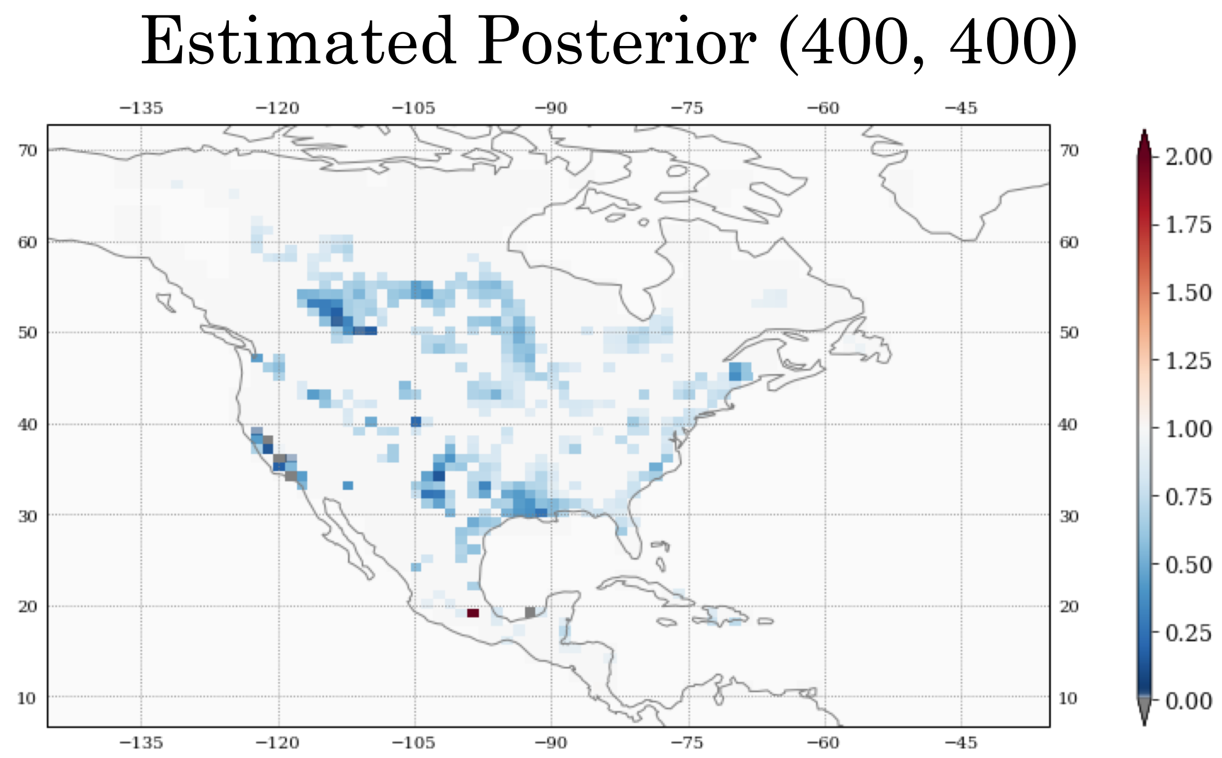
Iterating improves the Jacobian estimate

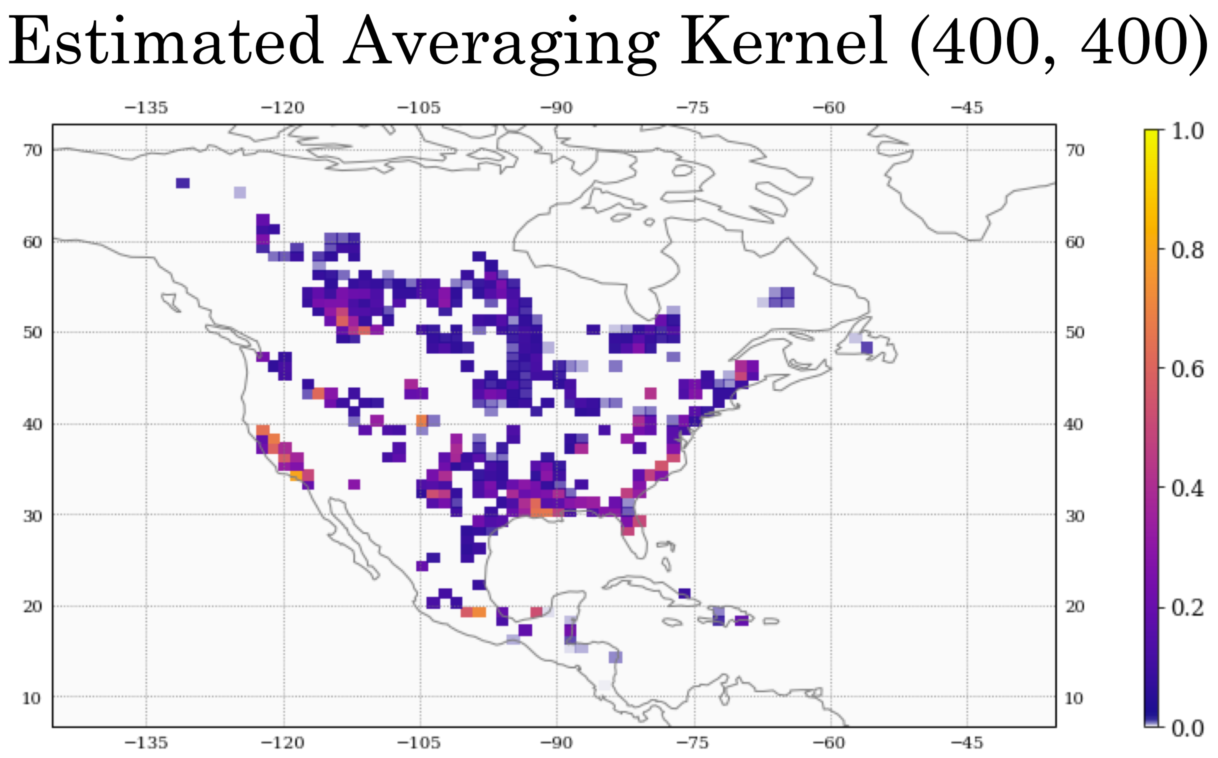


The resulting posterior approximates the true posterior with fewer than half the model runs



The resulting posterior approximates the true posterior best in areas with high information content





Reduced-Rank Jacobian Construction

Reduced-rank Jacobians optimize methane emissions in areas with high information content while significantly decreasing computational cost.

Next steps:

I. Define and justify an optimal iteration scheme, including convergence criteria;

II. Quantify the error associated with the reduced-rank Jacobian and the resulting posterior solutions.