GAR: Generalized Autoregression for Multi-Fidelity Fusion


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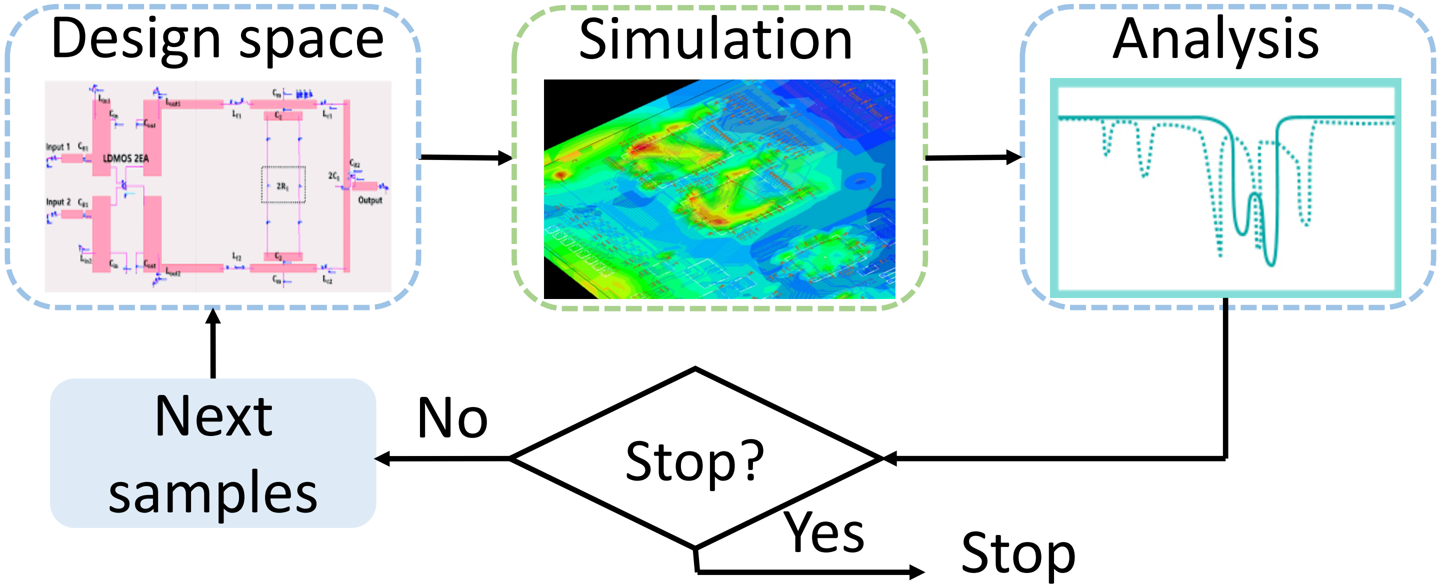
Zen Xing


Wei W. Xing

Multi-Fidelity Fusion Motivation

Circuit design optimization as an example:



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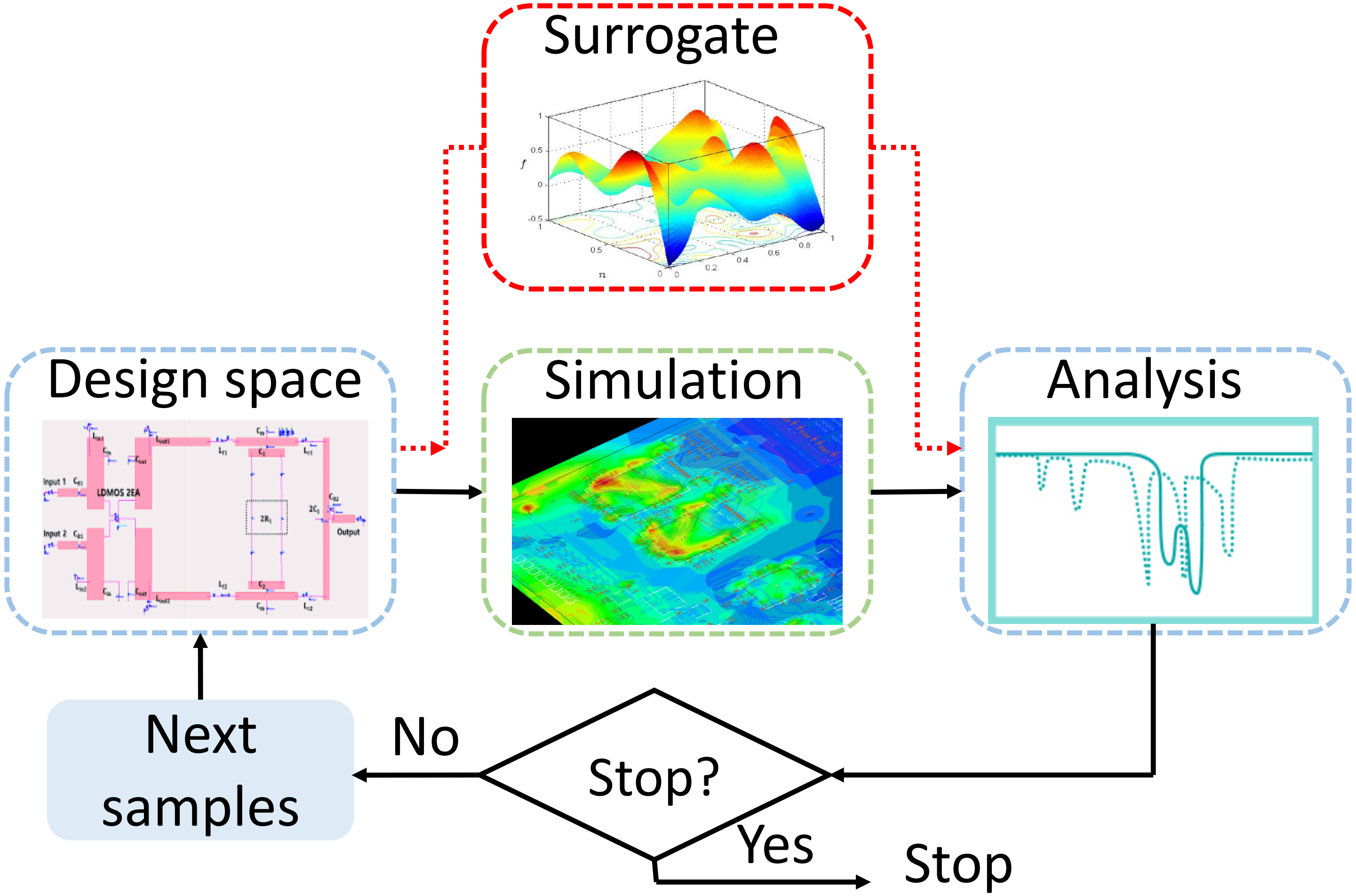
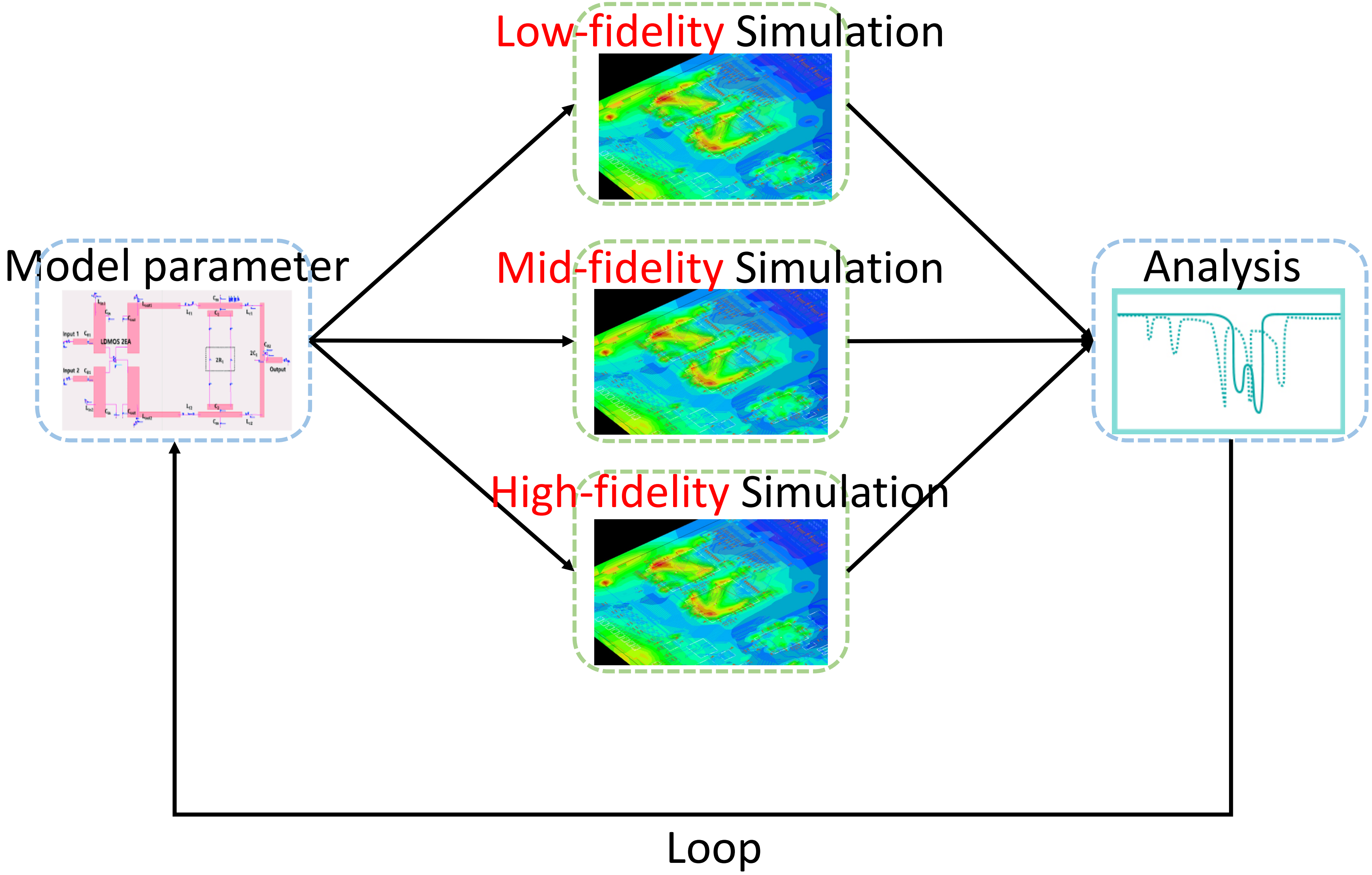


