Variational Data Assimilation and Regularization for Ill-posed Problems: A Common Framework

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Motivation

Wildfire smoke modeling

$$\frac{\partial q}{\partial t} + \nabla \cdot \vec{u}(\mathbf{x}, t) q(\mathbf{x}, t) = Q(\mathbf{x}, t)$$

Atmospheric winds *$PM_{2.5}$ concentration* *Wildfire plume rise*
Smoke emissions

- Fire related processes are difficult to simulate
  e.g. Pole Creek and Bald Mountain Fires, Central Utah, September, 2018

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JGR Atmospheres

Evaluating Wildfire Smoke Transport Within a Coupled Fire-Atmosphere Model Using a High-Density Observation Network for an Episodic Smoke Event Along Utah's Wasatch Front

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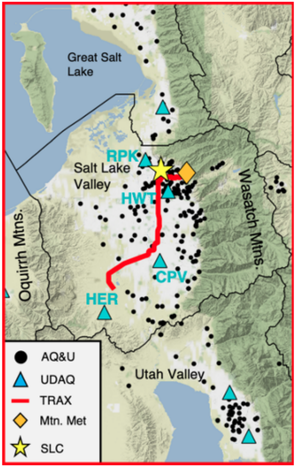
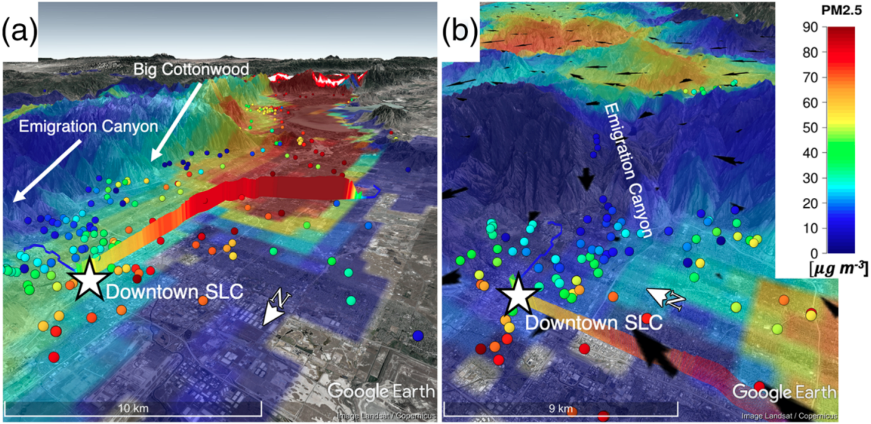
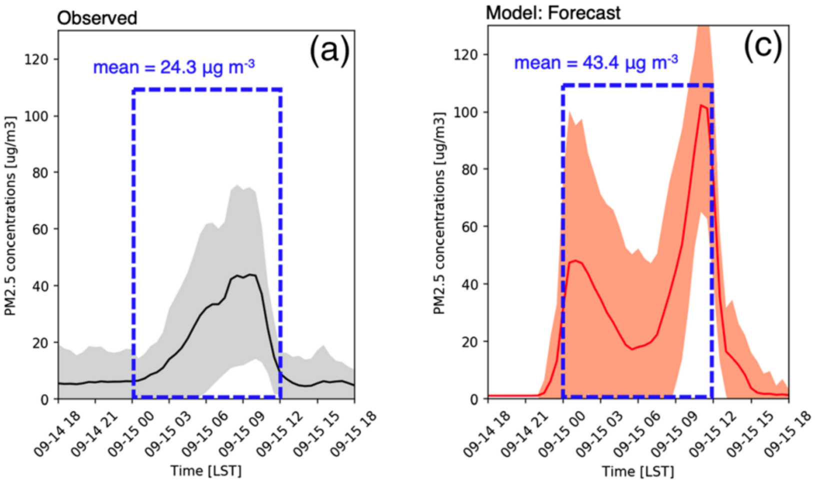


