ON THE TREATMENT AND CHALLENGES OF MODEL UNCERTAINTY

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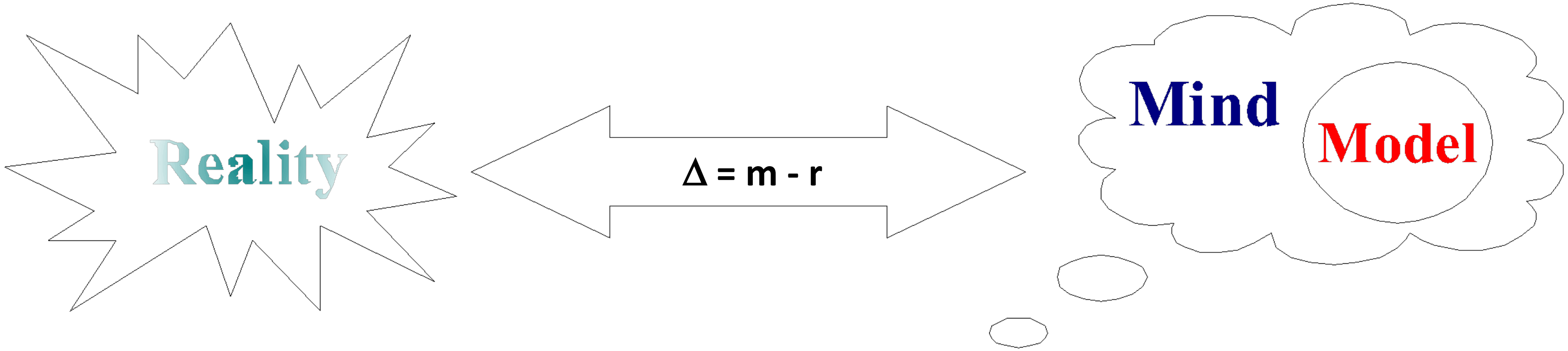
ROADMAP

- Fundamentals:
  - Models, Model Uncertainty and Parameter Uncertainty
  - Modeling Process and Model Uncertainty
  - Model Output Uncertainty
- Operationalization of Model Uncertainty
  - Bayesian and Non-Bayesian based approaches
  - Model performance
  - Model applicability
- Challenges ahead
  - Uncertainty is uncertainty?
  - Multiple models, submodels and dependency
  - Accounting for the unexpected
  - Massive and multidimensional data

FUNDAMENTALS

MODEL ERROR AND MODEL UNCERTAINTY



MODEL UNCERTAINTY AND PARAMETER UNCERTAINTY

- Models can be characterized as having a structure (*S*) and a set of parameters (Θ)

$$x = M(S, \Theta)$$

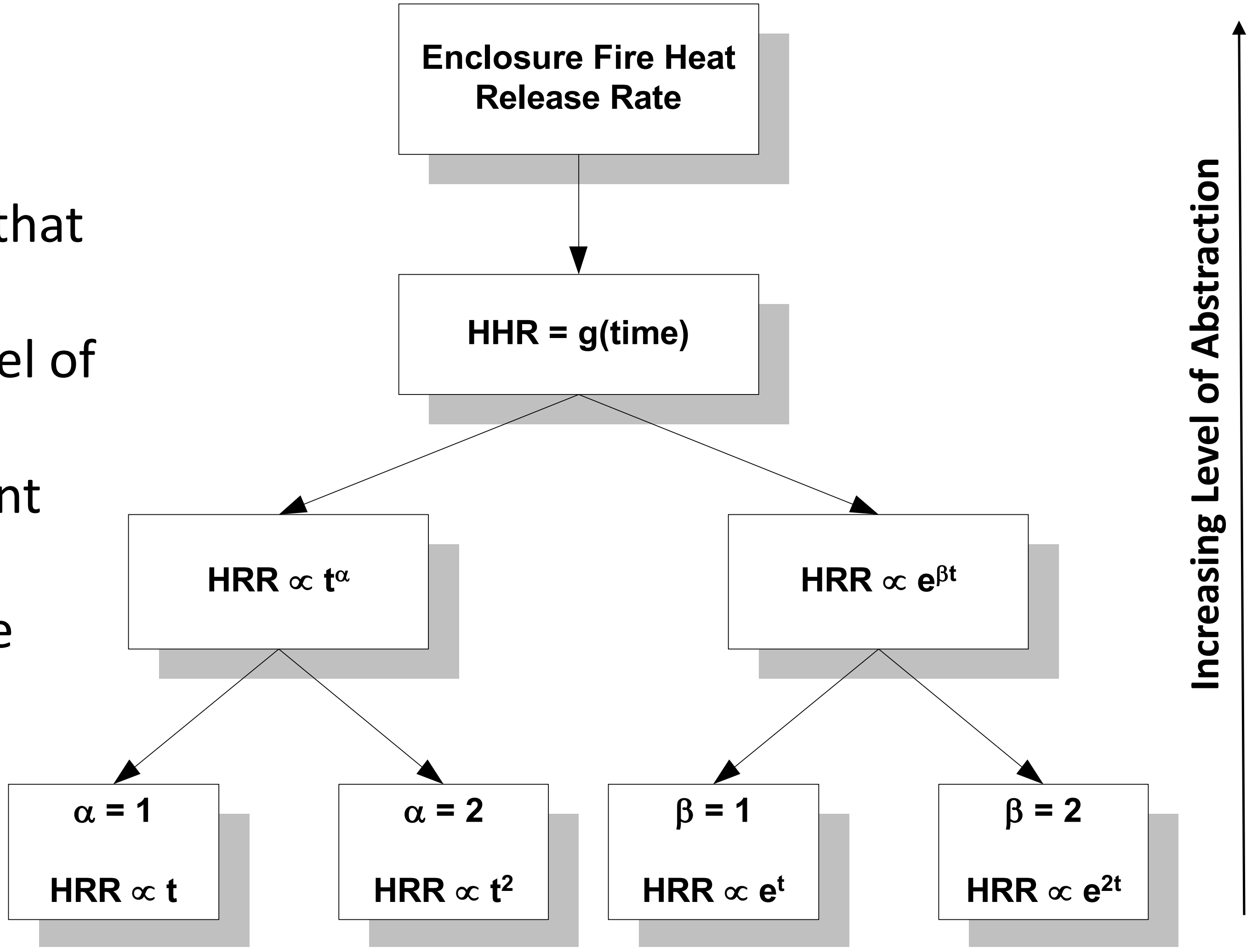
- Uncertainty attributed to the values of parameters is commonly referred to as "Parameter Uncertainty”