Multi-Fidelity Fusion Motivation



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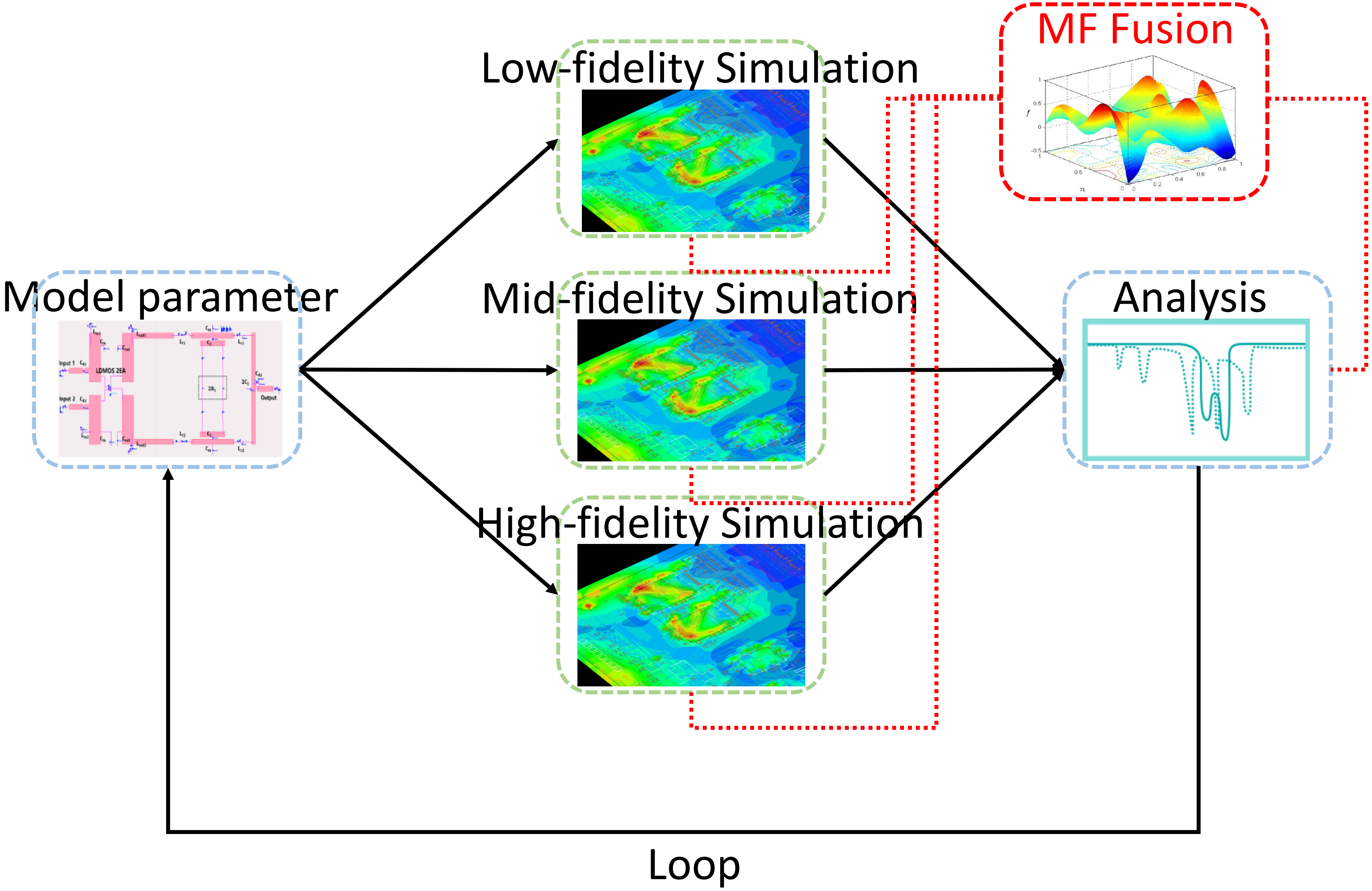

Classic Multi-Fidelity Fusion: Autoregression

$$f^h(\mathbf{x}) = \rho \underbrace{f^l(\mathbf{x})}_{\text{GP}} + \underbrace{f^r(\mathbf{x})}_{\text{GP}},$$

M. Kennedy. Predicting the output from a complex computer code when fast approximations are available. 87(1):1–13. ISSN 0006-3444, 1464-3510.

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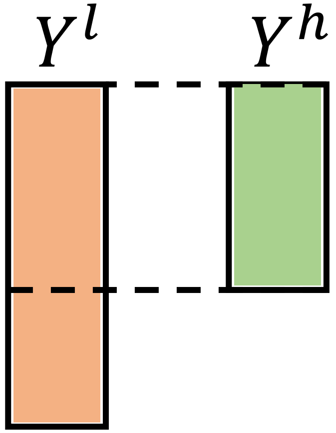