WRFSFC Forecast and Observations



Averaged $PM_{2.5}$ Concentrations

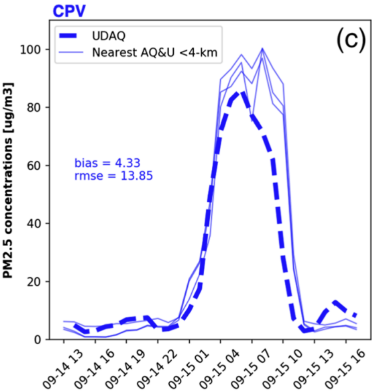


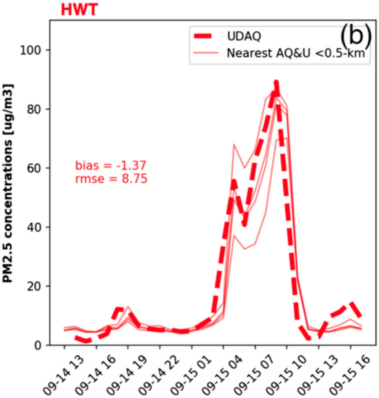
Outline

- Variational Data Assimilation (4DVAR)
  Weakly constrained dynamics and the Representer method
- Ill-posed Inverse Problems
  Regularization parameter selection
- Common Framework
  Uncertainty estimates using L-curve, GCV and χ^2 method
- Results
  1D transport model with simulated data

Observations

$$d_m = q(x_m, t_m) + \epsilon_m$$





Forward Problem

$$\frac{\partial q_F}{\partial t} + \nabla \cdot u(\mathbf{x},t) q_F(\mathbf{x},t) = Q(\mathbf{x},t)$$

$$q_F(\mathbf{x},0) = I(\mathbf{x})$$

$$q_F(\mathbf{x},t) = B(t) \qquad \text{for } \mathbf{x} \in \partial\Omega$$

Failure of the forward solution: $q_F(\mathbf{x}_m, t_m) \neq d_m$

Weakly constrained dynamics

$$\begin{cases} \dfrac{\partial q}{\partial t} + \nabla \cdot u(\mathbf{x},t) q(\mathbf{x},t) = Q(\mathbf{x},t) + f(\mathbf{x},t) \\ q(\mathbf{x},0) = I(\mathbf{x}) + i(\mathbf{x}) \\ q(\mathbf{x},t) = B(t) + b(t) \qquad \text{for } \mathbf{x} \in \partial\Omega \end{cases}$$

Normal Distribution Assumption

$$f(\mathbf{x},t) \sim \mathcal{N}(0, C_f(\mathbf{x},t))$$
$$i(\mathbf{x}) \sim \mathcal{N}(0, C_i(\mathbf{x}))$$
$$b(t) \sim \mathcal{N}(0, C_b(t))$$

$$\epsilon_m \sim \mathcal{N}(0, \sigma_{d_m})$$

e.g. probability density function of data error

$$(2\pi\sigma_{d_m}^2)^{-1/2} e^{-\frac{(d_m - q(x_m, t_m))^2}{2\sigma_{d_m}^2}}$$

Least Squares Fitting

Maximum likelihood estimate when errors are normally distributed

$$
\begin{aligned}
\mathcal{J}[q(\mathbf{x},t)] = & \int_0^T \int_\Omega \int_0^T \int_\Omega f(\mathbf{x},t) C_f^{-1}(\mathbf{x},t,\mathbf{x}',t') f(\mathbf{x}',t') \; d\mathbf{x}' dt' d\mathbf{x} dt \\
& + \int_\Omega \int_\Omega i(\mathbf{x}) C_i^{-1}(\mathbf{x},\mathbf{x}') i(\mathbf{x}') \; d\mathbf{x}' d\mathbf{x} \\
& + \int_0^T \int_0^T b(t) C_b^{-1}(t,t') b(t') \; dt' dt \\
& + \boldsymbol{\epsilon}^T \mathbf{C}_\epsilon^{-1} \boldsymbol{\epsilon}
\end{aligned}
$$

where

$$
\int_0^T \int_\Omega C_f^{-1}(\mathbf{x},t,\mathbf{x}',t') C_f(\mathbf{x}',t',\mathbf{x}'',t'') \; dx' dt' = \delta(\mathbf{x}-\mathbf{x}'')\delta(t-t'')
$$

Calculus of Variations

$\hat{q}(\mathbf{x}, t) = \arg\min_{q(\mathbf{x},t)} \mathcal{J}$ so that

$$\mathcal{J}[\hat{q} + \delta q] = \mathcal{J}[\hat{q}] + \mathcal{O}(\delta q)^2$$

