Hyper-parameter optimization for improving the performance of localization in an iterative ensemble smoother

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Outline

- Background
- Parameterized correlation-based localization
- Numerical examples
- Summary

Iterative ensemble smoother (IES)

- Basic iterative ensemble smoother (IES) without localization:

$$m_j^{i+1} = m_j^i + K\left(d^o - g\left(m_j^i\right)\right), j = 1, 2, \ldots, N_e$$

  - $d^o \in R^{p\times 1}$: p-dimensional observed field data
  - $m \in R^{n\times 1}$: n-dimensional reservoir model
  - i: iteration index
  - j: ensemble member index
  - g: reservoir simulator (ignoring model errors)
  - K: Kalman-gain matrix
  - N_e: ensemble size

Localization in the IES

- IES often runs with a small ensemble
  - Spurious correlations (sampling errors)
  - Rank deficiency
  - Degraded data assimilation (history matching) performance

- Localization often adopted for improved performance

- IES with (Kalman-gain) localization

$$m_j^{i+1} = m_j^i + (T \circ K)\left(d^o - g\left(m_j^i\right)\right), j = 1, 2, \ldots, N_e$$

  - $T \in [0,1]$: localization (or tapering) matrix
  - $T \circ K$: elementwise product between T and K

Localization in the IES

$$m_j^{i+1} = m_j^i + (T \circ K)\left(d^o - g\left(m_j^i\right)\right), j = 1, 2, \ldots, N_e$$

- Essential question: how to construct the tapering matrix T?

- Here the focus on correlation-based localization

Correlation-based localization

- Additional notations:

$$m_j^{i+1} = m_j^i + (T \circ K)\left(d^o - g\left(m_j^i\right)\right)$$

  - $\left[m_j^i\right]_s$: the s-th model variable of m_j^{i+1}
  - $\left[g\left(m_j^i\right)\right]_k$: the k-th element of $g\left(m_j^i\right)$
  - $T \equiv [t_{sk}]$
  - t_{sk}: element of T on the s-th row and the k-th column

- In correlation-based localization:

$$t_{sk} = h_\theta(\rho_{sk})$$

  - ρ_{sk}: sample correlation between the ensembles $\left[m_j^i\right]_s$ and $\left[g\left(m_j^i\right)\right]_k$, for $j = 1, 2, \ldots, N_e$
  - h_θ: tapering function, parameterized by a set of hyper-parameters θ

Correlation-based localization

- Example 1*:

$$t_{sk} = h_\theta(\rho_{sk})$$

$$h_\theta(\rho_{sk}) = h(|\rho_{sk}| > \theta) = \begin{cases} 1, if\ |\rho_{sk}| > \theta \\ 0, otherwise \end{cases} \quad \text{(Heaviside function)}$$

  - θ: threshold value (hard-thresholding)
  - θ empirically chosen, as in, e.g., Luo et. al*
  - Referred to as empirical tuning strategy hereafter

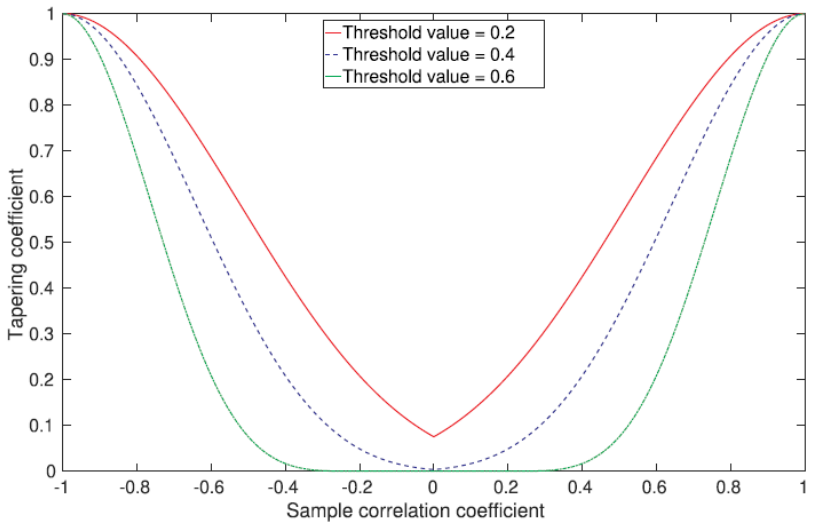
*Luo, X., Bhakta, T. and Naevdal, G., 2018. Correlation-based adaptive localization with applications to ensemble-based 4D-seismic history matching. *SPE Journal*, *23*(02), pp.396-427.

