Integrated Emulators for Systems of Computer Models†

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September 17, 2020
MASCOT-NUM PhD Students' Day

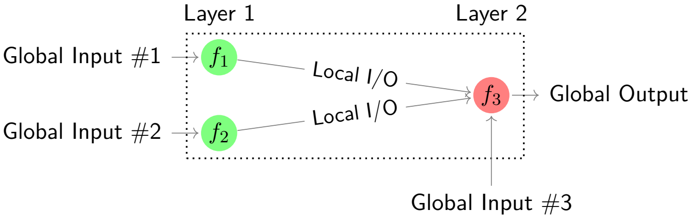
† Full manuscript at arXiv:1912.09468.

Examples of computer model systems

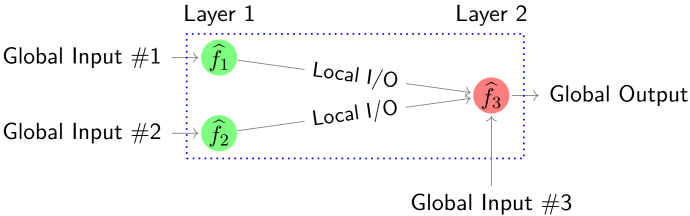
- **Multi-physics systems** of computer simulators, e.g., coupled tsunami simulators with earthquake and landslide sources;
- **Multi-disciplinary systems**, e.g., automotive and aerospace systems;
- **Other examples** include climate models, multi-disciplinary future biodiversity models, etc.

Composite vs integrated emulator

Composite emulator (single Gaussian process):



Integrated emulator (combined Gaussian processes):

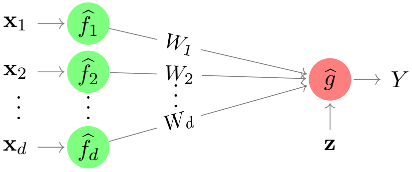


Method comparison

	System	Trend	Local I/O Dimension	Analytical Solutions	Adaptive Design
Kyzyurova et al. (2018)	two models	linear in one local input	≥ 1	SExp-ARD+nugget	No
Marque-Pucheu et al. (2019)	two models	linear in basis functions of global inputs	$=1$	SExp-ARD	Yes
Sanson et al. (2019)	multi-models	zero	≥ 1	No, by MC*	Yes
This study	multi-models	linear in local inputs and basis functions of global inputs	≥ 1	Exp-ARD SExp-ARD Matérn-1.5-ARD Matérn-2.5-ARD + nugget	Yes

†SExp = Squared exponential; ‡ARD = Automatic relevance determination; *MC = Monte Carlo

Integrated emulator at iteration i



Under a mild condition on the trend function and assume that

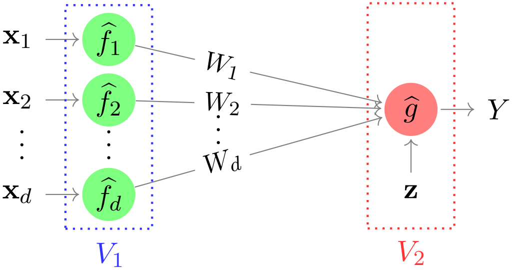
- $W_i(\mathbf{x}_i) \overset{ind}{\sim} \mathcal{N}(\mu_i(\mathbf{x}_i),\, \sigma_i^2(\mathbf{x}_i))$ for $k = 1, \dots, d$,

the output $Y(\mathbf{x}_1, \dots, \mathbf{x}_d, \mathbf{z})$ predicted at the input positions $\mathbf{x}_1, \dots, \mathbf{x}_d$ and $\mathbf{z}$ has its mean and variance

$$\begin{aligned}\mu_I =& \mathbb{E}(\mu_g(\mathbf{W}, \mathbf{z}))\\ \sigma_I^2 =& \mathrm{Var}(\mu_g(\mathbf{W}, \mathbf{z})) + \mathbb{E}(\sigma_g^2(\mathbf{W}, \mathbf{z}))\end{aligned}$$

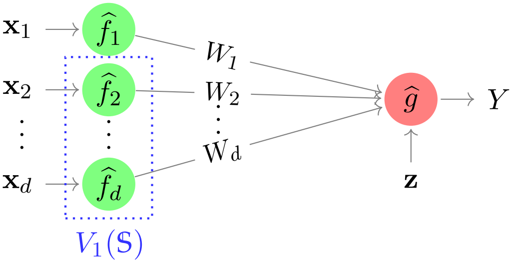
that can be expressed in closed-form for a wide range of kernels.

