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State-dependent Preconditioning for Data Assimilation

Victor Trappler, Arthur Vidard

► **To cite this version:**

Victor Trappler, Arthur Vidard. State-dependent Preconditioning for Data Assimilation: Application to a Shallow Water Assimilation system. ISDA 2023 - 9th International Symposium on Data Assimilation, Oct 2023, Bologna, Italy. , pp.1-1, 2023. hal-04309242

HAL Id: hal-04309242

<https://hal.science/hal-04309242>

Submitted on 27 Nov 2023

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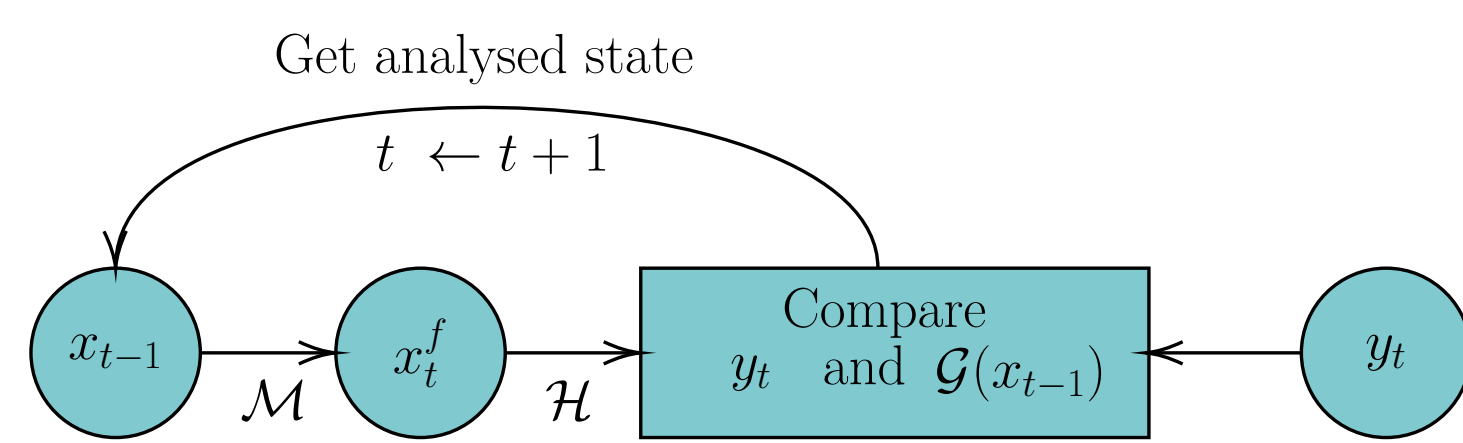
In short

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



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

$$\mathcal{G} : \mathbb{X} \subseteq \mathbb{R}^n \rightarrow \mathbb{X} \rightarrow \mathbb{R}^m \quad (1)$$

$$x \mapsto \mathcal{M}(x) \mapsto (\mathcal{H} \circ \mathcal{M})(x) = \mathcal{G}(x)$$

- The cost function to optimize to get the analysis is

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

and

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

Incremental 4DVar

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

- Linearize J around x (Linear Inverse Problem):

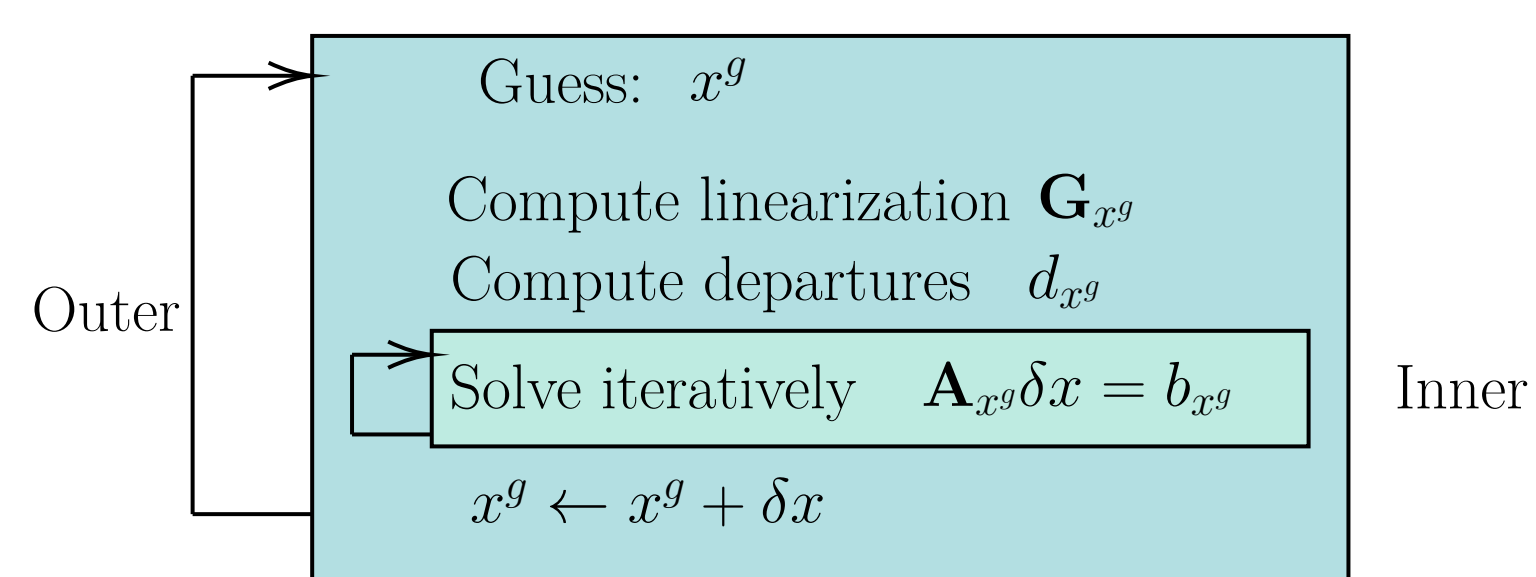
$$J_{\text{incr}}(x, \delta x) = \frac{1}{2} \|\mathbf{G}_x \delta x + \underbrace{(\mathcal{G}(x) - y)}_{-d_x}\|_{R^{-1}}^2 + \frac{1}{2} \|\delta x + x - x^b\|_{B^{-1}}^2 \quad (4)$$