Define adjoint variable

$$\lambda(\mathbf{x}, t) = \int_0^T \int_\Omega C_f^{-1}(\mathbf{x}, t, \mathbf{x}', t') f(\mathbf{x}', t')\ d\mathbf{x}' dt' \equiv C_f^{-1} \bullet f$$

and write the discrete term as $\hat{\boldsymbol{\epsilon}}^T \mathbf{C}_\epsilon^{-1} \delta \mathbf{q}$ or

$$\int_0^T \int_\Omega \sum_{m=1}^{M} (\hat{\boldsymbol{\epsilon}}^T \mathbf{C}_\epsilon^{-1})_m \delta q(\mathbf{x}, t) \delta(\mathbf{x} - \mathbf{x}_m) \delta(t - t_m)\ d\mathbf{x} dt$$

with $\hat{\boldsymbol{\epsilon}}, \delta \mathbf{q} \in \mathbb{R}^M$ and $\mathbf{C}_\epsilon^{-1} \in \mathbb{R}^{M \times M}$

Euler-Lagrange Equations

Coupled system of equations where

$$(B)\begin{cases} -\dfrac{\partial \lambda}{\partial t} - \nabla \cdot u(\mathbf{x},t)\lambda(\mathbf{x},t) = -\sum_m \left((\hat{\mathbf{q}}-\mathbf{b})^T \mathbf{C}_\epsilon^{-1}\right)_m \delta(\mathbf{x}-\mathbf{x}_m)\delta(t-t_m) \\ \lambda(\mathbf{x},T) = 0 \\ \lambda(\mathbf{x},t) = 0 \qquad \text{for } \mathbf{x} \in \partial\Omega \end{cases}$$

is solved backward in space and time for adjoint variable $\lambda(\mathbf{x},t)$ while

$$(F)\begin{cases} \dfrac{\partial \hat{q}}{\partial t} + \nabla \cdot u(\mathbf{x},t)\hat{q}(\mathbf{x},t) = Q(\mathbf{x},t) + C_f \bullet \lambda \\ \hat{q}(\mathbf{x},0) = I(\mathbf{x}) + C_i \circ \lambda(\mathbf{x},0) \\ \hat{q}(\mathbf{x},t) = u(\mathbf{x},t)B(t) + C_b * \lambda(\mathbf{x},t) \qquad \text{for } \mathbf{x} \in \partial\Omega \end{cases}$$

is solved forward in space and time for optimal state estimate $\hat{q}(\mathbf{x},t)$

Representer Theorem

Let

$$\hat{q}(\mathbf{x}, t) = \arg\min_{q \in \mathcal{H}} \left\{ \boldsymbol{\epsilon}^T \mathbf{C}_\epsilon^{-1} \boldsymbol{\epsilon} + \mathcal{R}(q) \right\}$$

with $\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1$ where $\mathcal{H}_0 = \{q : \mathcal{R}(q) = 0\}$ is a finite dimensional space with basis $\phi_1, \ldots, \phi_N$ and $\mathcal{H}_1$ is a Reproducing Kernel Hilbert Space (RKHS) with reproducing kernel Γ. Let $r_m(x, t) = \Gamma(\mathbf{x}, t, \mathbf{x}_m, t_m)$ be representers. Then

$$\hat{q}(\mathbf{x}, t) = \sum_{n=1}^{N} c_n \phi_n(\mathbf{x}, t) + \sum_{m=1}^{M} \beta_m r_m(\mathbf{x}, t).$$

Note that for $\mathcal{J} = \boldsymbol{\epsilon}^T \mathbf{C}_\epsilon^{-1} \boldsymbol{\epsilon} + \mathcal{R}(q)$, $\mathcal{R}(q_F) = 0$ so that

$$\hat{q}(\mathbf{x}, t) = q_F(\mathbf{x}, t) + \sum_{m=1}^{M} \beta_m r_m(\mathbf{x}, t).$$

Reproducing Kernel Hilbert Space (RKHS)