- Uncertainty arising from lack of confidence in model structure or alternative structures is commonly referred to as "Model Uncertainty”

MODELING PROCESS: MODEL FORM AND PARAMETERS

Parameter:

- An aspect of the model that relates it to its specific instances in the next level of the modeling process
- A parameter in the parent model can become a structural element in the child model



SOURCES OF MODEL UNCERTAINTY

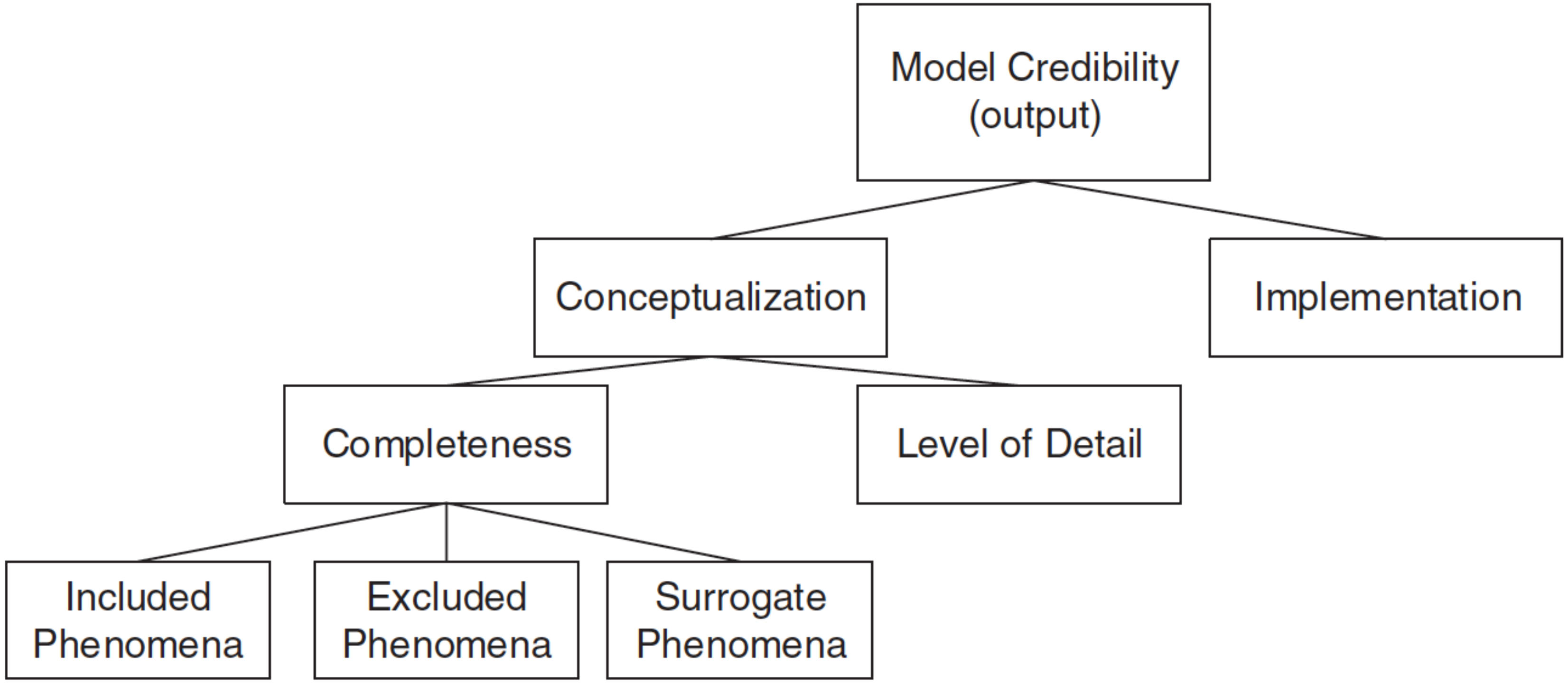
- Alternative plausible hypotheses for describing the phenomena

- A single model:
  - Generally accepted but not completely validated
  - Conceptually accepted and validated but its implementation is of uncertain quality
  - Recognized to only partially cover the relevant aspects of the problem
  - Composed of sub-models of different degrees of accuracy and credibility

