Complex Computer Models: Leveraging Methods for Physical Experiments

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Latest Advances in the Theory and Applications of
Design and Analysis of Experiments
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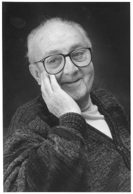
- High dimensionality of factors
- Nonlinear relationships (factors with many levels)
- High-order interaction effects
- Substantial random variation

Physical Experiments: Good Guys (Statisticians)

- Effect sparsity (Box and Meyer, 1985).
  - Only some factors are active
  - Only some (low-order) effects are important



DavidMCEddy at en.wikipedia

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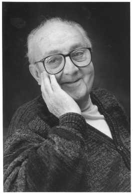

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- Effect heredity:
  significant interaction $\Rightarrow$ at least one of its factors has a significant main effects (Yates, 1937; Hamada and Wu, 1992)
- Effect hierarchy: lower-order effects tend to be more significant than higher-order effects (Yates, 1937; Wu and Hamada, 2009)

Physical Experiments: Tools

- Many, many other contributors . . .
- Main effects plans
- Resolution IV and V designs give up up on estimation of 3-factor and higher-order interaction effects
- etc., etc.

Physical Experiments: Tools

- Many, many other contributors . . .
- Main effects plans
- Resolution IV and V designs give up up on estimation of 3-factor and higher-order interaction effects
- etc., etc.
- What is the point here for computer experiments?

Computer Experiments: Bad Boys

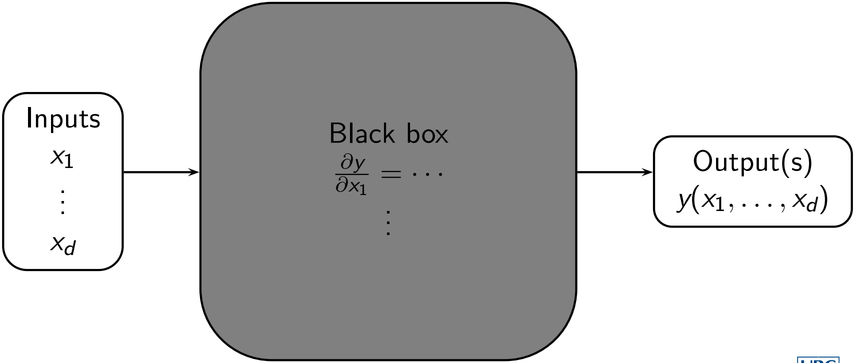
- High dimensionality of inputs
- Nonlinear relationships
- High-order interaction effects
- ~~Substantial random variation~~
- WHATCHA GONNA DO?

Computer Experiments: Bad Boys

- High dimensionality of inputs
- Nonlinear relationships
- High-order interaction effects
- WHATCHA GONNA DO?
  - You can cope with 2 bad boys but not 3
  - Standard GP approaches try to deal with all 3 simultaneously

Computer Model

- Inputs $\mathbf{x} = (x_1, \ldots, x_d)$
- Output $y = y(\mathbf{x})$



Gaussian Process (GP) Model

- Model $y(\mathbf{x})$ as a realization of

$$Y(\mathbf{x}) = \mu + Z(\mathbf{x})$$

- μ is a constant mean; regression model rarely helpful (Chen et al., 2016)
- $Z(\mathbf{x})$ is a multivariate normal random function with
  - Marginal distribution $\mathrm{N}\left(0, \sigma^2\right)$
  - Covariance $\mathrm{Cov}(Z(\mathbf{x}), Z(\mathbf{x}')) = \sigma^2 R(\mathbf{x}, \mathbf{x}')$ at two input vectors $\mathbf{x}$ and $\mathbf{x}'$

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  - Correlation function $R(\mathbf{x}, \mathbf{x}')$ is critical

Correlation Function

- Two sets of inputs $\mathbf{x}$ and $\mathbf{x}'$
- Standard (Std) correlation structure has a product form in 1-dimensional functions

$$R^{\mathrm{Std}}(\mathbf{x}, \mathbf{x}') = \prod_{j=1}^{d} R(h_j) \quad \in [0, 1],$$

  a function of the distance $h_j = |x_j - x_j'|$ for input j
- We will use the squared-exponential (Gaussian) function

$$R(h_j) = \exp(-\theta_j h_j^2),$$

  where $\theta_j \geq 0$ controls the sensitivity (nonlinearity) of input j.
- Following arguments apply to correlation functions other than squared exponential