Define adjoint representer $\alpha_m(\mathbf{x}, t)$ as the Green's Function

$$(B) \begin{cases} -\frac{\partial \alpha_m}{\partial t} - \nabla \cdot u(\mathbf{x}, t)\alpha_m(\mathbf{x}, t) = \delta(\mathbf{x} - \mathbf{x}_m)\delta(t - t_m) \\ \alpha_m(\mathbf{x}, T) = 0 \\ \alpha_m(\mathbf{x}, t) = 0. \qquad \text{for } \mathbf{x} \in \partial\Omega \end{cases}$$

and let $r_m(\mathbf{x}, t)$ satisfy

$$(F) \begin{cases} \frac{\partial r_m}{\partial t} + \nabla \cdot u(\mathbf{x}, t) r_m(\mathbf{x}, t) = C_f \bullet \alpha_m(\mathbf{x}, t) \\ r_m(\mathbf{x}, 0) = C_i \circ \alpha_m(\mathbf{x}, 0) \\ r_m(\mathbf{x}, t) = u(0, t) C_b * \alpha_m(\mathbf{x}, t) \text{for } \mathbf{x} \in \partial\Omega \end{cases}$$

Then $r_m(\mathbf{x}_l, t_l) = r_l(\mathbf{x}_m, t_m)$ is a reproducing kernel.

Representer Coefficients

Substituting $\hat{q}(\mathbf{x},t) = q_F(\mathbf{x},t) + \sum_{m=1}^{M} \beta_m r_m(\mathbf{x},t)$ into E-L equations decouples them and we get

$$(\mathbf{R} + \mathbf{C}_\epsilon)\,\boldsymbol{\beta} = \mathbf{d} - \mathbf{q}_F$$

where $\mathbf{R}$ is the representer matrix with elements $\mathbf{R}_{ml} = r_m(\mathbf{x}_l, t_l)$.

This gives the optimal estimate

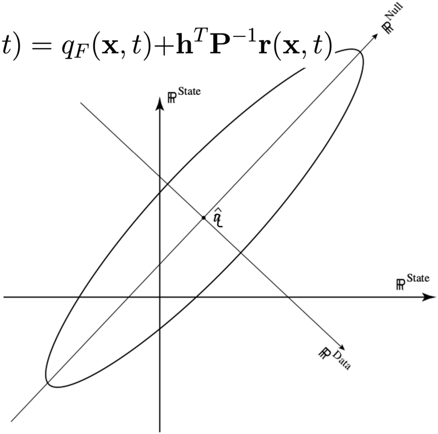
$$\hat{q}(\mathbf{x},t) = q_F(\mathbf{x},t) + (\mathbf{d} - \mathbf{q}_F)^T(\mathbf{R} + \mathbf{C}_\epsilon)^{-1}\mathbf{r}(\mathbf{x},t)$$

with $\mathbf{r}(\mathbf{x},t)$ the vector of the m representers evaluated at $(\mathbf{x},t)$.

Representer Method for 4DVAR*

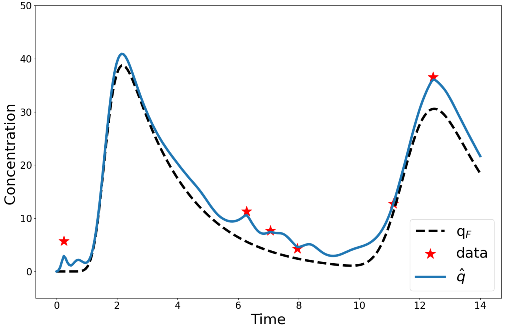
Define $\mathbf{h} = \mathbf{d} - \mathbf{q}_F$ and $\mathbf{P} = \mathbf{R} + \mathbf{C}_\epsilon$ so that

$$\hat{q}(\mathbf{x}, t) = q_F(\mathbf{x}, t) + \mathbf{h}^T \mathbf{P}^{-1} \mathbf{r}(\mathbf{x}, t)$$

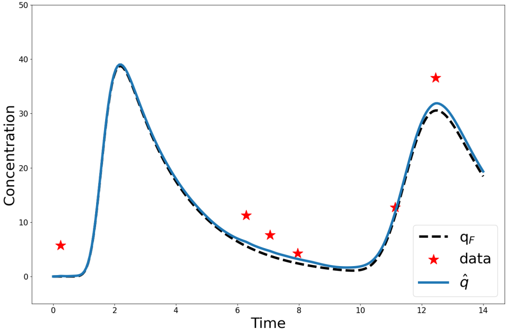


*Bennett, 2005

Effect of Error Covariance on Optimal Estimates



C_f is “larger" than $\mathbf{C}_\epsilon$



$\mathbf{C}_\epsilon$ is “larger" than C_f

Simplifying Assumptions

$$\mathcal{J}[q(\mathbf{x},t)] = \sigma_f^{-2}\int_0^T\int_\Omega\left(\frac{\partial q}{\partial t} + \nabla\cdot u(\mathbf{x},t)q(\mathbf{x},t) - Q(\mathbf{x},t)\right)^2 \, d\mathbf{x}dt$$
$$+\boldsymbol{\epsilon}^T\mathbf{C}_\epsilon^{-1}\boldsymbol{\epsilon}$$

i.e. initial and boundary conditions are exact while errors in PDE can be represented with a scalar σ_f.