- Multiple models, each covering different aspects of the reality

- Surprising events, change of a known pattern

MODEL CREDIBILITY



MODEL OUTPUT UNCERTAINTY

- Uncertainty associated to the difference between the model output values and the true values of the quantities of interest (Bjerga, Aven, Zio; 2014):

$$\Delta G(X) = G(X) - Z$$

STRUCTURAL MODEL UNCERTAINTY

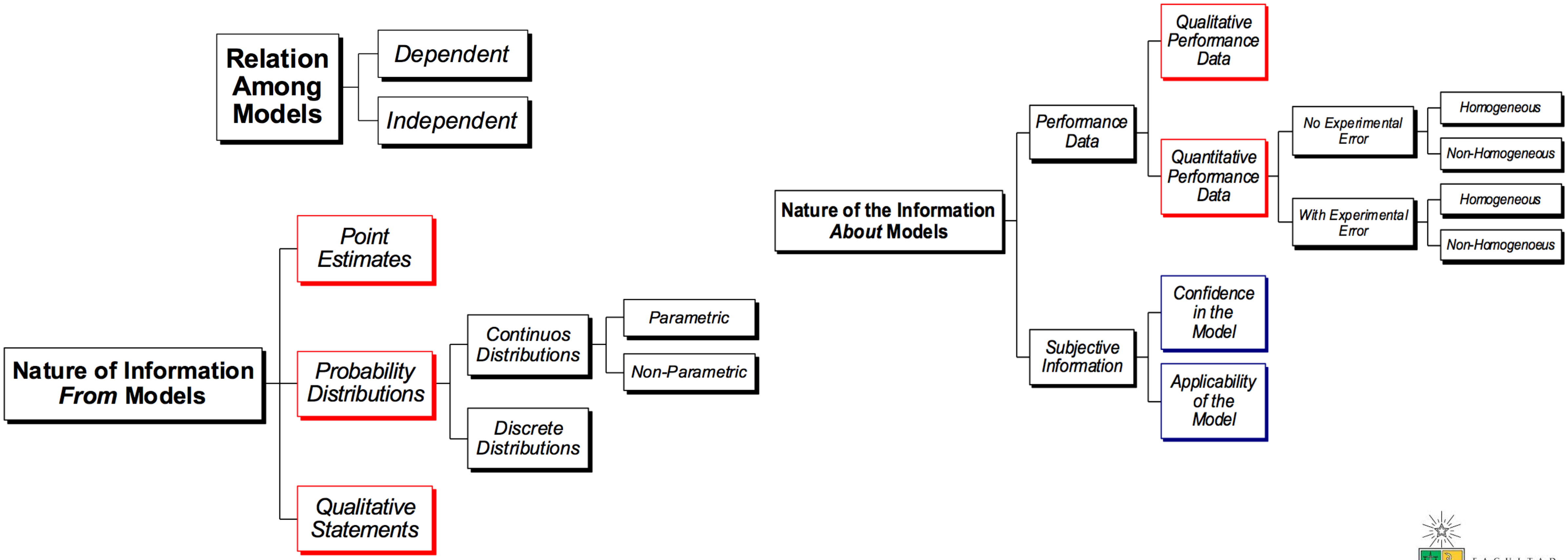
- Model output uncertainty results from the combination of two components:
  - Structural model uncertainty
  - Parameter uncertainty

- Structural model uncertainty:
  - Fundamentally, model uncertainty is model structural uncertainty
  - It is a source of uncertainty
  - In practice, both sources (model and parameter uncertainties) usually get confounded
  - And this is reflected in the model output error

OPERATIONALIZATION

DIFFERENT REALITIES - DIFFERENT SOLUTIONS

- Available information, context of application, objective of the analysis



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UNCERTAINTY FACTOR APPROACH

- It introduces a correction factor directly on the predictions provided by a single model (Siu and Apostolakis, 1986 and 1992):