Estimation

- μ, σ^2, and the correlation parameters $(\theta_1, \ldots, \theta_d)$ estimated by MLE or Bayes
- For the results shown later, $\theta_1, \ldots, \theta_d$ optimized numerically via the `mlegp` package (Dancik, 2013)
- All standard stuff
- (`mlegp` is adapted for the new correlation structures introduced later)

Prediction

- Predict $y(\mathbf{x}^*)$ at some new input vector $\mathbf{x}^*$
- More standard stuff ...
- The best linear unbiased predictor or posterior mean (given the correlation parameters) is of the form

$$\hat{y}(\mathbf{x}^*) = \hat{\mu} + \mathbf{a}^T \mathbf{r}(\mathbf{x}^*)$$

  - the vector $\mathbf{a}$ does not depend on $\mathbf{x}^*$
  - $\mathbf{r}(\mathbf{x}^*) = \left(R(\mathbf{x}^*, \mathbf{x}^{(1)}), \dots, R(\mathbf{x}^*, \mathbf{x}^{(n)})\right)^T$ is a vector of correlations between $Y(\mathbf{x}^*)$ and $Y(\mathbf{x}^{(i)})$ at the training design points $\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}$

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  - The predictor has the same form for any legal correlation function
  - The predictor is a linear combination of basis functions $R(\mathbf{x}^*, \mathbf{x}^{(i)})$

Prediction Accuracy of $\hat{y}$

- Measured by root mean squared error (RMSE) over a new test set
- Normalized version compares with the RMSE of the trivial predictor $\bar{y}$, the sample mean of the training data:

$$e_{\text{N-RMSE}} = \frac{\text{RMSE of } \hat{y}}{\text{RMSE of } \bar{y}}$$

- $e_{\text{N-RMSE}} = 0$ says perfect accuracy
- $e_{\text{N-RMSE}} = 1$ says $\hat{y}$ no better than $\bar{y}$

Additive Correlation Structures

- Recall

$$R^{\mathrm{Std}}(\mathbf{x}, \mathbf{x}') = \prod_{j=1}^{d} \exp(-\theta_j h_j^2) \quad (\text{where } h_j = x_j - x_j')$$

- Instead, additive correlation structure with equal weights (A-EW)

$$R^{\mathrm{A-EW}}(\mathbf{x}, \mathbf{x}') = \frac{1}{d} \sum_{j=1}^{d} \exp(-\theta_j h_j^2)$$

- Or additive correlation structure with unequal weights (A-UW)

$$R^{\mathrm{A-UW}}(\mathbf{x}, \mathbf{x}') = \sum_{j=1}^{d} \omega_j \exp(-\theta_j h_j^2)$$

  - weights $\omega_1, \ldots, \omega_d$ have to be estimated too, subject to $\omega_j \geq 0$ and $\sum_{j=1}^{d} \omega_j = 1$

Michalewicz Test Function (Ba and Joseph, 2012)

- Michalewicz function in d dimensions:

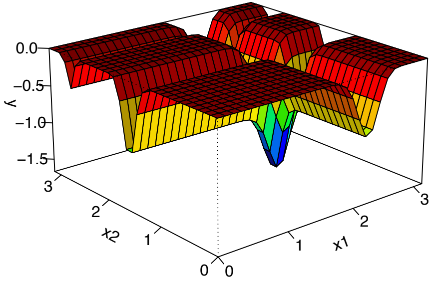
$$y_{\mathrm{u}}(\mathbf{x}) = -\sum_{j=1}^{d} \sin(x_j)\left[\sin\left(\frac{jx_j^2}{\pi}\right)\right]^{20} \quad \text{where} \quad x_j \in [0, \pi].$$

- Has $d!$ local minima (highly nonlinear)
- Weighted form:

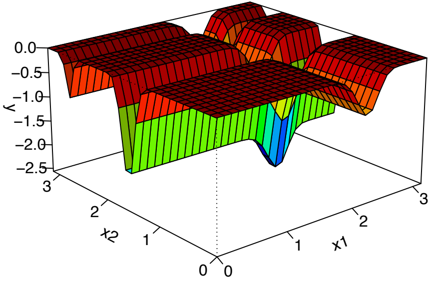
$$y_{\mathrm{w}}(\mathbf{x}) = -\sum_{j=1}^{d} j \sin(x_j)\left[\sin\left(\frac{jx_j^2}{\pi}\right)\right]^{20} \quad \text{where} \quad x_j \in [0, \pi].$$

