State-dependent Preconditioning for Data Assimilation

Victor Trappler [1,2] Arthur Vidard [1]

[1]AIRSEA Research team – Inria – Laboratoire Jean Kuntzmann
[2]AI4Sim R&D team – Eviden (ex Bull/Atos)

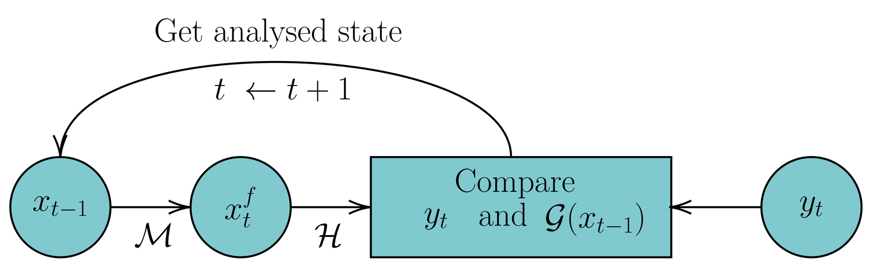
In short

Variational Data Assimilation requires the optimization of a high-dimensional function. This is usually done by linearizing the problem, and then inverting the Gauss-Newton matrix

¿ Can we build a state-dependent preconditioner which would help for the inversion of the linear system ?

Variational Data Assimilation

- $x \in \mathbb{R}^n$: state
- $\mathcal{M}: \mathbb{R}^n \to \mathbb{R}^n$: time propagator
- $\mathcal{H}: \mathbb{R}^n \to \mathbb{R}^m$: observation operator
- $y \in \mathbb{R}^m$: observations



- $\mathcal{G}$ composes the forward model and the observation operator, to compare with the available observation

$$\begin{aligned} \mathcal{G}: \mathbb{X} \subseteq \mathbb{R}^n &\longrightarrow \quad \mathbb{X} \quad \longrightarrow \quad \mathbb{R}^m \\ x &\longmapsto \mathcal{M}(x) \longmapsto (\mathcal{H}\circ\mathcal{M})(x) = \mathcal{G}(x) \end{aligned} \tag{1}$$

- The cost function to optimize to get the analysis is

$$J_{4D}(x) = \frac{1}{2}\|\mathcal{G}(x) - y\|^2_{R^{-1}} + \frac{1}{2}\|x - x^b\|^2_{B^{-1}} \tag{2}$$

and

$$x^a_{t-1} = \arg\min_{x\in\mathbb{X}} J_{4D}(x) \tag{3}$$

Incremental 4DVar

Outer and Inner loops: Minimization as a sequence of Linear Systems

- Linearize J around x (Linear Inverse Problem):

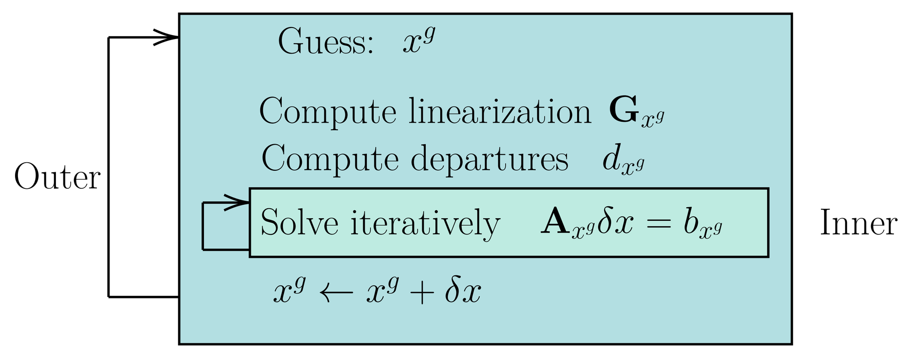
$$J_{\text{incr}}(x, \delta x) = \frac{1}{2}\|\mathbf{G}_x\delta x + \underbrace{(\mathcal{G}(x) - y)}_{-d_x}\|^2_{R^{-1}} + \frac{1}{2}\|\delta x + x - x^b\|^2_{B^{-1}} \tag{4}$$