Correlation-based localization

- Example 2 (AutoAdaLoc)*:

$$t_{sk} = h_\theta(\rho_{sk})$$

$$h_\theta(\rho_{sk}) = h_{GC}\left(\frac{1 - |\rho_{sk}|}{1 - \theta}\right)$$



- h_{GC}: Gaspari-Cohn (GC) function
- θ: threshold value (soft-thresholding)
- θ chosen based on statistical analyses, before data assimilation starts;
- Referred to as prior tuning strategy hereafter

*Luo, X. and Bhakta, T., 2020. Automatic and adaptive localization for ensemble-based history matching. *Journal of Petroleum Science and Engineering*, *184*, p.106559.

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Hyper-parameters in correlation-based localization

$$t_{sk} = h_{GC}\left(\frac{1 - |\rho_{sk}|}{1-\theta}\right) \Rightarrow t_{sk} = h_{GC}\left(\frac{1 - |\rho_{sk}|}{\ell_k}\right)$$

- $\theta \equiv \{\ell_k, k = 1,2,\dots,p\}$: localization length scales varying for each observation data point (θ in the same size as field data d^o)
- Hyper-parameters can also vary over each model variable and each data point (i.e., $\theta \equiv \{\ell_{sk}, s = 1,2,\dots,n;\ k = 1,2,\dots,p\}$), but maybe too many to be practical (a lighter choice: $\theta \equiv \{\ell_s, s = 1,2,\dots,n\}$, i.e., varying over each model variable)
- Localization called parameterized AutoAdaLoc (P-AutoAdaLoc) scheme hereafter
- θ iteratively updated during data assimilation
- Referred to as posterior tuning strategy hereafter

Continuous hyper-parameter optimization (CHOP)*

- CHOP designed to estimate (an ensemble of) algorithmic hyper-parameters $\{\theta_j^i\}_{j=1}^{N_e}$ in a generic model update formula $m_j^{i+1} = f(m_j^i, \theta_j^i | d^o)$

- Containing as a special case an IES with parameterized localization

$$m_j^{i+1} = f\left(m_j^i, \theta_j^i \middle| d^o\right) \equiv m_j^i + (T(\theta_j^i) \circ K)\left(d^o - g\left(m_j^i\right)\right)$$

*Luo, X. and Xia, C.A, 2022. Continuous Hyper-parameter OPtimization (CHOP) in an ensemble Kalman filter. Frontiers in Applied Mathematics and Statistics, 2022, 8, p. 1021551.

Continuous hyper-parameter optimization (CHOP)

- Two-step update procedure: Given ensembles of $\{m_j^i\}_{j=1}^{N_e}$ and $\{\theta_j^i\}_{j=1}^{N_e}$ at the i-th iteration step

  - Step 1: model update (through an IES): ← existing in the original IES algorithm

$$m_j^{i+1} = m_j^i + \left(T\left(\theta_j^i\right) \circ K\right)\left(d^o - g\left(m_j^i\right)\right), j = 1, 2, \dots, N_e$$

K computed with respect to $\{m_j^i\}_{j=1}^{N_e}$ and $\{g(m_j^i)\}_{j=1}^{N_e}$

  - Forward simulations to obtain $\{g(m_j^{i+1})\}_{j=1}^{N_e}$: ← existing in the original IES algorithm

  - Step 2: hyper-parameter update (also through an IES): ← new component

$$\theta_j^{i+1} = \theta_j^i + \left(T\left(\theta_j^i\right) \circ \widetilde{K}\right)\left(d^o - g\left(m_j^{i+1}\right)\right), j = 1, 2, \dots, N_e$$

$\widetilde{K}$ computed with respect to $\{\theta_j^i\}_{j=1}^{N_e}$ and $\{g(m_j^{i+1})\}_{j=1}^{N_e}$

Continuous hyper-parameter optimization (CHOP)*

$$\theta_j^{i+1} = \theta_j^i + \left(T\left(\theta_j^i\right) \circ \widetilde{K}\right)\left(d^o - g\left(m_j^{i+1}\right)\right), j = 1, 2, \ldots, N_e$$

- Optimization criterion: $\left\{\theta_j^{i+1}\right\}_{j=1}^{N_e}$ chosen to minimize/reduce average data mismatch between $\left\{g\left(m_j^{i+1}\right)\right\}_{j=1}^{N_e}$ and d^o

- CHOP converted to a normal parameter estimation problem (and solved by IES)

For those who are interested: $\left\{\theta_j^{i+1}\right\}_{j=1}^{N_e}$ approximate solution to the following minimum-average cost (MAC) problem

$$\min_{\left\{\theta_j^{i+1}\right\}_{j=1}^{N_e}} \frac{1}{N_e}\sum_j L\left(\theta_j^{i+1}\right)$$

$$L\left(\theta_j^{i+1}\right) = \frac{1}{2}\left(d^o - g\left(f\left(m_j^i, \theta_j^{i+1}|d^o\right)\right)\right)^T C_d^{-1}\left(d^o - g\left(f\left(m_j^i, \theta_j^{i+1}|d^o\right)\right)\right) + \frac{\gamma}{2}\left(\theta_j^{i+1} - \theta_j^i\right)^T C_\theta^{-1}\left(\theta_j^{i+1} - \theta_j^i\right)$$

*Luo, X., Cruz, W., Zhang, X. L., & Xiao, H. Hyper-Parameter Optimization for Improving the Performance of Localization in an Iterative Ensemble Smoother. Preprint, *available at SSRN 4388296*.