$$X = X_M - \xi_a \qquad\qquad X = X_M / \xi_m$$

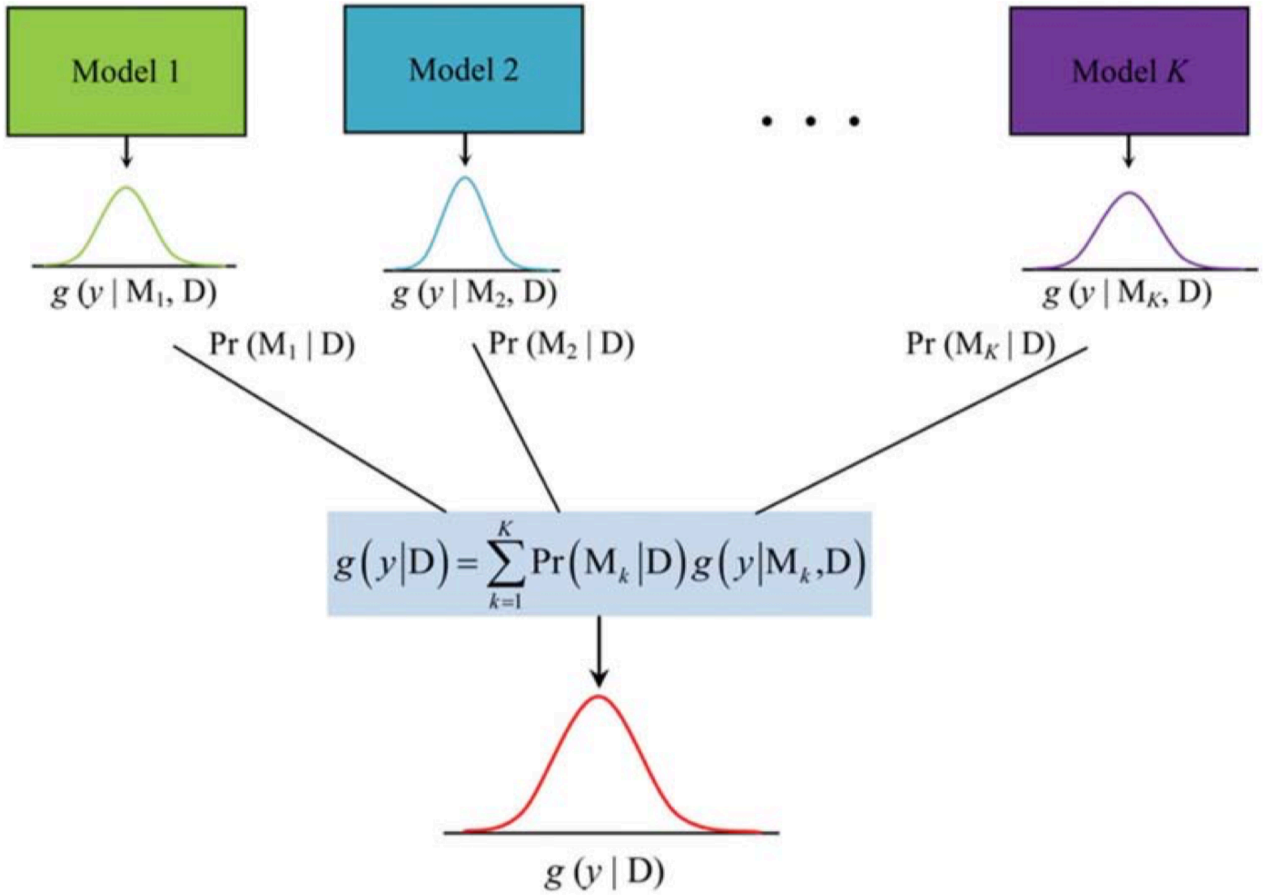
- The correction factor translates the modeler's confidence in the model's *M* prediction X_M about the quantity of interest *X*

$$f(\xi_m|E) = \int_\Lambda f(\xi_m|\Lambda)\pi(\Lambda|E)d\Lambda$$

- It allows for the use of a model outside its intended domain of application (extrapolation)

- Usually applicable to situations where only one model is available

MODEL AVERAGING

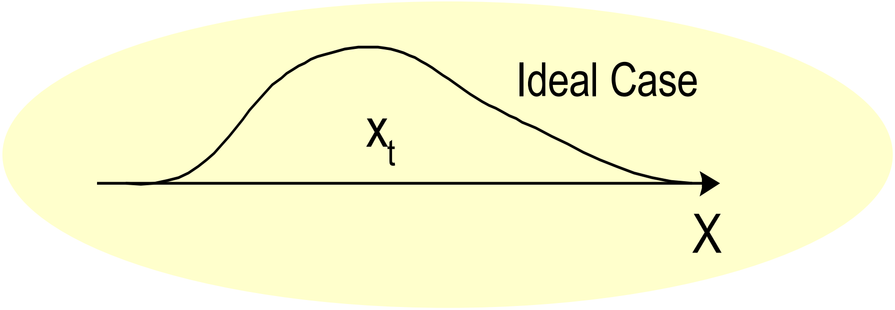


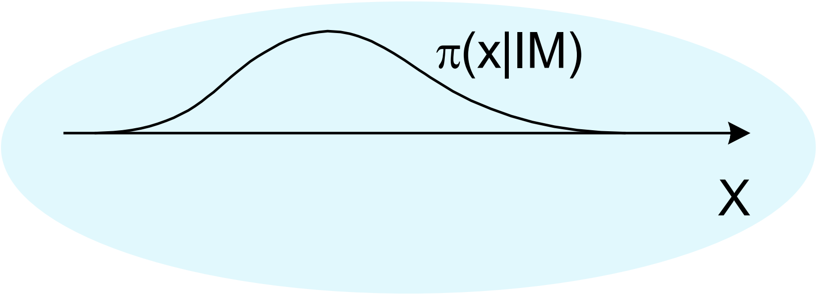
- The set of models should be mutually exclusive and collectively exhaustive
- The model weights should sum up to one
- The collective exhaustiveness implies that not only the probability attributed to a model is interpreted as the probability that model M_i is "correct", but also the "correct" model should necessarily be one of the alternate models

I. PARK, "Quantification of Multiple Types of Uncertainty Physics-Based in Simulation," PhD Thesis, Wright State University, 2012

BAYESIAN PERSPECTIVE

- In assessing the uncertainty about X, the objective is to ensure that the true but unknown value x_t falls within some uncertainty range characterized by a probability distribution $\pi(x)$
- We could settle for a probability distribution given the available evidence relevant to the estimation of the unknown X, $\pi(x|IM)$





BAYESIAN ASSESSMENT

$$\pi(x \mid IM) = \frac{L(IM \mid x)\,\pi_0(x)}{\int_x L(IM \mid x)\,\pi_0(x)\,dx}$$

$$IM = (IM_1, IM_2, \ldots, IM_n)$$

$$L(IM \mid x) = L(\underline{x}^* \mid \underline{D}, x)\,L(\underline{D} \mid x)$$

Model Estimate

Information about Model

SINGLE MODEL

- Model *M* provides an estimate *u** about an unknown *u*

- Evidence *D* about the model *M:*

$$\pi(u \mid u^*, D) = \frac{L(u^* \mid D, u)\pi_o(u)}{\int_u L(u^* \mid D, u)\pi_o(u)\, du}$$