- The optimal increment solves

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

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

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



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 $\delta x = L z$

- $H = LL^T$ 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

$$x \mapsto H(x) \quad (7)$$

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 $\text{TL}(x, z) = \mathbf{A}_x z$) 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 $\Lambda_\theta = \text{diag}(\lambda_1, \dots, \lambda_r) \in \mathbb{R}_+^{r \times r}$

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

Low-rank approximation is optimal wrt to the Frobenius norm

$$\min_\theta \|\mathbf{A}_x - \tilde{\mathbf{A}}_\theta(x)\|_F^2 \quad (9)$$

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

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

Possibility of **online training**:

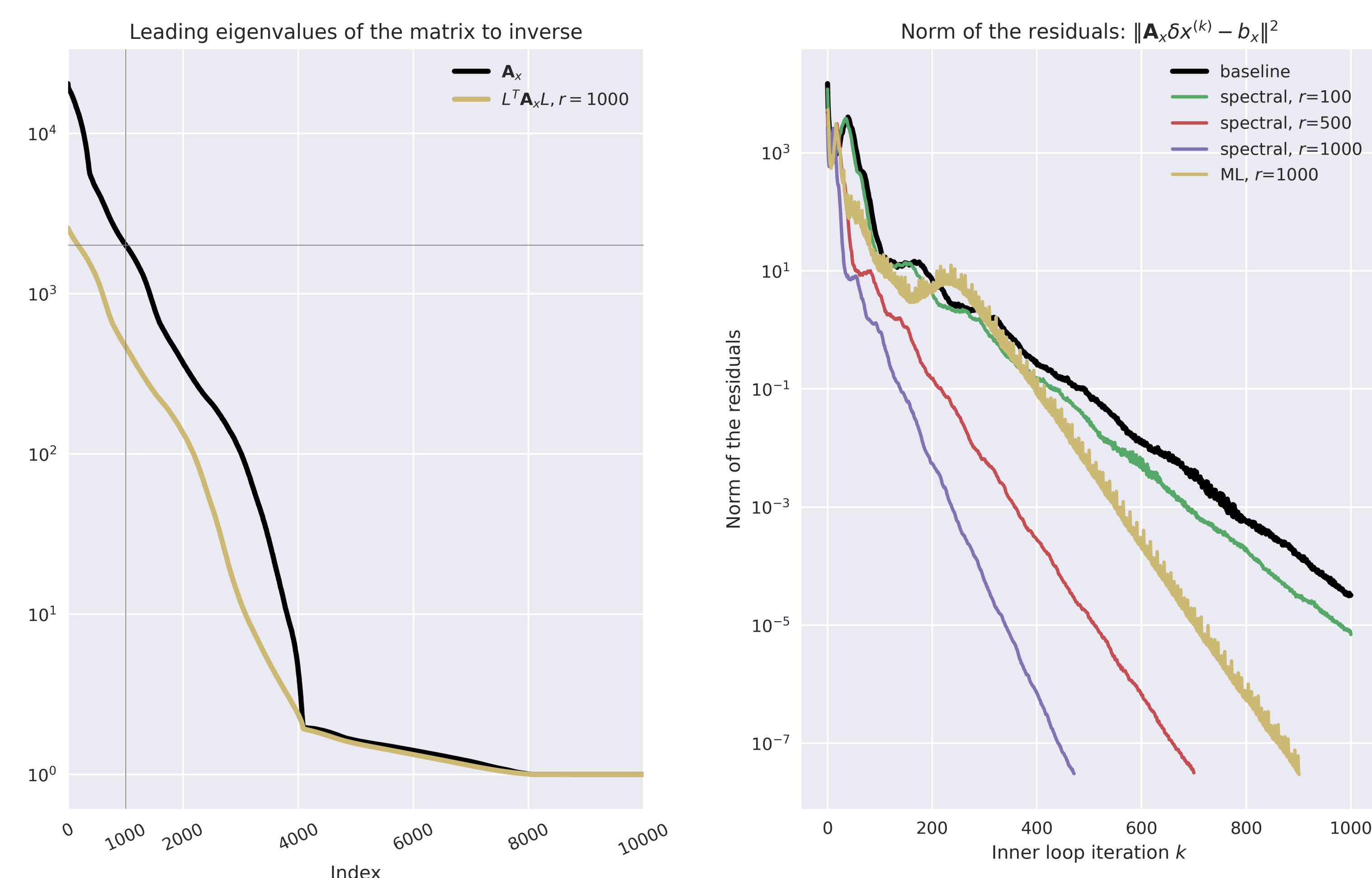
- Only $\mathbf{A}_x z_j$ needed instead of constructing and storing \mathbf{A}_x explicitly

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

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

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 ?

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