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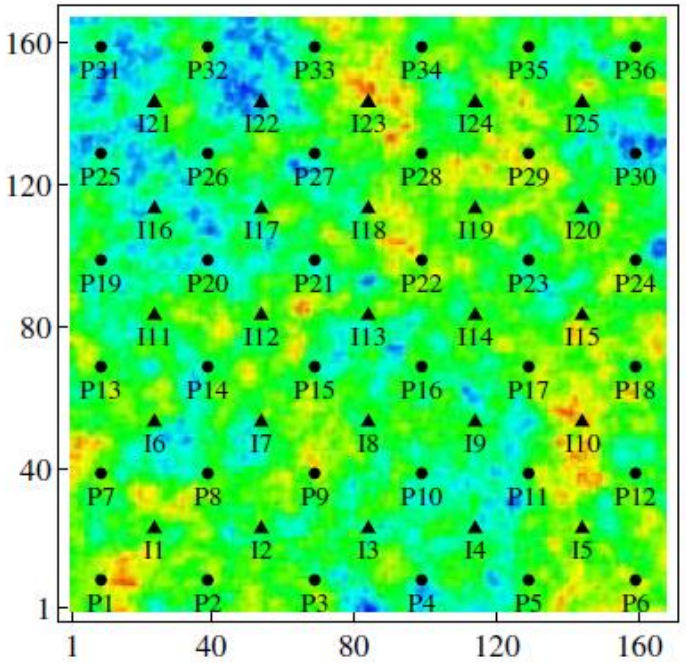
2D case: multiple 5spots (M-5Spots)*



Experimental settings	
Model information	167 x 167 36 producers + 25 injectors Uncertain parameters: PERMX
Production data used for history matching	WOPR, WWPR, WBHP, WWIR total number = 1098
HM algorithm	IES with AutoAdaLoc vs. IES with P-AutoAdaLoc Ensemble size: 100
Initial ensemble of localization length scales	i.i.d samples from the uniform distribution on the interval [0.23, 0.43] (manual choice)

*Chen, Y. and Oliver, D.S., 2010. Cross-covariances and localization for EnKF in multiphase flow data assimilation. *Computational Geosciences*, *14*(4), pp.579-601.

2D case: multiple 5spots (M-5Spots)

Table 2: Data mismatch (DM), root mean squared error (RMSE) and ensemble spread in the M-5Spots case.

	Initial ensemble	Final ensemble (AutoAdaLoc)	Final ensemble (P-AutoAdaLoc)
DM (mean $\pm$ STD)	$(1.7091 \pm 0.3517) \times 10^7$	$(1.7896 \pm 0.5328) \times 10^5$	$\mathbf{(7.2535 \pm 1.1881) \times 10^4}$
RMSE (mean $\pm$ STD)	1.6647 ± 0.0707	1.3811 ± 0.0357	$\mathbf{1.2550 \pm 0.0340}$
Spread	1.1864	0.9293	**0.5819**

2D case: multiple 5spots (M-5Spots)