- With an appropriate likelihood parameterization:

$$\pi(u \mid u^*, D) = \frac{\left[\int_{\underline{\theta}} L(u^* \mid \underline{\theta}, u)\pi(\underline{\theta} \mid D)\, d\underline{\theta}\right]\pi_o(u)}{\int_u \left[\int_{\underline{\theta}} L(u^* \mid \underline{\theta}, u)\pi(\underline{\theta} \mid D)\, d\underline{\theta}\right]\pi_o(u)\, du}$$

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MODEL UNCERTAINTY QUANTIFICATION IN LIGHT OF PERFORMANCE DATA

- *D* corresponds to the available information about *M*:
  - Performance data: experimental results $x_1^e, \ldots, x_n^e$ and corresponding model estimates $x_1^*, \ldots, x_n^*$

- Additive model error:

$$E_i = x_i^* - x_i^t$$

- Likelihood:

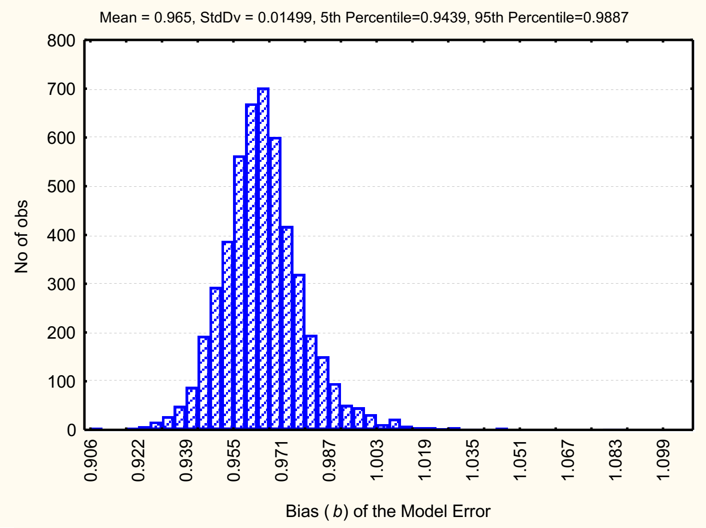
$$L(x^* \mid x, \underline{\theta}) = L(x^* \mid x, b, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\left(\frac{x^* - (x+b)}{\sigma}\right)^2},$$

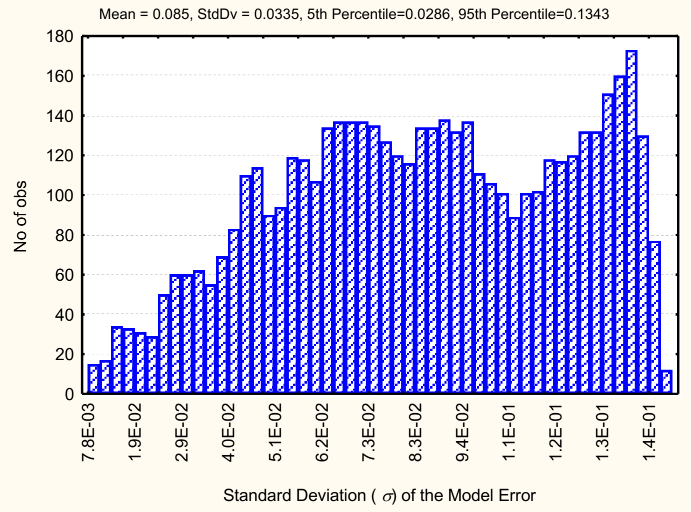
FIRE HAZARD WITH HOMOGENEOUS PERFORMANCE DATA

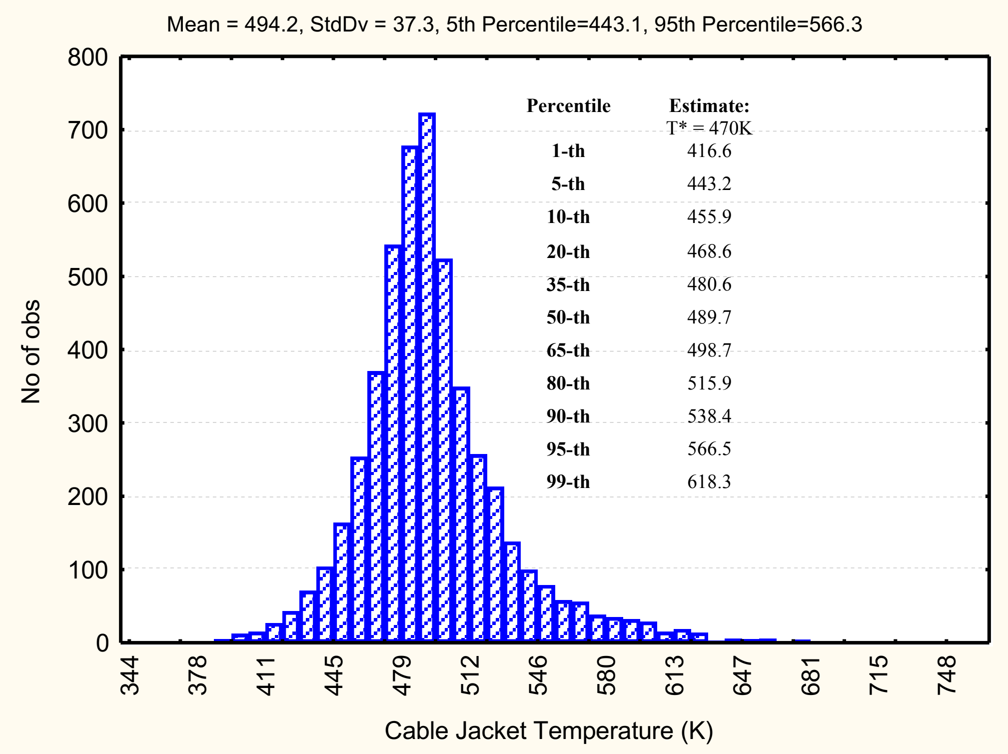
- Fire hazard model for estimating cable jacket temperatures. The model provides a new estimate of 470 K at 300 seconds
- Homogeneous performance data:

	Cable Jacket Temperature (K)		
Time (sec)	Experimental Result (T^e)	Model Predictions	
		T_{cj}^p	T_{cj}^p / T_{cj}^e
60	360	375	1.042
180	425	430	1.012
300	455	470	1.033
480	505	500	0.990
720	575	520	0.904
900	575	500	0.870

FIRE HAZARD WITH HOMOGENEOUS PERFORMANCE DATA







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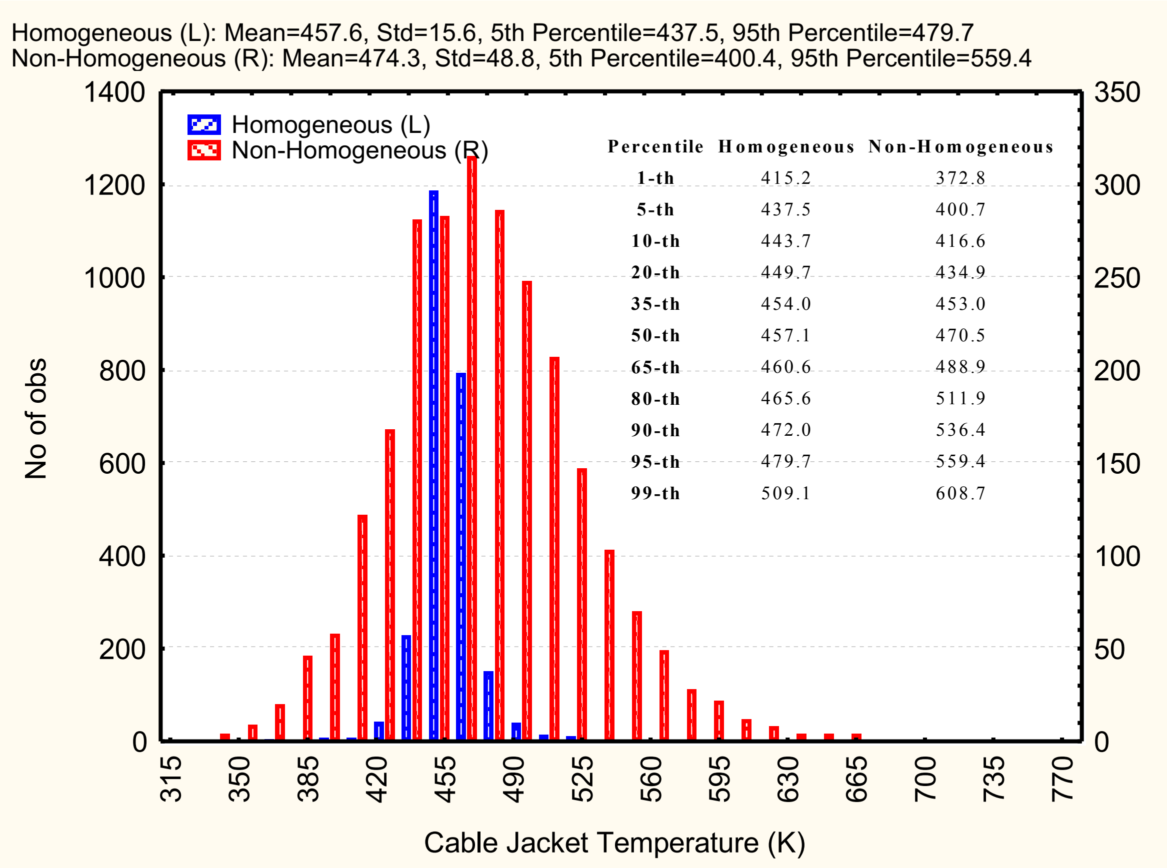
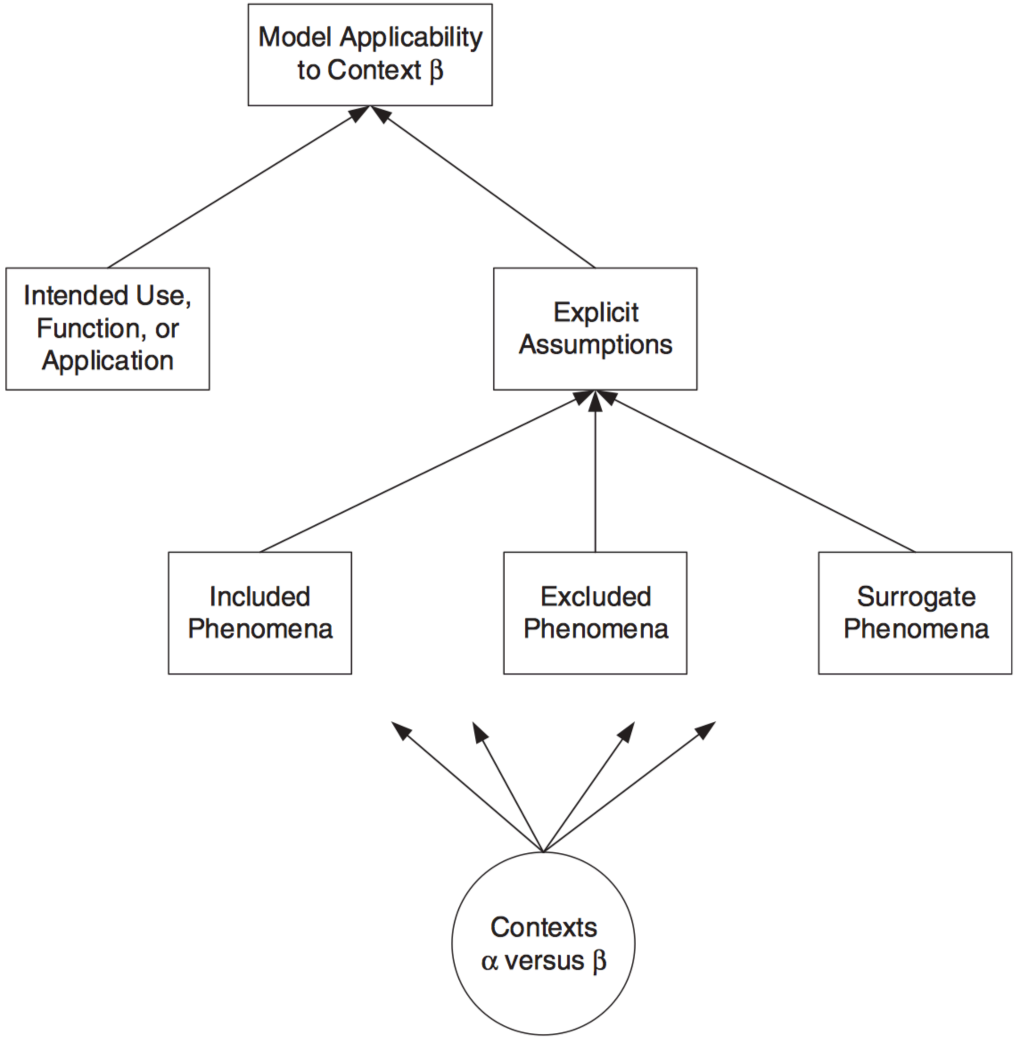
NON-HOMOGENEOUS PERFORMANCE DATA