Note that

$$\min_{q(\mathbf{x},t)} \ \boldsymbol{\epsilon}^T\mathbf{C}_\epsilon^{-1}\boldsymbol{\epsilon}$$

is ill-posed in continuous intervals $\mathbf{x}\in\Omega$, $t\in[0,T]$. Weakly constrained 4DVAR regularizes it as long as σ_f is "small" enough.

Well-posed Problems

The problem of finding $q(\mathbf{x}, t)$ from $\mathbf{d}$ is called well-posed (Hadamard, 1923) if the following hold

- Existence - a solution $q(\mathbf{x}, t)$ exists for any $\mathbf{d}$ in data space
- Uniqueness - the solution is unique
- Stability - continuous dependence of $q(\mathbf{x}, t)$ on $\mathbf{d}$, the inverse mapping $\mathcal{A}^{-1} : \mathbf{d} \rightarrow q(\mathbf{x}, t)$ is continuous

The first two conditions are equivalent to saying that the operator $\mathcal{A}$ has a well defined inverse $\mathcal{A}^{-1}$. Moreover, we require that the domain of $\mathcal{A}^{-1}$ is the data space.

Well-conditioned Problems

For condition number $\kappa(x)$

$$\text{variation in output} \approx \kappa(x) \text{ perturbation in input}$$

Example

Let $\mathbf{A} \in \mathbb{R}^{M\times M}$, then

$$\kappa(\mathbf{A}) = \begin{cases} \|\mathbf{A}\|\|\mathbf{A}^{-1}\| & \text{if } \mathbf{A} \text{ is invertible} \\ \infty & \text{otherwise} \end{cases}$$

Regularization

$$\mathbf{A}\mathbf{x} = \mathbf{b}$$

Existence: Least squares

$$\min_{\mathbf{x}} \|\mathbf{C}_\epsilon^{-1/2}(\mathbf{b} - \mathbf{A}\mathbf{x})\|_2^2 \Rightarrow \mathbf{A}^T\mathbf{C}_\epsilon^{-1}\mathbf{A}\hat{\mathbf{x}} = \mathbf{A}^T\mathbf{C}_\epsilon^{-1/2}\mathbf{b}$$

However, $\mathbf{A}^T\mathbf{C}_\epsilon^{-1}\mathbf{A}$ may not be invertible and so we use regularization.

<u>Tikhonov Regularization</u>

Introduce a regularization parameter $\eta > 0$ such that small η gives a problem "close" to original e.g.

$$\min_{\mathbf{x}} \{\|\mathbf{C}_\epsilon^{-1/2}(\mathbf{b} - \mathbf{A}\mathbf{x})\|_2^2 + \eta\|\mathbf{L}\mathbf{x}\|_2^2\} \Rightarrow (\mathbf{A}^T\mathbf{C}_\epsilon^{-1}\mathbf{A} + \eta\mathbf{L}^T\mathbf{L})\hat{\mathbf{x}} = \mathbf{A}^T\mathbf{C}_\epsilon^{-1/2}\mathbf{b}$$

where $\mathbf{L}$ can be a differential operator and $\|\mathbf{L}\mathbf{x}\|$ an approximation to a Sobolev norm.

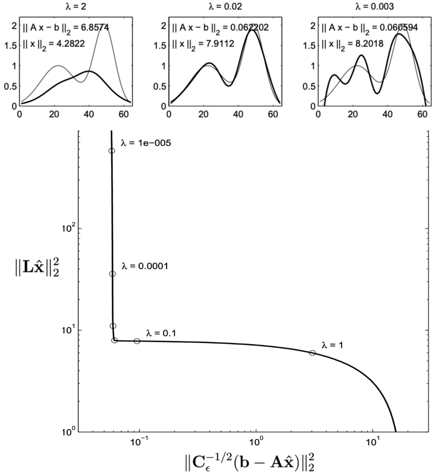
L-curve* Choice of Regularization Parameter

Methodology: Find the best trade-off between the size of a regularized estimate and its fit to the given data, as the regularization parameter varies.