The subset structure

Likelihood

$$\log p(\mathbf{Y}^l, \mathbf{Y}^h) = \underbrace{-\frac{N^L}{2} log(2\pi) - \frac{1}{2}\log|\mathbf{K}^l| - \frac{1}{2}(\mathbf{Y}^l)^T(\mathbf{K}^l)^{-1}\mathbf{Y}^l}_{\mathcal{L}^l} \underbrace{-\frac{N^h}{2} log(2\pi) - \frac{1}{2}\log|\mathbf{K}^r| - \frac{1}{2}(\mathbf{Y}^r)^T(\mathbf{K}^r)^{-1}\mathbf{Y}^r}_{\mathcal{L}^r}$$

Posterior

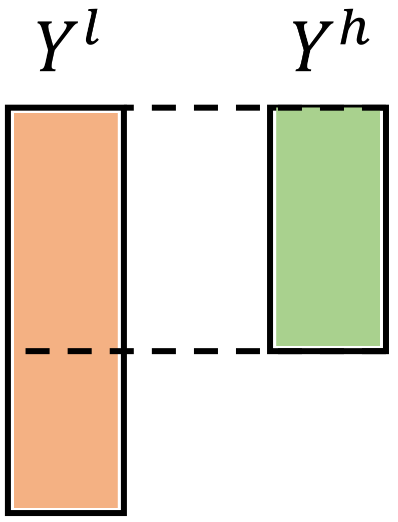
$$\mu^h_* = \left[\rho \mathbf{k}^l(\mathbf{x}_*, \mathbf{X}^l)(\mathbf{K}^l)^{-1}\right]\mathbf{Y}^l + \mathbf{k}^r(\mathbf{x}_*, \mathbf{X}^h)(\mathbf{K}^r)^{-1}\mathbf{Y}^r$$

$$\sigma^h_* = \rho^2\left(\mathbf{k}^l(\mathbf{x}_*, x_*) - (\mathbf{k}^l_*)^T(\mathbf{K}^l)^{-1}\mathbf{k}^l_*\right) + \left(\mathbf{k}^r(\mathbf{x}_*, \mathbf{x}_*) - (\mathbf{k}^r_*)^T(\mathbf{K}^r)^{-1}\mathbf{k}^r_*\right)$$

Classic Multi-Fidelity Fusion: Autoregression

$$f^h(\mathbf{x}) = \rho f^l(\mathbf{x}) + f^r(\mathbf{x}),$$

GP_1 + GP_2



The subset structure

Limitation:

- Scalar output only
- Subset Structure

Contribution 1: Vector Output AR

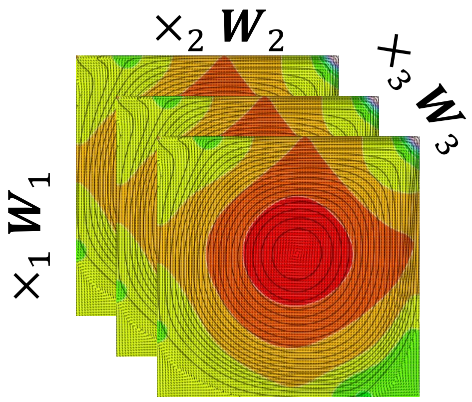
$$f^h(\mathbf{x}) = \rho f^l(\mathbf{x}) + f^r(\mathbf{x}),$$

$$\mathbf{F}^h(\mathbf{x}) = \mathbf{F}^l(\mathbf{x}) \times_1 \mathbf{W}_1, \ldots, \times_M \mathbf{W}_M + \mathbf{F}^r(\mathbf{x}),$$

Tensor GP

Tensor matrix product

Tensor GP



Sequential velocity fields

Zhe, Shandian, Wei Xing, and Robert M. Kirby. "Scalable high-order gaussian process regression." *The 22nd International Conference on Artificial Intelligence and Statistics*. PMLR, 2019.

