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State-dependent Preconditioning for Data Assimilation



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In short

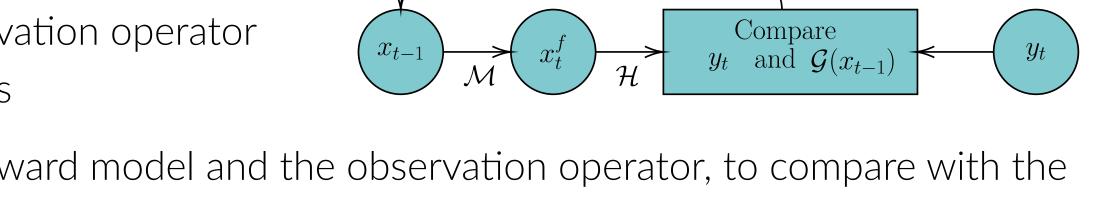
Variational Data Assimilation requires the optimization of a high-dimensional function. This is usually done by linearizing the problem, and then inverting the Gauss-Newton matrix **Can we build a state-dependent preconditioner which would help for the inversion of the linear system?**

(6)

Variational Data Assimilation



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



Get analysed state

 $t \leftarrow t + 1$

ullet composes the forward model and the observation operator, to compare with the available observation

$$\mathcal{G}: \mathbb{X} \subseteq \mathbb{R}^n \longrightarrow \mathbb{X} \longrightarrow \mathbb{R}^m$$

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

$$(1)$$

The cost function to optimize to get the analysis is

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

and

$$x_{t-1}^a = \underset{x \in \mathbb{X}}{\operatorname{arg\,min}} J_{4D}(x) \tag{3}$$

Incremental 4DVar

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

• Linearize J around x (Linear Inverse Problem):

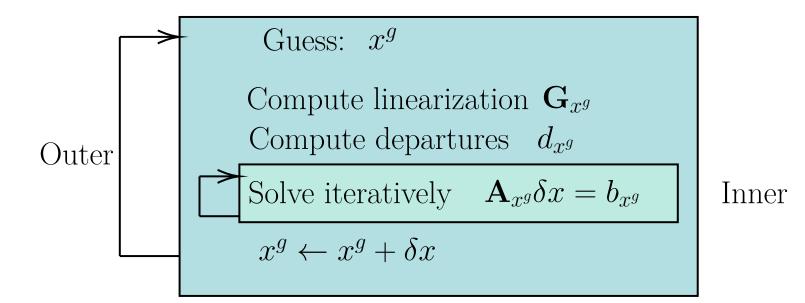
$$J_{\text{incr}}(x, \delta x) = \frac{1}{2} \|\mathbf{G}_x \delta x + \underbrace{(\mathcal{G}(x) - y)}_{-d_x}\|_{R^{-1}}^2 + \frac{1}{2} \|\delta x + x - x^b\|_{B^{-1}}^2$$
(4)

The optimal increment solves

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

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

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



In the Inner Loop

- \mathbf{A}_x is spd, so **Conjugate Gradient** can be used
- lacktriangle Convergence rate depends on the spectrum of ${f A}_x$ 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}
- $1 \le \kappa(H\mathbf{A}_x) \le \kappa(\mathbf{A}_x)$

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

State-dependent preconditioner

We propose to construct a mapping

$$x \longmapsto H(x)$$
 (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 A_x when in use
- No access to ${\bf A}_x^{-1}$ during the training, no explicit construction of ${\bf A}_x$

Low-rank approximation

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

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

(9)

Low-rank approximation is optimal wrt to the Frobenius norm

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

but A_x cannot be explicitely constructed in practice: estimation of F-norm

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

Possibility of online training:

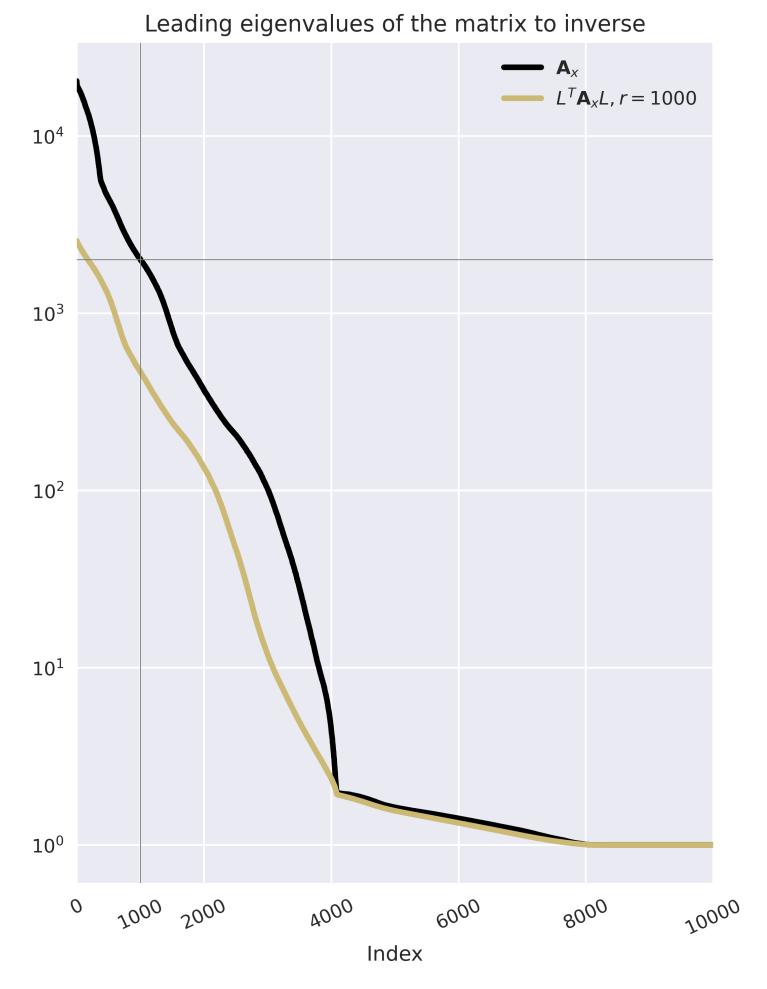
• Only $\mathbf{A}_x z_j$ needed instead of constructing and storing \mathbf{A}_x explicitely

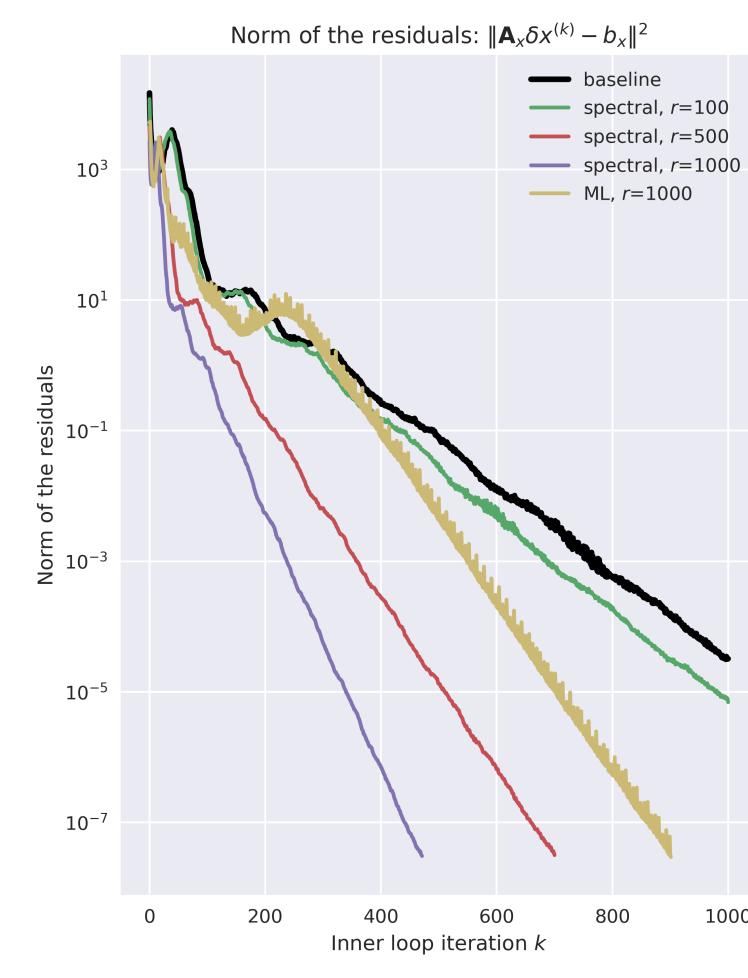
When trained, we can construct the preconditioner as ([5])

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