Approach: For a range of values of η, create a log-log plot of the norm of a regularized solution versus the the corresponding residual norm.

*Hansen, 2000

L-curve example ($\lambda = \eta$)



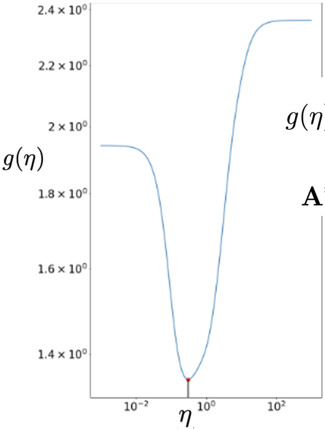
Generalized Cross Validation (GCV)* Choice of η

Methodology: Hold back data and the optimal regularization parameter is the one which minimizes the predictive error for all other data.

Approach: Minimize the sum of predictive error by applying the leave-one-out lemma to speed up computation.

*Golub et al, 1979

GCV Example



$$g(\eta) = \frac{m\|\mathbf{A}\hat{\mathbf{x}} - \mathbf{b}\|^2}{\left(\text{trace}(\mathbf{I} - \mathbf{A}\mathbf{A}^{\#})\right)^2}$$

$$\mathbf{A}^{\#} = (\mathbf{A}^T\mathbf{A} + \eta\mathbf{I})^{-1}\mathbf{A}^T$$

χ^{2*} Discrepancy for Choice of η

Methodology: Find the regularization parameter for which the objective function evaluated at the optimal state estimate follows a χ^2_M distribution.

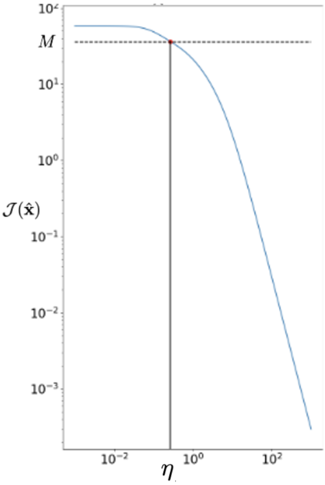
Morozov's discrepancy principle: $\|\mathbf{C}_\epsilon^{-1/2}(\mathbf{b} - \mathbf{A}\hat{\mathbf{x}})\|_2^2 \approx M$

χ^2 Method: $\mathcal{J}(\hat{\mathbf{x}}) = \|\mathbf{C}_\epsilon^{-1/2}(\mathbf{b} - \mathbf{A}\hat{\mathbf{x}})\|_2^2 + \eta\|\mathbf{L}\hat{\mathbf{x}}\|^2 \sim \chi^2_M$

Approach: For a given data set, solve the nonlinear equation $\mathcal{J}[\hat{\mathbf{x}}] = M$ for η.

*Mead, 2006

χ^2 Method Example



Common Framework - Optimal Estimates

Regularized Inverse Problem

$$\mathcal{J}[\mathbf{x}] = (\mathbf{b} - \mathbf{A}\mathbf{x})^T \mathbf{C}_\epsilon^{-1} (\mathbf{b} - \mathbf{A}\mathbf{x}) + \eta \|\mathbf{L}(\mathbf{x} - \mathbf{x}_0)\|^2$$

$$\hat{\mathbf{x}} \equiv \arg\min_{\mathbf{x}} \mathcal{J}[\mathbf{x}] = \mathbf{x}_0 + (\mathbf{A}^T\mathbf{A} + \eta \mathbf{L}^T\mathbf{L})^{-1}\mathbf{A}^T(\mathbf{b} - \mathbf{A}\mathbf{x}_0)$$

Weakly Constrained 4DVAR with Representers

$$\begin{aligned}\mathcal{J}[q(x,t)] = & \sum_{m=1}^{M} \sigma_{\epsilon_m}^{-2} (d_m - q(x_m, t_m))^2 \\ & + \sigma_f^{-2} \int_0^T \int_0^L \left(\frac{\partial q}{\partial t} + \frac{\partial}{\partial x} (u(x,t) q(x,t)) - Q(x,t) \right)^2 dx dt\end{aligned}$$

$$\hat{q}(x,t) \equiv \arg\min_{q(x,t)} \mathcal{J}[q(x,t)] = q_F(x,t) + \mathbf{r}(x,t)^T (\mathbf{R} + \sigma_\epsilon^{-2}\mathbf{I})^{-1} (\mathbf{d} - \mathbf{q}_F)$$