- Posterior expected distribution:

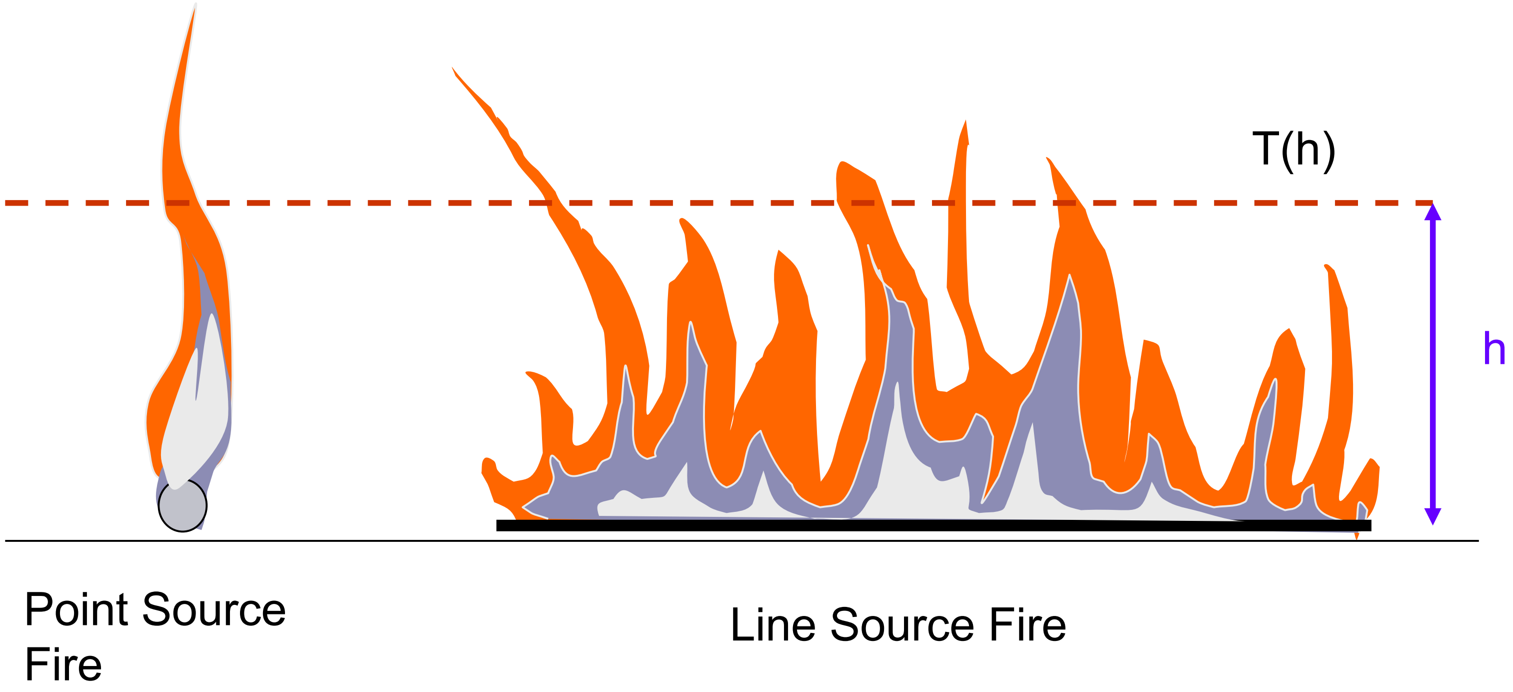
$$\pi(x|x^*,D) \propto \left[\int_{\underline{\theta}} L(x^*|\underline{\theta},x)\bar{g}(\underline{\theta}|D)\,d\underline{\theta}\right]\times \pi_o(x)$$