  - Complexity and more importance of x_j increases with j

Michalewicz Test Function

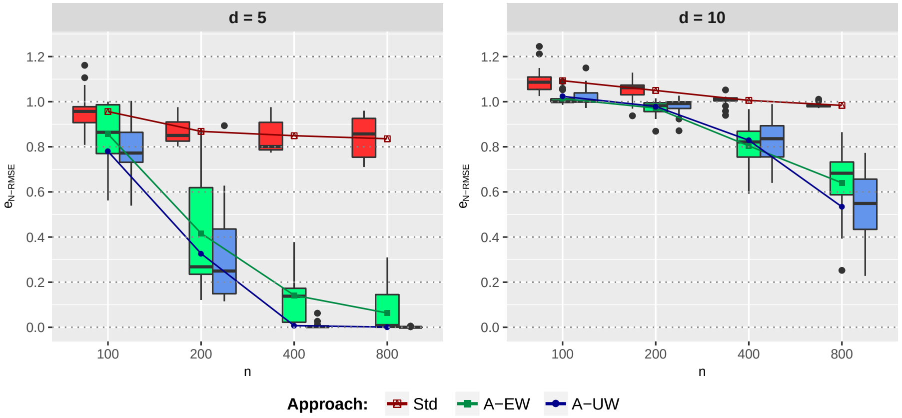


(a) Unweighted



(b) Weighted

Weighted Michalewicz Function ($e_{\text{N-RMSE}}$ for 20 Repeat Training Experiments)



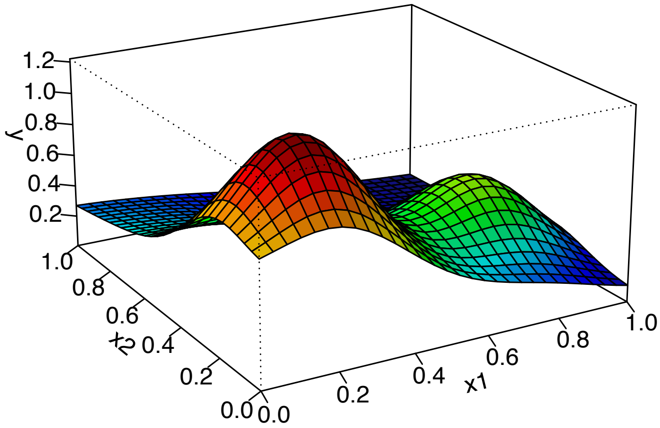
Franke's Function (Franke, 1979; Haaland and Qian, 2011)

- Most functions are not perfectly additive
- Franke's function in 2 dimensions:

$$
\begin{aligned}
y_{\mathrm{F}}(x_1, x_2) = 0.75 \exp\left[-\frac{(9x_1-2)^2}{4} - \frac{(9x_2-2)^2}{4}\right] \\
+ 0.75 \exp\left[-\frac{(9x_1+1)^2}{49} - \frac{9x_2+1}{10}\right] \\
+ 0.5 \exp\left[-\frac{(9x_1-7)^2}{4} - \frac{(9x_2-3)^2}{4}\right] \\
- 0.2 \exp[-(9x_1-4)^2 - (9x_2-7)^2] \\
\text{where} \quad x_1, x_2 \in [0, 1].
\end{aligned}
$$

- Nonlinear with interaction

Franke's Function in 2 Dimensions



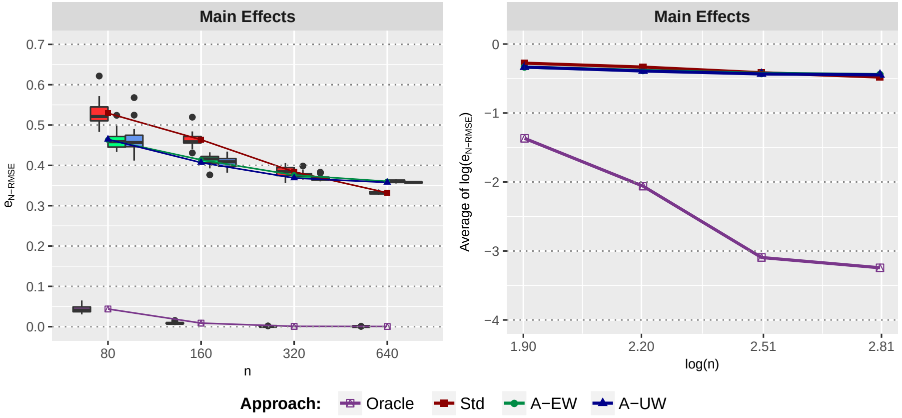
New Franke's Function in 8 Dimensions

- $y_{\mathrm{F8}}(\mathbf{x}) = y_{\mathrm{F}}(x_1, x_2) + y_{\mathrm{F}}(x_3, x_4) + y_{\mathrm{F}}(x_5, x_6) + y_{\mathrm{F}}(x_7, x_8)$
- Nonlinear with moderate interaction (x_1 with x_2, x_3 with x_4, etc.)