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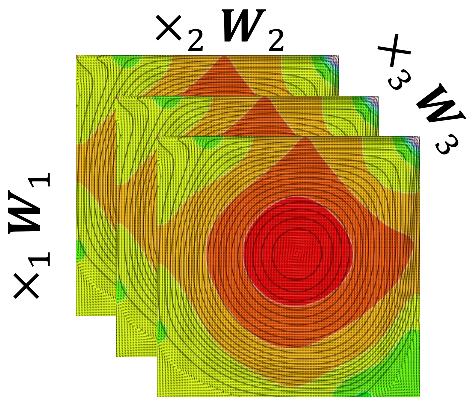
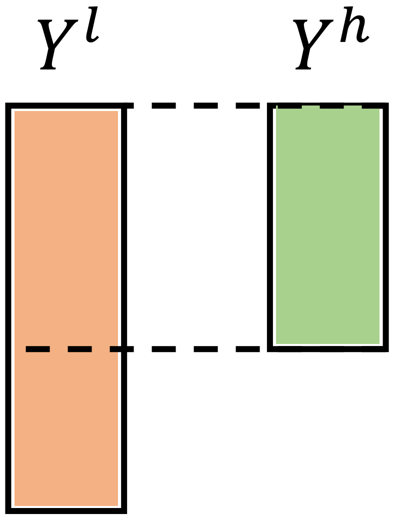


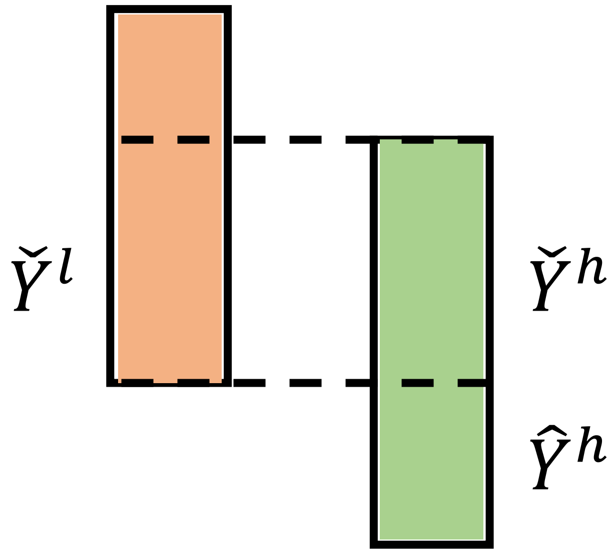
Sequential velocity fields

TGP_1 + TGP_2



The subset structure

Contribution 2: Non-Subset Decomposition



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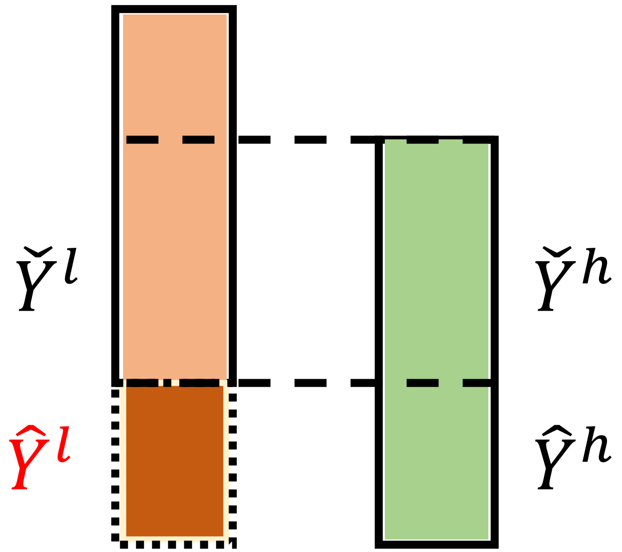


$$\log p(\mathbf{Y}^l, \mathbf{Y}^h) = \log \int p(\mathbf{Y}^l, \mathbf{Y}^h, \hat{\mathbf{Y}}^l) d\hat{\mathbf{Y}}^l = \log \int \left(p(\mathbf{Y}^h | \hat{\mathbf{Y}}^l, \mathbf{Y}^l) p(\hat{\mathbf{Y}}^l | \mathbf{Y}^l) p(\mathbf{Y}^l) \right) d\hat{\mathbf{Y}}^l$$

$$= \log \int p(\mathbf{Y}^h | \hat{\mathbf{Y}}^l, \mathbf{Y}^l) p(\hat{\mathbf{Y}}^l | \mathbf{Y}^l) d\hat{\mathbf{Y}}^l + \log p(\mathbf{Y}^l),$$