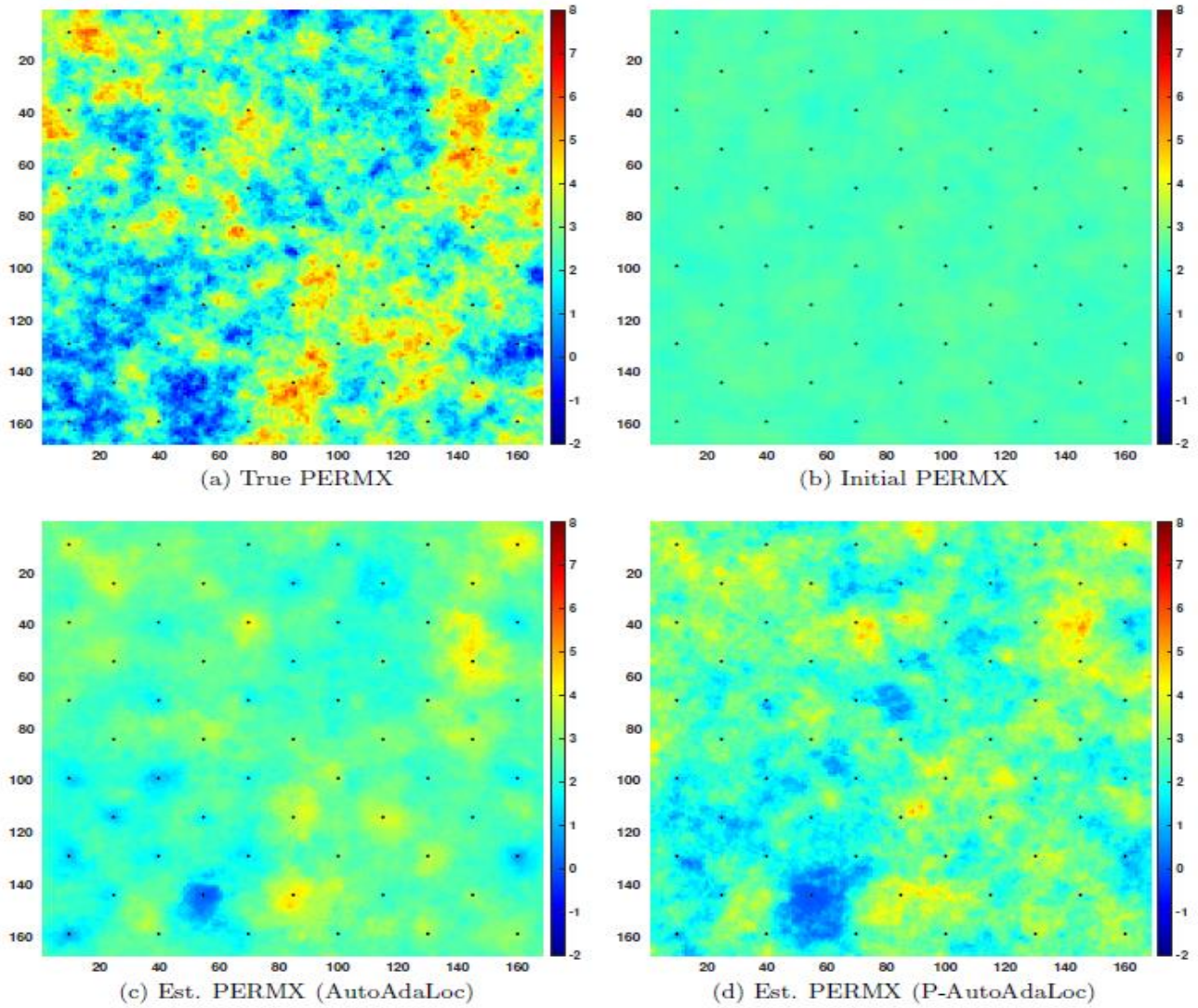
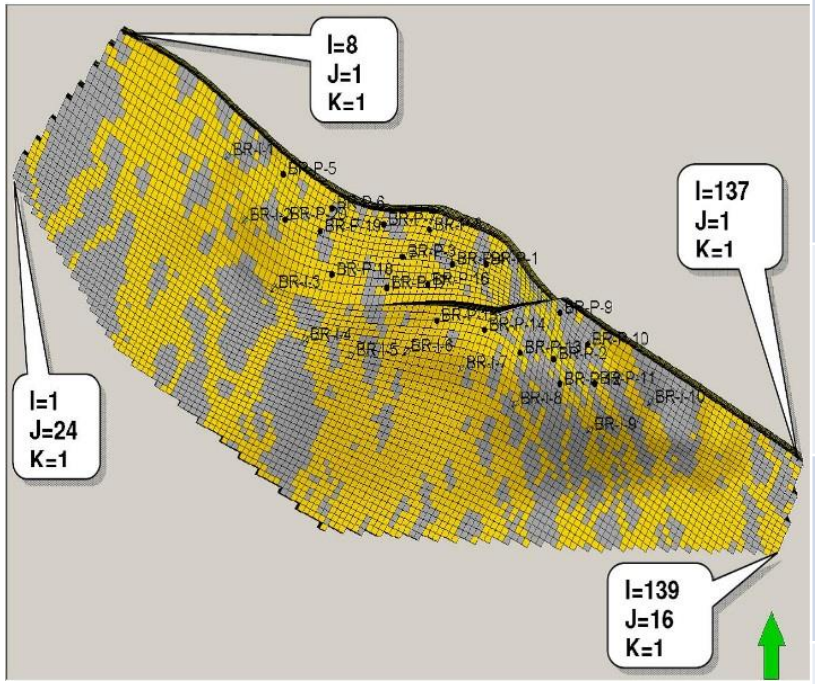


Figure 5: PERMX maps (in the natural logarithmic scale) with respect to (a) the reference model; (b) the mean of the initial ensemble; (c) – (d) the means of the final estimated (est.) ensembles obtained by the IES algorithm with the AutoAdaLoc and the P-AutoAdaLoc schemes, respectively, in the M-5Spots case. In all the maps, the small dots indicate the locations of wells.