Choice of PDE Error Estimates

The PDE error

$$\int_0^T \int_0^L \left(\frac{\partial q}{\partial t} + \frac{\partial}{\partial x} \left(u(x,t) q(x,t) \right) - Q(x,t) \right)^2 \; dx dt$$

in the cost function is weighted by its uncertainty estimate σ_f^{-2}. Existing approaches to specifying σ_f^{-2} include

- Order of numerical approximation
- Order of error in physics

Here we propose using regularization parameter selection methods. We assume the data uncertainty $\mathbf{C}_\epsilon$ is known.

Results for 4DVAR with Representers

L-curve

Plot

$$\mathcal{J}_{mod}[\hat{q}] = \sigma_f^{-2} \int_{T_0}^{T} \int_{\Omega} \left(\frac{\partial \hat{q}}{\partial t} + \nabla \cdot \vec{u}(x,t)\hat{q}(x,t) - Q(x,t) \right)^2 dx\, dt$$
$$= \sigma_f^{-2} \mathbf{h}^T \mathbf{P}^{-1} \mathbf{R} \mathbf{P}^{-1} \mathbf{h}$$

vs

$$\mathcal{J}_{data}[\hat{q}] = \sum_{m=1}^{M} \sigma_{\epsilon_m}^{-2} (d_m - \hat{q}(x_m, t_m))^2$$
$$= \mathbf{h}^T \mathbf{P}^{-1} \mathbf{C}_\epsilon \mathbf{P}^{-1} \mathbf{h}$$

and estimate the value of σ_f at the corner.

Results for 4DVAR with Representers

GCV

Optimal σ_f is the one that minimizes the GCV function

$$g(\sigma_f) = M \frac{\mathbf{h}^T \mathbf{P}^{-1} \mathbf{C}_\epsilon \mathbf{P}^{-1} \mathbf{h}}{\text{trace}(\mathbf{I} - \mathbf{R}^{\#})}$$

where the influence matrix is $\mathbf{R}^{\#} = \mathbf{R}(\mathbf{R} + \mathbf{C})^{-1}$.

χ^2 Discrepancy

Solve the nonlinear equation

$$\mathcal{J}[\hat{\mathbf{q}}] = \mathcal{J}_{data}[\hat{\mathbf{q}}] + \mathcal{J}_{mod}[\hat{\mathbf{q}}] = \mathbf{h}^T \mathbf{P}^{-1} \mathbf{h}$$

for σ_f.

Numerical Experiments

$$\frac{\partial q}{\partial t} + \nabla \cdot u(\mathbf{x},t)q(\mathbf{x},t) = S_0 exp(-kt - ar_0^2) + S_1 exp(-kt - ar_1^2)$$

where $r_i = x - x_i$. In all experiments $k = 0.5$, $x_0 = 32$ and $x_1 = 40$.

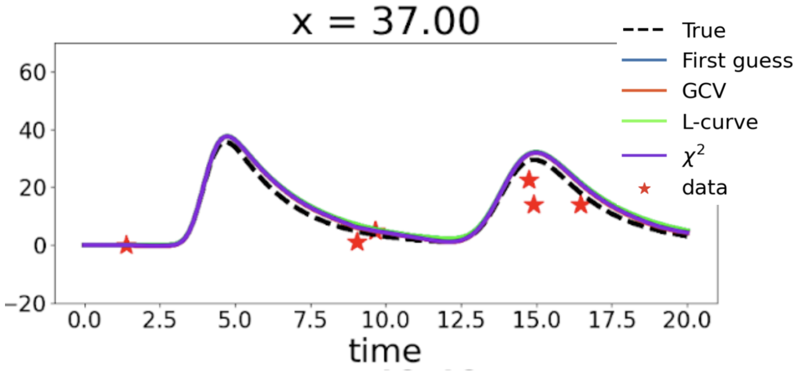
Experiment	B.C.	S_0	S_1	a
1	periodic	100	0	10
2	periodic	100	0	5
3	no flux	100	50	10
4	no flux	100	100	10