Variance decomposition (I)



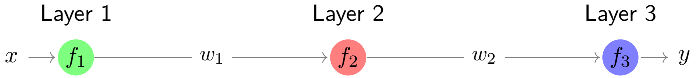
$$\sigma_I^2 = \underbrace{\mathrm{Var}\left(\mu_g(\mathbf{W},\mathbf{z})\right)}_{V_1} + \underbrace{\mathbb{E}\left[\sigma_g^2(\mathbf{W},\mathbf{z})\right]}_{V_2}$$

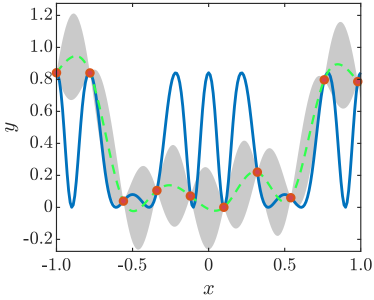
Variance decomposition (II)



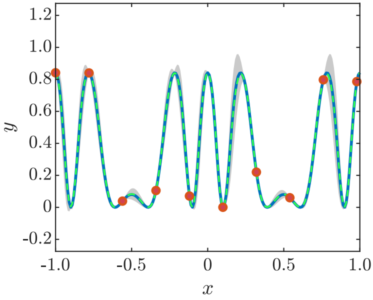
$$V_1(\mathbb{S}) = \mathrm{Var}_{W_{k\in\mathbb{S}}}\left(\mathbb{E}_{W_{k\in\mathbb{S}^c}}\left[\mu_g(\mathbf{W},\mathbf{z})\right]\right), \quad \mathbb{S} \subseteq \{1,\ldots,d\}$$