Oracle

- Just for a best possible baseline; cannot be done in practice
- Knows the structure of $y_{\mathrm{F8}}(\mathbf{x})$ and fits 4 separate GPs
  - Training data for x_1, x_2, $y_{\mathrm{F}}(x_1, x_2)$ gives $\hat{y}_{\mathrm{F},12}(x_1, x_2)$
  - $\cdots$
  - Training data for x_7, x_8, $y_{\mathrm{F}}(x_7, x_8)$ gives $\hat{y}_{\mathrm{F},78}(x_7, x_8)$
- $\hat{y}_{\mathrm{F8}}^{(\mathrm{Oracle})}(\mathbf{x}^*) = \hat{y}_{\mathrm{F},12}(x_1^*, x_2^*) + \cdots + \hat{y}_{\mathrm{F},78}(x_7^*, x_8^*)$

Franke's Function in 8 Dimensions: Additive (Main Effects) Model



Normalized RMSE versus *n* and log-log plot to show rate of convergence

Composite Correlation Structures (Additive and All 2-Input Interactions)

- Composite, equal weights

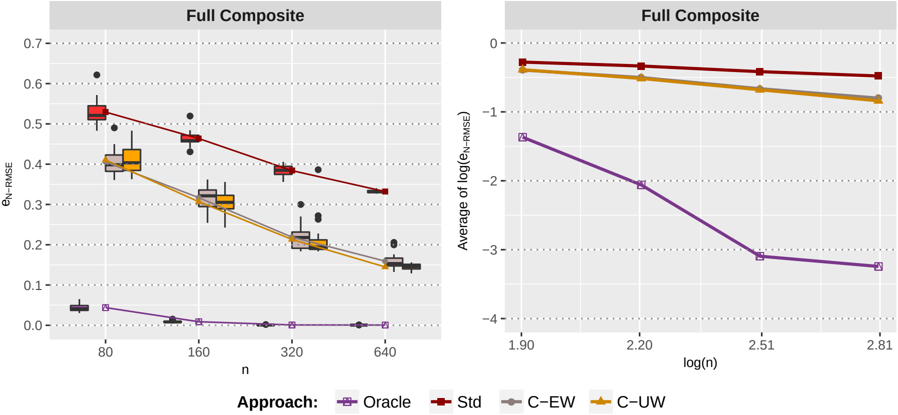
$$R^{\mathrm{C-EW}}(\mathbf{x}, \mathbf{x}') = \frac{1}{2} \cdot \frac{1}{d} \sum_{j=1}^{d} e^{-\theta_j h_j^2} + \frac{1}{2} \cdot \frac{2}{d(d-1)} \sum_{j=1}^{d} \sum_{j'=j+1}^{d} e^{-\theta_j h_j^2} e^{-\theta_{j'} h_{j'}^2}$$

- Composite, unequal weights

$$R^{\mathrm{C-UW}}(\mathbf{x}, \mathbf{x}') = \lambda_1 \cdot \frac{1}{d} \sum_{j=1}^{d} e^{-\theta_j h_j^2} + \lambda_2 \cdot \frac{2}{d(d-1)} \sum_{j=1}^{d} \sum_{j'=j+1}^{d} e^{-\theta_j h_j^2} e^{-\theta_{j'} h_{j'}^2}$$

(λ_1 and λ_2 estimated subject to $\lambda_1 + \lambda_2 = 1$)

Franke's Function: Composite Correlation Structures (Additive and All 2-Input Interactions)



Normalized RMSE versus n and log-log plot to show rate of convergence

Composite Select Correlation Structures (Additive and Some 2-Input Interactions)

- Composite with select 2-input interactions, equal weights

$$R^{\mathrm{CS-EW}}(\mathbf{x}, \mathbf{x}') = \frac{1}{2} \cdot \frac{1}{d} \sum_{j=1}^{d} e^{-\theta_j h_j^2} + \frac{1}{2} \cdot \frac{1}{|B|} \sum_{\{j,j'\} \in B} e^{-\theta_j h_j^2} e^{-\theta_{j'} h_{j'}^2}$$