Estimates of PDE uncertainty σ_f

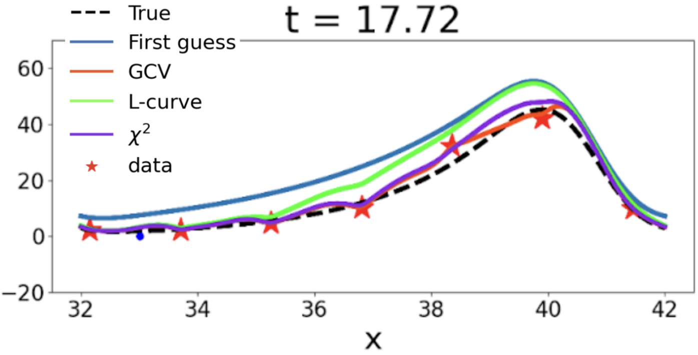
Random is noise added to k and a with standard deviation σ.
The mean of standard deviation of data noise is σ_ϵ.

Experiment	σ_ϵ	σ	L-curve	GCV	χ^2
1	0.5	0.1	2.66	0.09	0.07
2	0.15	0.5	0.04	18.7	2.0
3	0.35	0.2	0.498	0.018	0.001
4	0.22	0.6	0.0025	1.520	1.520

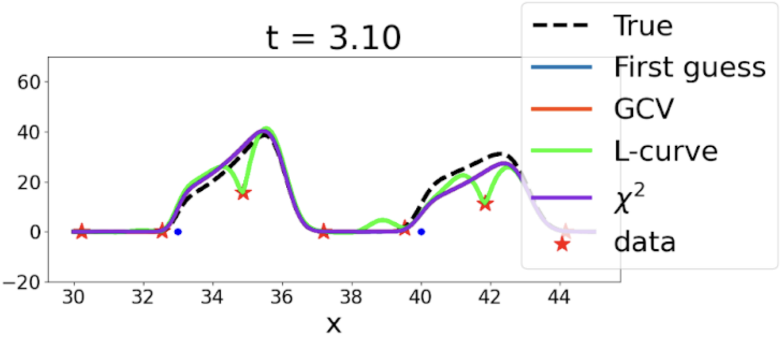
Experiment 1 - optimal concentration estimates over time



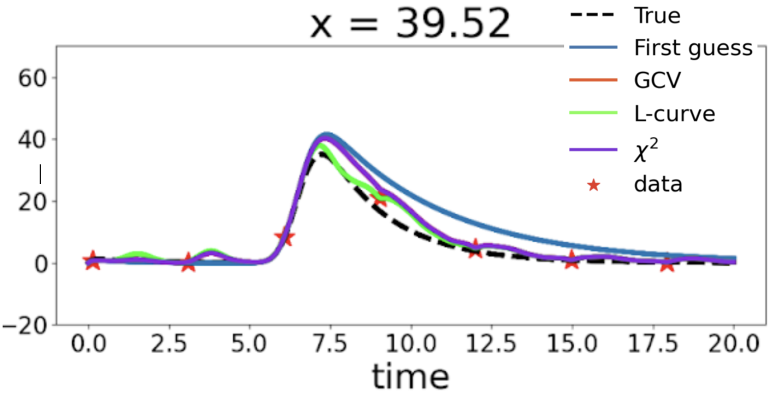
Experiment 2 - optimal concentration estimates over space



Experiment 3 - optimal concentration estimates over space



Experiment 4 - optimal concentration estimates over time



RMSE

Experiment	Data	Forward (q_F)	L-curve	GCV	χ^2
1	5.0944	2.0625	2.0625	1.7402	1.7930
2	3.4272	8.4616	3.2877	3.2040	3.5306
3	4.2152	2.1465	2.6059	2.1299	2.1431
4	2.5433	5.8943	3.0762	3.8050	3.8050

Summary and Conclusions

We present a new approach to estimating model errors or uncertainty for four dimensional variational data assimilation (4DVAR).

The approach

- utilizes the Representer Method which reduces the search space of state estimates to the size of the data space,
- formulates 4DVAR as an ill-posed inverse problem in order to use regularization parameter selection methods to estimate error or uncertainty in the forward PDE model.

Results include

- formulations for L-curve, GCV and χ^2 discrepancy principle methods for 4DVAR with Representers,
- error or uncertainty estimates for the PDE that accurately reflect if more weight should be given to the PDE or to the data,
- optimal state estimates that improve those from the forward PDE model or data.