3D case: Brugge benchmark



Grid geometry of the Brugge field

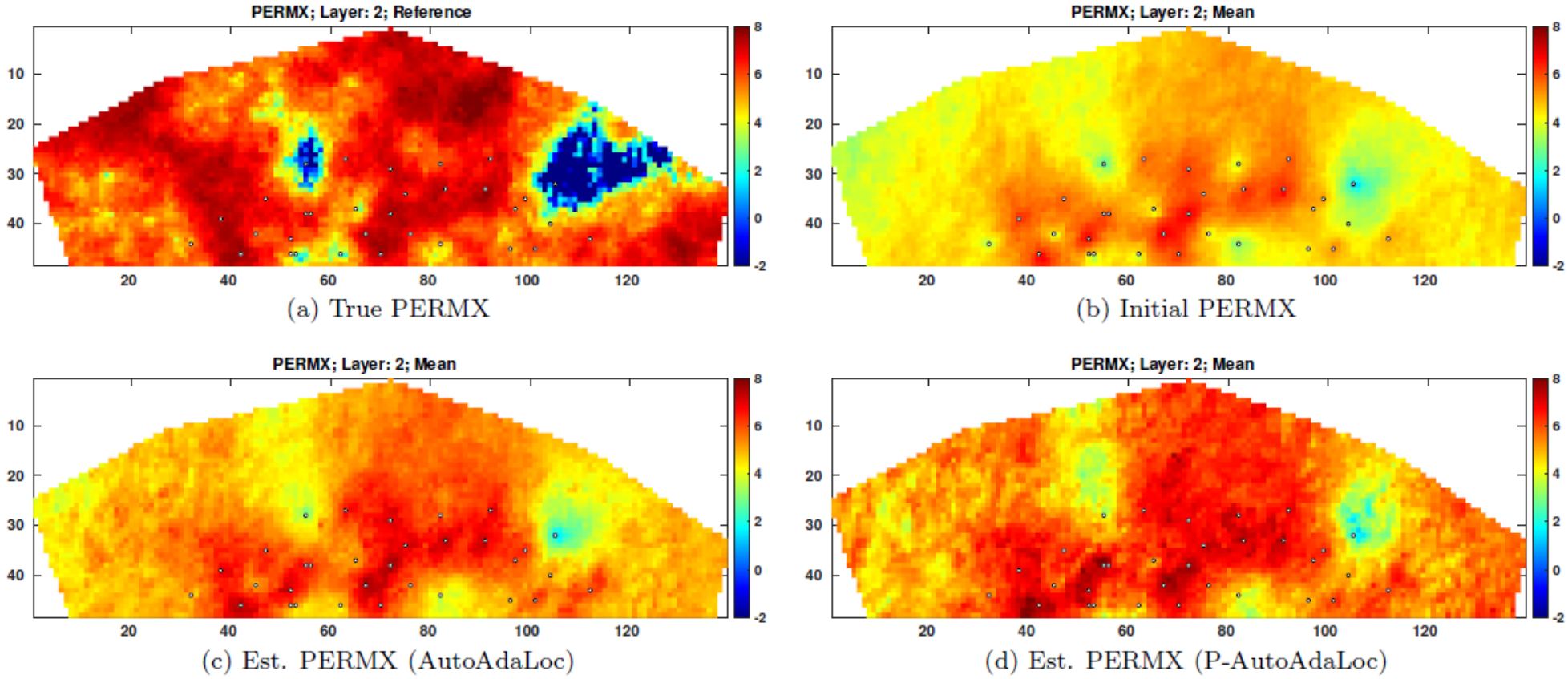
Experimental settings	
Model information	139 x 48 x 9 20 producers + 10 injectors Uncertain parameters: PERMX, PERMY, PERMZ, PORO
Production data used for history matching	WOPR, WWCT, WBHP total number = 1400
HM algorithm	IES with AutoAdaLoc vs. IES with P-AutoAdaLoc Ensemble size: 103
Initial ensemble of localization length scales	i.i.d samples from the uniform distribution on the interval [0.23, 0.43] (manual choice)

3D case: Brugge benchmark

Table 3: Data mismatch (DM), root mean squared error (RMSE) and ensemble spread in the Brugge benchmark case.

	Initial ensemble	Final ensemble (AutoAdaLoc)	Final ensemble (P-AutoAdaLoc)
DM (mean $\pm$ STD)	$(0.3623 \pm 1.4900) \times 10^{10}$	$(0.9481 \pm 1.9730) \times 10^{7}$	$\mathbf{(3.9842 \pm 7.0173) \times 10^{5}}$
Total RMSE (mean $\pm$ STD)	1.5450 ± 0.3362	1.2610 ± 0.1663	$\mathbf{1.1645 \pm 0.1046}$
RMSE of PERMX (mean $\pm$ STD)	1.6585 ± 0.3827	1.3498 ± 0.1982	$\mathbf{1.2399 \pm 0.1205}$
RMSE of PERMY (mean $\pm$ STD)	1.6612 ± 0.3794	1.3546 ± 0.1959	$\mathbf{1.2444 \pm 0.1197}$
RMSE of PERMZ (mean $\pm$ STD)	2.0077 ± 0.4096	1.6426 ± 0.1937	$\mathbf{1.5282 \pm 0.1307}$
RMSE of PORO (mean $\pm$ STD)	0.0302 ± 0.0033	0.0298 ± 0.0031	$\mathbf{0.0259 \pm 0.0018}$
Spread	0.8661	0.6308	**0.5435**