TGP_1 + TGP'_2

Contribution 3: Autokrigeability In AR and CIGAR

Autokrigeability[1] also holds in AR

$$\mathbf{S}_m^h = \mathbf{I}, \mathbf{S}_m^l = \mathbf{I}$$

$$\mathbf{Z}^l(\mathbf{x}, \mathbf{x}') \sim \mathcal{TGP}\left(\mathbf{0}, k^l(\mathbf{x}, \mathbf{x}'), \mathbf{S}_1^l, \ldots, \mathbf{S}_M^l\right), \mathbf{Z}^r(\mathbf{x}, \mathbf{x}') \sim \mathcal{TGP}\left(\mathbf{0}, k^r(\mathbf{x}, \mathbf{x}'), \mathbf{S}_1^r, \ldots, \mathbf{S}_M^r\right),$$

Conditional Independent GAR

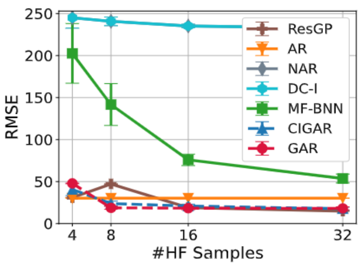
$$\mathbf{W}_m^T \mathbf{W}_m = \mathbf{I}$$

$$\mathcal{O}(\textstyle\sum_i \sum_{m=1}^M (d_m^i)^3 + (N^i)^3) \quad \Rightarrow \quad \mathcal{O}(\textstyle\sum_i (N^i)^3)$$

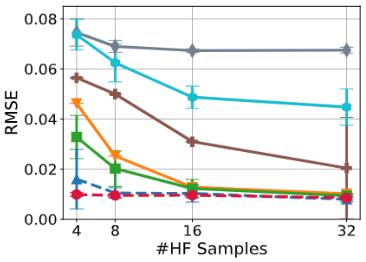
[1] Wackernagel, Hans. *Multivariate geostatistics: an introduction with applications*. Springer Science & Business Media, 2003.

Fast & SOTA Performance

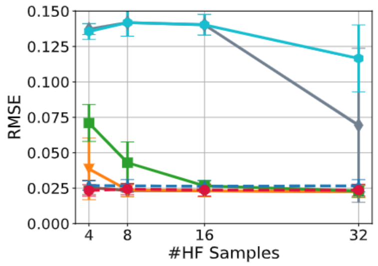
Almost always the best, with up to 6x improvements



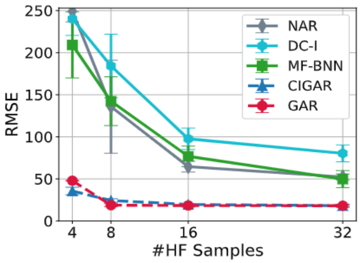
(a)



(b)



(c)



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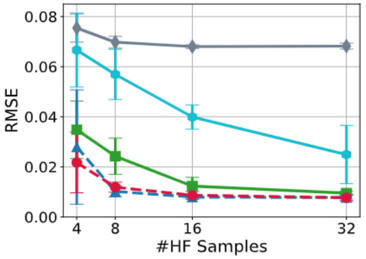

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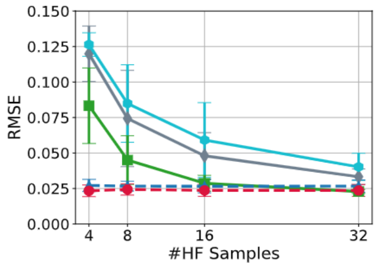

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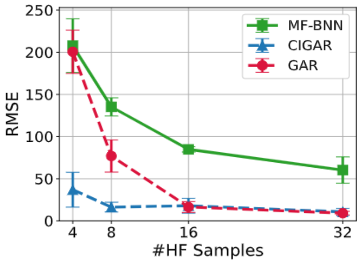