- Composite with select 2-input interactions, unequal weights

$$R^{\mathrm{CS-UW}}(\mathbf{x}, \mathbf{x}') = \lambda_1 \cdot \frac{1}{d} \sum_{j=1}^{d} e^{-\theta_j h_j^2} + \lambda_2 \cdot \frac{1}{|B|} \sum_{\{j,j'\} \in B} e^{-\theta_j h_j^2} e^{-\theta_{j'} h_{j'}^2}$$

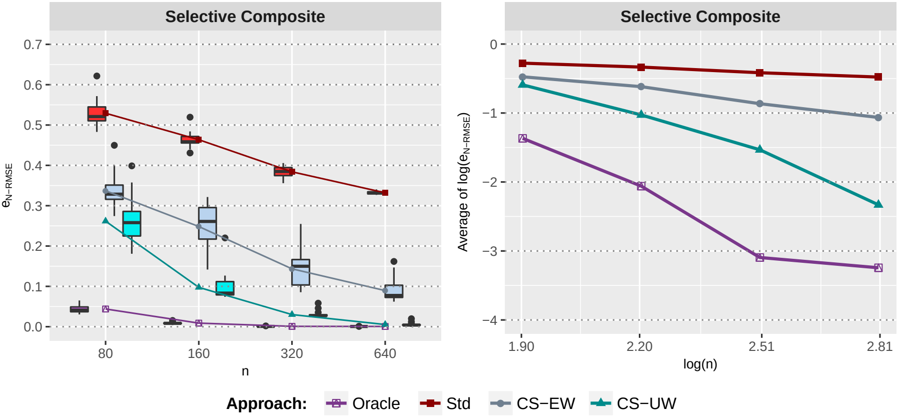
Choosing the 2-Input Interactions: FANOVA (Schonlau and Welch, 2006)

- Choose the interaction effects for the 8-dimensional Franke's function data adaptively
- Functional ANOVA (FANOVA) based on a training set with $n = 640$
- Percent contributions to total variance of the function

Effect	%	Effect	%	Effect	%
x_1	8.1	x_2	15.8	$x_1 \times x_2$	2.4
x_3	7.5	x_4	13.5	$x_3 \times x_4$	2.3
x_5	7.9	x_6	15.1	$x_5 \times x_6$	2.4
x_7	7.4	x_8	14.5	$x_7 \times x_8$	2.3

- These effects account for 99.2% of the variation (others negligible)
- $B = \{\{1,2\},\{3,4\},\{5,6\},\{7,8\}\}$.

Franke's Function: Select Composite (Main Effects and Select 2-Input Interaction Effects)



Normalized RMSE versus *n* and log-log plot to show rate of convergence

Bad Boys: The Math

- High dimensionality: $d \gg 1$ inputs are active, say $x_1, \ldots, x_d$
- Nonlinearity: their θ_j are large
- What does the product correlation function do?

$$
\begin{aligned}
R^{\mathrm{Std}}(\mathbf{x}, \mathbf{x}') = \prod_{j=1}^{d} R(h_j) = \prod_{j=1}^{d} e^{-\theta_j h_j^2} &= \prod_{j=1}^{d} (1 - \theta_j h_j^2 + \frac{1}{2}(\theta_j h_j^2)^2 + \cdots) \\
&= 1 - \theta_1 h_1^2 + \frac{1}{2}(\theta_1 h_1^2)^2 + \text{similar terms for } x_2, \text{ etc.} \\
&+ \theta_1 h_1^2 \theta_2 h_2^2 + \text{similar terms for } x_3, x_4, \text{ etc.} \\
&+ \cdots \pm \prod_{j=1}^{d} \theta_j h_j^2
\end{aligned}
$$

- The higher-order products will not disappear if the $\theta_j \gg 0$ unless all $h_j \simeq 0$ (huge sample size)

Conclusions

- With high dimensionality and nonlinearity, the product correlation function automatically introduces high-order interactions, needed or not

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  - Useful accuracy with a main-effects model
- New Franke function: nonlinear, moderate dimension
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  - More accuracy with limited, 2-input interactions
- Work by Alexi Rodríguez to extend these ideas to real applications is also taking account of the science (Dennis Lin's paper in JQT)

THANK YOU! ⌣̈

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