3D case: Brugge benchmark

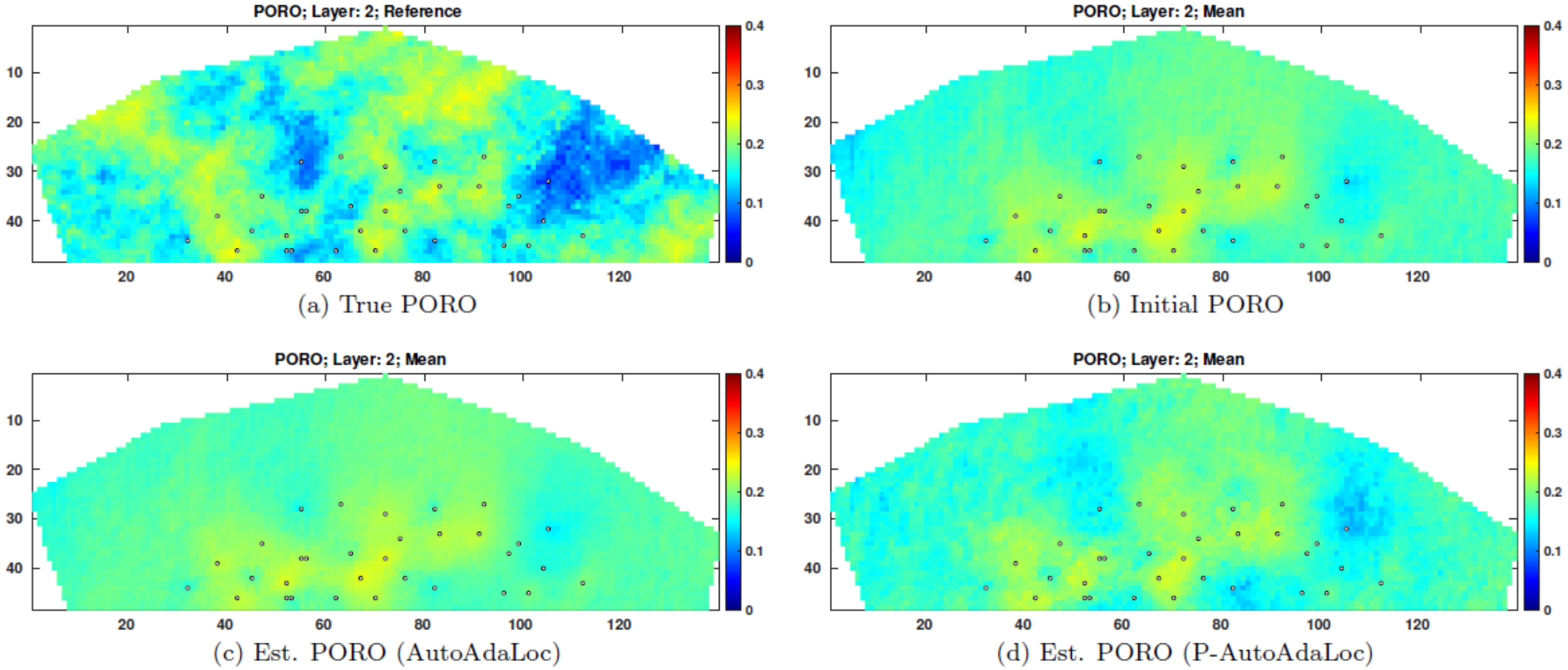


(a) True PERMX (b) Initial PERMX

(c) Est. PERMX (AutoAdaLoc) (d) Est. PERMX (P-AutoAdaLoc)

Figure 8: PERMX maps (in the natural logarithmic scale) on Layer 2 of (a) the reference model; (b) the mean reservoir model of the initial ensemble; (c) – (d) the mean reservoir models of the final estimated (est.) ensembles obtained by the IES algorithm with the AutoAdaLoc and the P-AutoAdaLoc schemes, respectively, in the Brugge benchmark case. In all the maps, the small dots indicate the locations of wells.

3D case: Brugge benchmark



(a) True PORO (b) Initial PORO

(c) Est. PORO (AutoAdaLoc) (d) Est. PORO (P-AutoAdaLoc)

Figure 9: As in Figure 8, but for PORO map on Layer 2 of the Brugge benchmark case.