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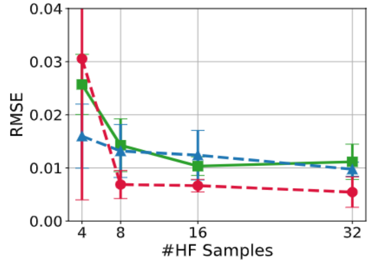

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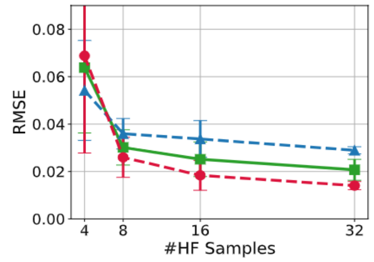
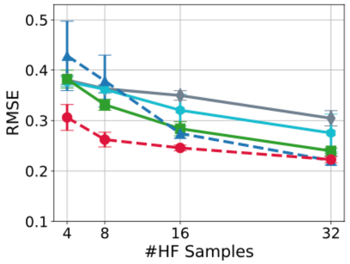


(i)



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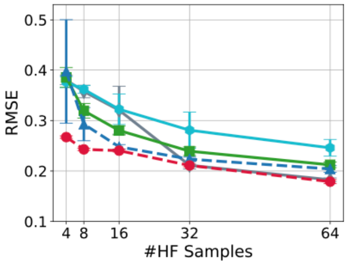

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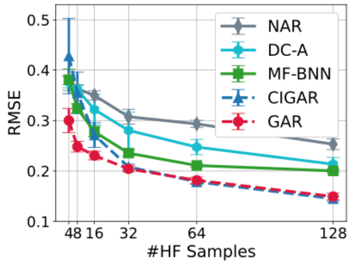

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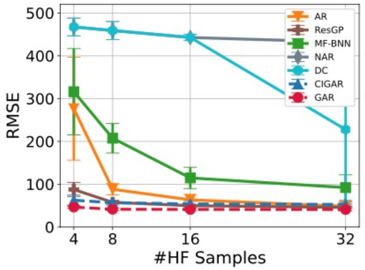

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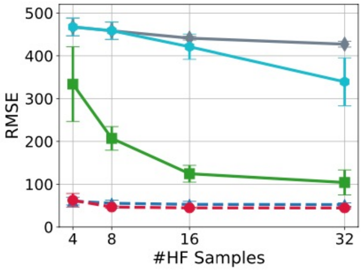

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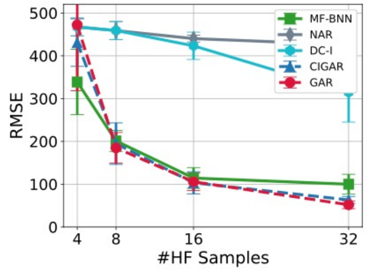

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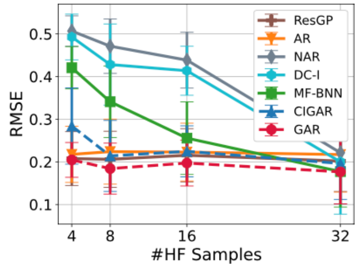

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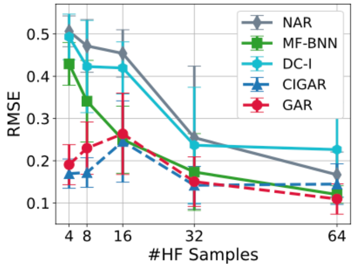

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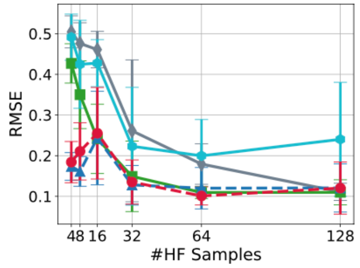

(c)

Thank You

Codes available at:
https://github.com/zen-xingle/ML_gp

Find more about our work on AI+Engineering at
wxing.me