Synthetic experiment I – graphical comparison



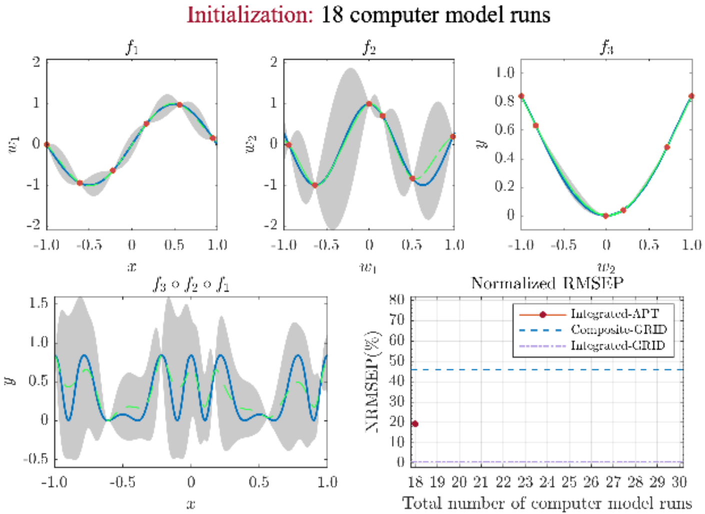


(a) Composite Emulator

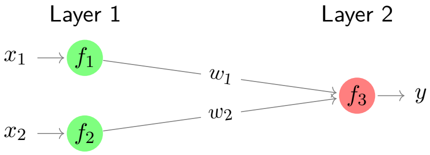


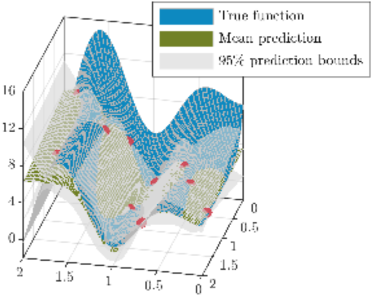
(b) Integrated Emulator

Synthetic experiment I – Smart design

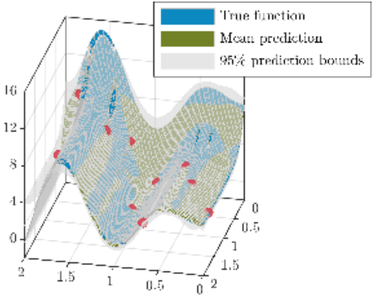


Experiment II – graphical comparison





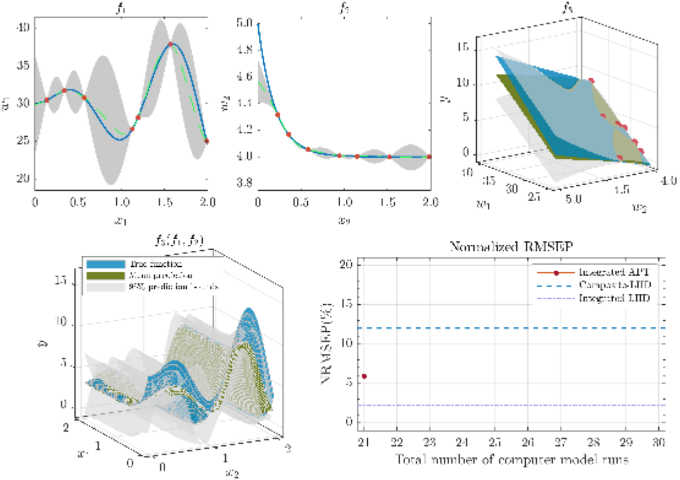
(c) Composite Emulator



(d) Integrated Emulator

Synthetic experiment II – Smart design

Initialization: 21 computer model runs



Feed-back coupled satellite model – (I)

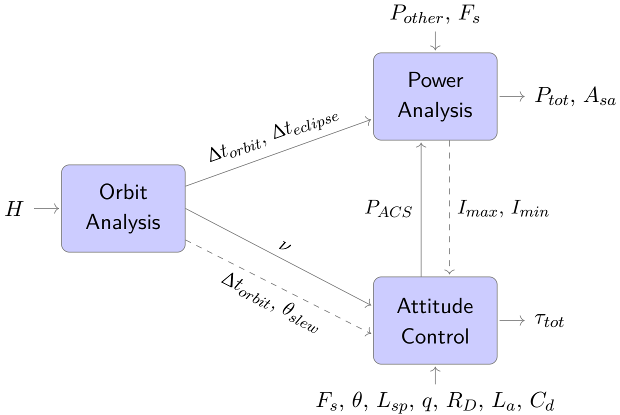
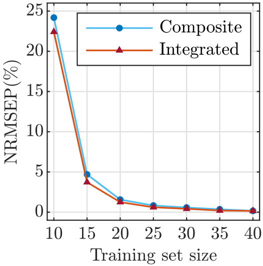
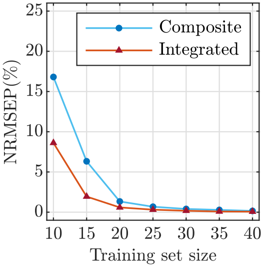


Figure 1: Fire-detection satellite model from Sankararaman and Mahadevan (2012). The decoupling is implemented by the algorithm from Baptista et al. (2018).

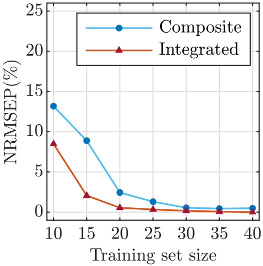
Feed-back coupled satellite model – (II)



(a) τ_{tot}

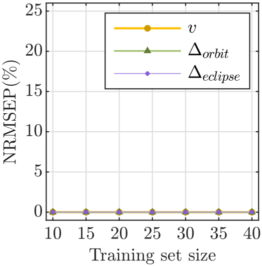


(b) P_{tot}

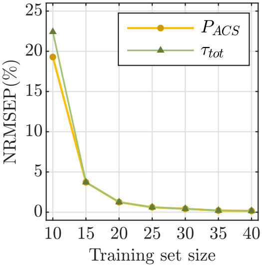


(c) A_{sa}

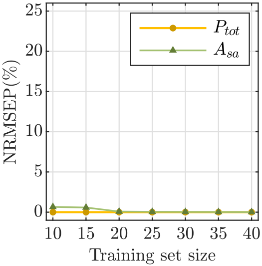
Feed-back coupled satellite model – (III)



(d) Orbit Analysis



(e) Attitude Control



(f) Power Analysis

Summary

Comparing to the composite emulator, the integrated emulator

1. produces better predictive performance with moderate-size designs;
2. achieves similar predictive error levels with reduced computational costs;
3. allows a smart adaptive designing strategy that can further reduce the predictive errors (or computational cost) remarkably by recognising the heterogeneous functional complexity of different computer models.

However, it may not show significant predictive improvement when a single computer model dominates the functional complexity of the whole system.

Thank you for your attention!

References

Baptista, R., Marzouk, Y., Willcox, K., and Peherstorfer, B. (2018). Optimal approximations of coupling in multidisciplinary models. *AIAA Journal*, 56(6):2412–2428.

Kyzyurova, K. N., Berger, J. O., and Wolpert, R. L. (2018). Coupling computer models through linking their statistical emulators. *SIAM/ASA Journal on Uncertainty Quantification*, 6(3):1151–1171.

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