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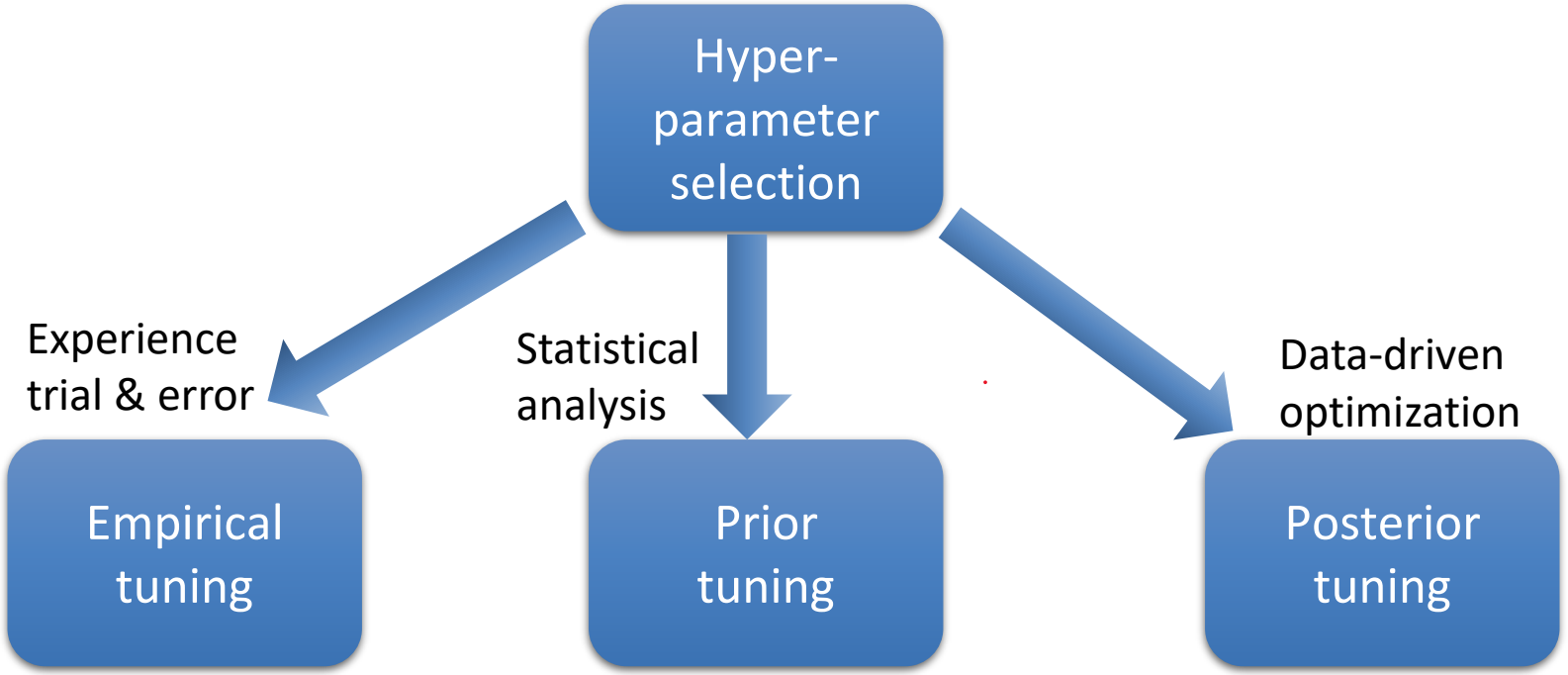
Summary



Example:	Correlation-based localization with hard-thresholding (Luo et. al 2018)	AutoAdaLoc (Luo & Bhakta 2020)	P-AutoAdaLoc (current work)

Q&A

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- *The NCS2030 petro-center, which is funded by the Research Council of Norway (project number 331644) and industry partners AkerBP, DNO, Equinor, Halliburton, Okea, SLB, Vår Energy and Wintershall DEA.*

Continuous hyper-parameter optimization (CHOP)

Algorithm 1 Pseudo-code of the IES algorithm equipped with the original AutoAdaLoc localization scheme. The texts in red highlight places where differences take place, in comparison to the pseudo-code in Algorithm 2.

Require: Initial ensembles of reservoir models $\mathbf{M}^0 = \{\mathbf{m}_j^0\}_{j=1}^{N_e}$, simulated observations $\{\mathbf{g}(\mathbf{m}_j^0)\}_{j=1}^{N_e}$ and $\mathbf{g}(\overline{\mathbf{m}}^0)$; Initial regularization parameter γ^0