- The optimal increment solves

$$\underbrace{\left(\mathbf{G}_x^T R^{-1}\mathbf{G}_x + B^{-1}\right)}_{\mathbf{A}_x}\delta x = \underbrace{-\mathbf{G}_x^T R^{-1} d_x - B^{-1}\left(x - x^b\right)}_{b_x} \tag{5}$$

where $\mathbf{A}_x$ Gauss-Newton Matrix $\iff$ Inverse of the posterior error cov matrix

$$\mathbf{A}_x = \mathbf{G}_x^T R^{-1}\mathbf{G}_x + B^{-1} \in \mathbb{R}^{n\times n} \text{ symmetric and spd} \tag{6}$$



In the Inner Loop

- $\mathbf{A}_x$ is spd, so **Conjugate Gradient** can be used
- Convergence rate depends on the spectrum of $\mathbf{A}_x$ *ie*
  - Condition number: $\kappa(\mathbf{A}_x) = \sigma_{\max}/\sigma_{\min} = \|\mathbf{A}_x\|\cdot\|\mathbf{A}_x^{-1}\|$
  - Clustering of eigenvalues at 1

State Dependent Preconditioner

Preconditioning

Instead of solving $\mathbf{A}_x\delta x = b_x$, solve $(L^T\mathbf{A}_x L)z = L^T b$ and $\delta x = Lz$

- $H = LL^T$ symmetric, positive definite, cheap to compute and to apply
- H should be *close* to $\mathbf{A}_x^{-1}$
- $1 \leq \kappa(H\mathbf{A}_x) \leq \kappa(\mathbf{A}_x)$

"One-fits-all" preconditioner do not exist, most include information on *spectrum* of $\mathbf{A}_x$, which depends on x

State-dependent preconditioner

We propose to construct a mapping

$$x \longmapsto H(x) \tag{7}$$

where $H(x)$ is a preconditioner well-suited for the linear system $\mathbf{A}_x\delta x = b_x$

Challenges

- $H(x) \in \mathbb{R}^{n\times n}$ is spd (ie $n(n+1)/2$ "free" parameters)
- $\mathbf{A}_x$ is not stored explicitly (only accessible as $\mathrm{TL}(x, z) = \mathbf{A}_x z$) and high-dimensional
- Independence with respect to the observations (thus to b_x)
- $H(x)$ should contain spectral information of $\mathbf{A}_x$

ML framework

Objective

- Construct a preconditioner using DNN, which requires **no** call to $\mathbf{A}_x$ when in use
- No access to $\mathbf{A}_x^{-1}$ during the training, no explicit construction of $\mathbf{A}_x$

Low-rank approximation

Let $U_\theta \in \mathbb{R}^{n\times r}$ whose columns are orthonormal vectors, and $\Lambda_\theta = \mathrm{diag}(\lambda_1, \dots, \lambda_r) \in \mathbb{R}_+^{r\times r}$

$$\tilde{\mathbf{A}}_\theta(x) = U_\theta\Lambda_\theta U_\theta^T \tag{8}$$

Low-rank approximation is optimal wrt to the Frobenius norm

$$\min_\theta \|\mathbf{A}_x - \tilde{\mathbf{A}}_\theta(x)\|^2_{\mathrm{F}} \tag{9}$$

but $\mathbf{A}_x$ cannot be explicitely constructed in practice: estimation of F-norm

$$\hat{\mathcal{L}}(\theta, x_i) = \frac{1}{n_z}\sum_{j=1}^{n_z}\|\mathbf{A}_{x_i}z_j - \tilde{\mathbf{A}}_\theta(x_i)z_j\|_2^2 \quad \text{with } z_j \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, I_n) \tag{10}$$

Possibility of **online training**:

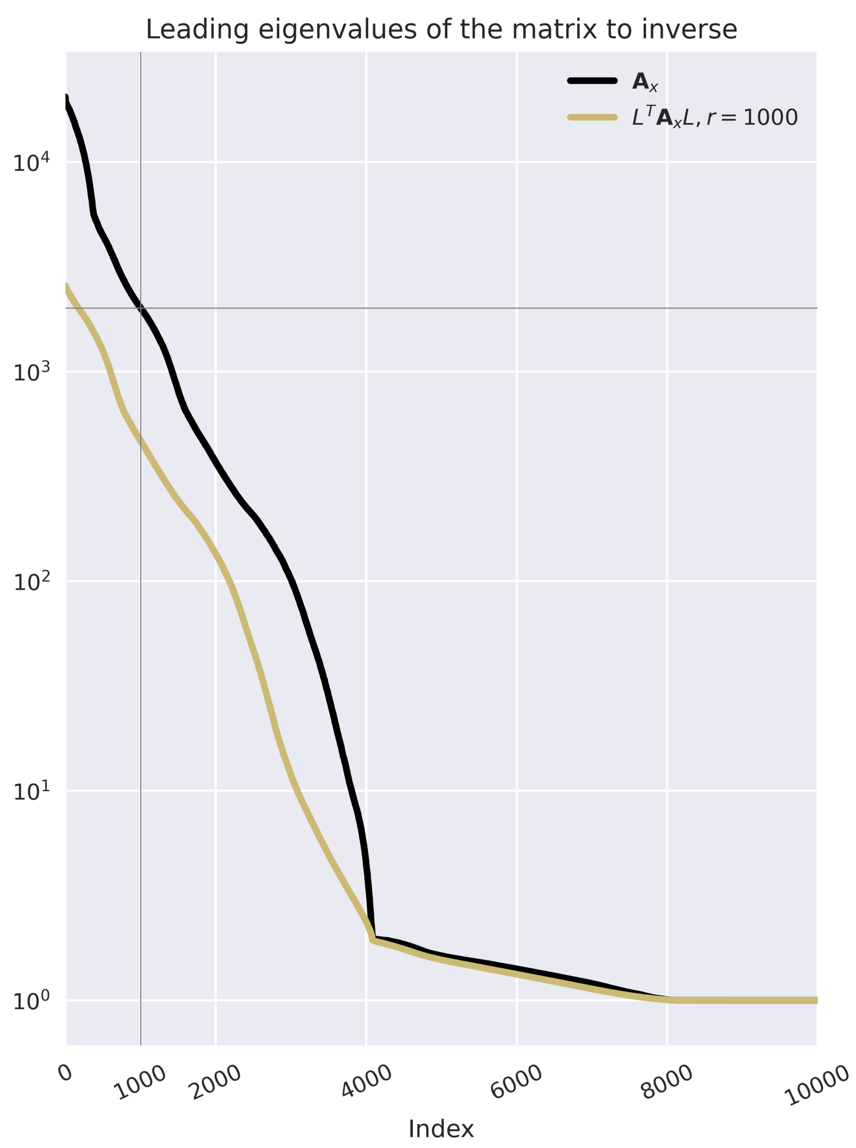
- Only $\mathbf{A}_x z_j$ needed instead of constructing and storing $\mathbf{A}_x$ explicitely