Construct the tapering matrix $\mathbf{T}$ ▷ cf. Eqs. 14 – 16
Iteration index $i \leftarrow 0$; IES not stopped $\leftarrow$ True
while IES not stopped **do**
  Calculate the Kalman-gain like matrix $\mathbf{K}^i$ for reservoir model update, e.g.,
    $\mathbf{K}^i = \mathbf{S}_m^i(\tilde{\mathbf{S}}_g^i)^T \left(\tilde{\mathbf{S}}_g^i(\tilde{\mathbf{S}}_g^i)^T + \gamma^i \mathbf{I}_p\right)^{-1}$ ▷ cf. Eqs. 4 – 9
  Update the reservoir models $\mathbf{m}_j^i$, e.g.,
    $\mathbf{m}_j^{i+1} = \mathbf{m}_j^i + \left(\mathbf{T} \circ \mathbf{K}^i\right)\left(\tilde{\mathbf{d}}_j^o - \tilde{\mathbf{g}}\left(\mathbf{m}_j^i\right)\right)$ ▷ cf. Eq. 18
  Run reservoir simulations to get the simulated observations $\{\mathbf{g}(\mathbf{m}_j^{i+1})\}_{j=1}^{N_e}$ and $\mathbf{g}(\overline{\mathbf{m}}^{i+1})$,
  Check data mismatch and update the value of γ^i ▷ cf. Luo et al. (2015)
  Apply stopping criteria to decide whether to stop the IES or not ▷ cf. Luo et al. (2015)
  $i \leftarrow i+1$
end while

Algorithm 2 Pseudo-code of the IES algorithm equipped with the P-AutoAdaLoc localization scheme. The texts in red highlight places where differences take place, in comparison to the pseudo-code in Algorithm 1.

Require: Initial ensembles of reservoir models $\mathbf{M}^0 = \{\mathbf{m}_j^0\}_{j=1}^{N_e}$, simulated observations $\{\mathbf{g}(\mathbf{m}_j^0)\}_{j=1}^{N_e}$ and $\mathbf{g}(\overline{\mathbf{m}}^0)$, localization length scales $\mathbf{L}^0 = \{\boldsymbol{\ell}_j^0\}_{j=1}^{Ne}$; Initial regularization parameter γ^0

Iteration index $i \leftarrow 0$; IES not stopped $\leftarrow$ True
while IES not stopped **do**
  Calculate the Kalman-gain like matrix $\mathbf{K}^i$ for reservoir model update, e.g.,
    $\mathbf{K}^i = \mathbf{S}_m^i(\tilde{\mathbf{S}}_g^i)^T \left(\tilde{\mathbf{S}}_g^i(\tilde{\mathbf{S}}_g^i)^T + \gamma^i \mathbf{I}_p\right)^{-1}$ ▷ cf. Eqs. 4 – 9
  for $j = 1, 2, \cdots, N_e$ **do**
    Construct the tapering matrix $\mathbf{T}\left(\boldsymbol{\ell}_j^i\right)$ with the set of length scales $\boldsymbol{\ell}_j^i$ ▷ cf. Eq. 19
    Update the reservoir models $\mathbf{m}_j^i$, e.g.,
      $\mathbf{m}_j^{i+1} = \mathbf{m}_j^i + \left(\mathbf{T}\left(\boldsymbol{\ell}_j^i\right) \circ \mathbf{K}^i\right)\left(\tilde{\mathbf{d}}_j^o - \tilde{\mathbf{g}}\left(\mathbf{m}_j^i\right)\right)$ ▷ cf. Eq. 18
  end for
  Run reservoir simulations to get the simulated observations $\{\mathbf{g}(\mathbf{m}_j^{i+1})\}_{j=1}^{N_e}$ and $\mathbf{g}(\overline{\mathbf{m}}^{i+1})$,
  Calculate the Kalman-gain like matrix $\mathbf{K}_\ell^i$ for hyper-parameter update, e.g.,
    $\mathbf{K}_\ell^i = \mathbf{S}_\ell^i(\tilde{\mathbf{S}}_g^{i+1})^T \left(\tilde{\mathbf{S}}_g^{i+1}(\tilde{\mathbf{S}}_g^{i+1})^T + \gamma^i \mathbf{I}_p\right)^{-1}$ ▷ cf. Eqs. 25 – 30
  for $j = 1, 2, \cdots, N_e$ **do**
    Construct the tapering matrix $\mathbf{T}_\ell\left(\boldsymbol{\ell}_j^i\right)$ with the set of length scales $\boldsymbol{\ell}_j^i$ ▷ similar to Eq. 19
    Update the set of localization length scale $\boldsymbol{\ell}_j^i$, e.g.,
      $\boldsymbol{\ell}_j^{i+1} = \boldsymbol{\ell}_j^i + \left(\mathbf{T}_\ell\left(\boldsymbol{\ell}_j^i\right) \circ \mathbf{K}_\ell^i\right)\left(\tilde{\mathbf{d}}_j^o - \tilde{\mathbf{g}}\left(\mathbf{m}_j^{i+1}\right)\right)$ ▷ cf. Eq. 31
  end for
  Check data mismatch and update the value of γ^i ▷ cf. Luo et al. (2015)
  Apply stopping criteria to decide whether to stop the IES or not ▷ cf. Luo et al. (2015)
  $i \leftarrow i+1$
end while