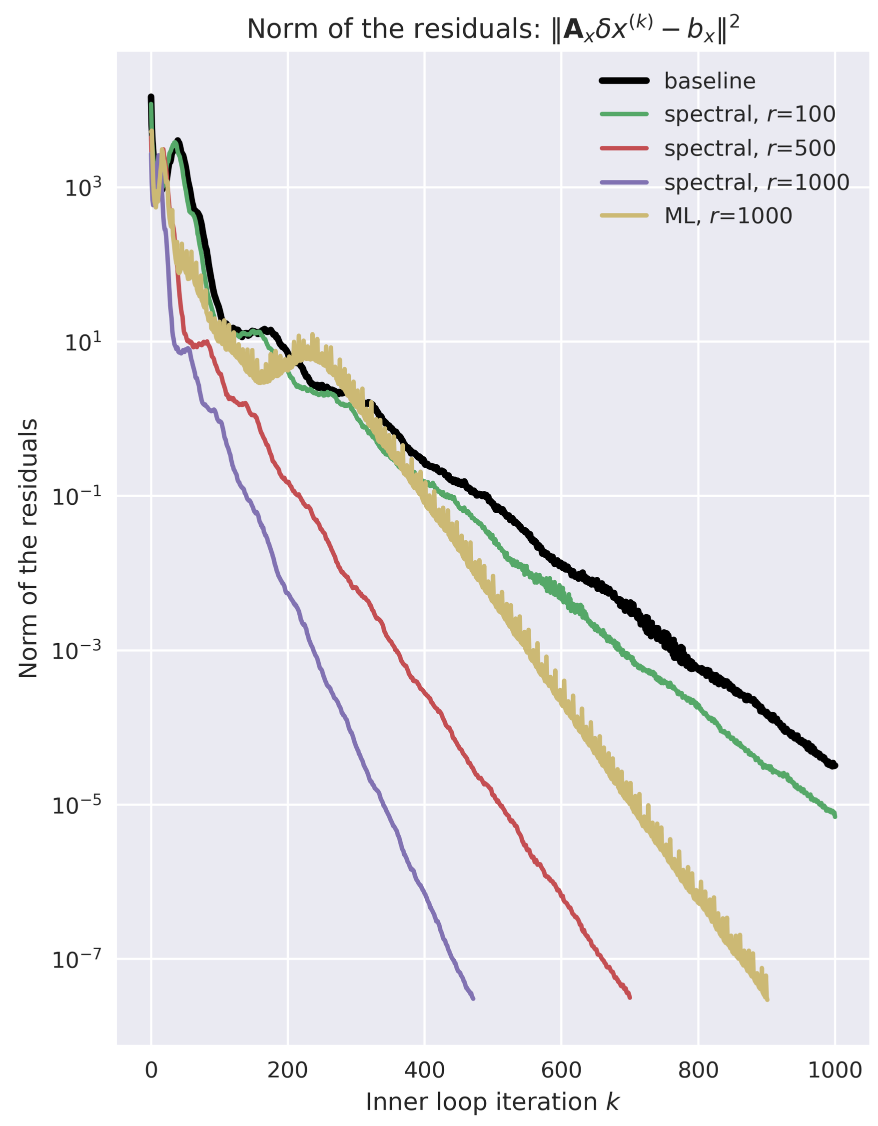
When trained, we can construct the preconditioner as ([5])

$$L_\theta = U_\theta\left(\Lambda_\theta^{\frac{1}{2}} - I_r\right)U_\theta^T + I_n, \quad \mathrm{sp}(H_\theta) = \left(1, \dots, 1, \lambda_r^{-1}, \dots, \lambda_1^{-1}\right) \tag{11}$$

Numerical Results

SW assimilation system, $n \approx 12000$, UNet-like architecture: η, u, v as features





Conclusion and further work

- We propose to use DNN in order to build a preconditioner for inverting the Gauss-Newton matrix, which is **state-dependent** (or parametrized spd matrices in general)
- Make use of spectral information
- Use this information for dimension reduction (with Bayesian inverse problem point of view) [3]
- Appropriate ML architecture to output large numbers of eigenvectors ?
- How to deal with changing observation operator ?

References

[1] N. Bousserez and Daven K. Henze. Optimal and scalable methods to approximate the solutions of large-scale Bayesian problems: Theory and application to atmospheric inversion and data assimilation. *Quarterly Journal of the Royal Meteorological Society*, 144(711):365–390, 2018.

[2] S. Gratton, A. S. Lawless, and N. K. Nichols. Approximate Gauss–Newton Methods for Nonlinear Least Squares Problems. *SIAM Journal on Optimization*, 18(1):106–132, January 2007.

[3] Alessio Spantini, Antti Solonen, Tiangang Cui, James Martin, Luis Tenorio, and Youssef Marzouk. Optimal low-rank approximations of Bayesian linear inverse problems. *arXiv:1407.3463 [math, stat]*, July 2015.

[4] Jemima M. Tabeart, Sarah L. Dance, Stephen A. Haben, Amos S. Lawless, Nancy K. Nichols, and Joanne A. Waller. The conditioning of least-squares problems in variational data assimilation. *Numerical Linear Algebra with Applications*, 25(5):e2165, 2018.

[5] J. Tshimanga, S. Gratton, A. T. Weaver, and A. Sartenaer. Limited-memory preconditioners, with application to incremental four-dimensional variational data assimilation. *Quarterly Journal of the Royal Meteorological Society*, 134(632):751–769, 2008.