DEVIATION FROM INTENDED USE

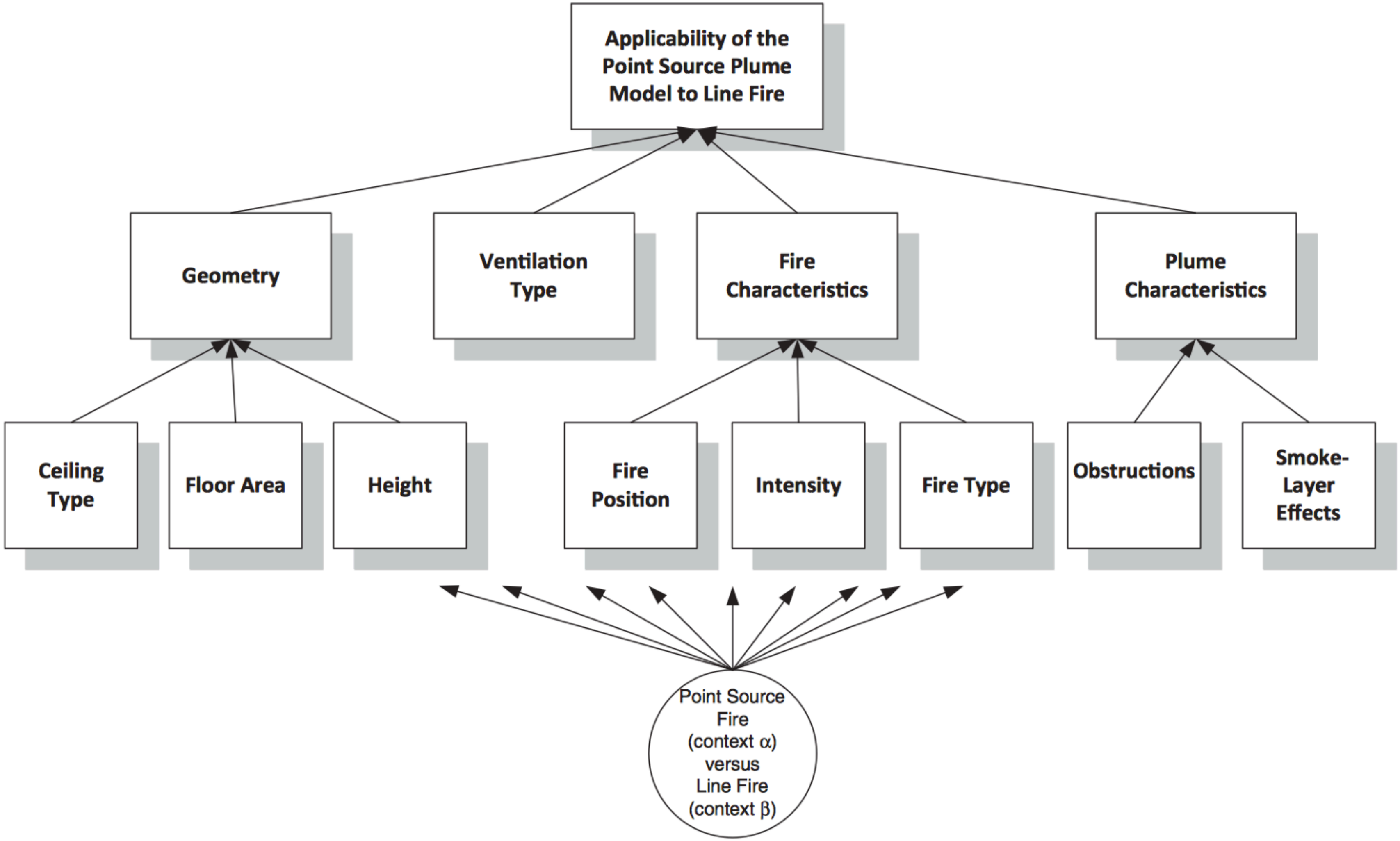


APPLICABILITY OF A MODEL



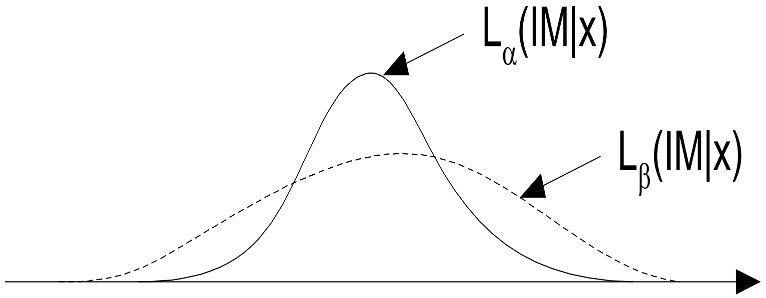
Predicting Fire Plume Temperature of a *Line Source* Using *Point Source* Model

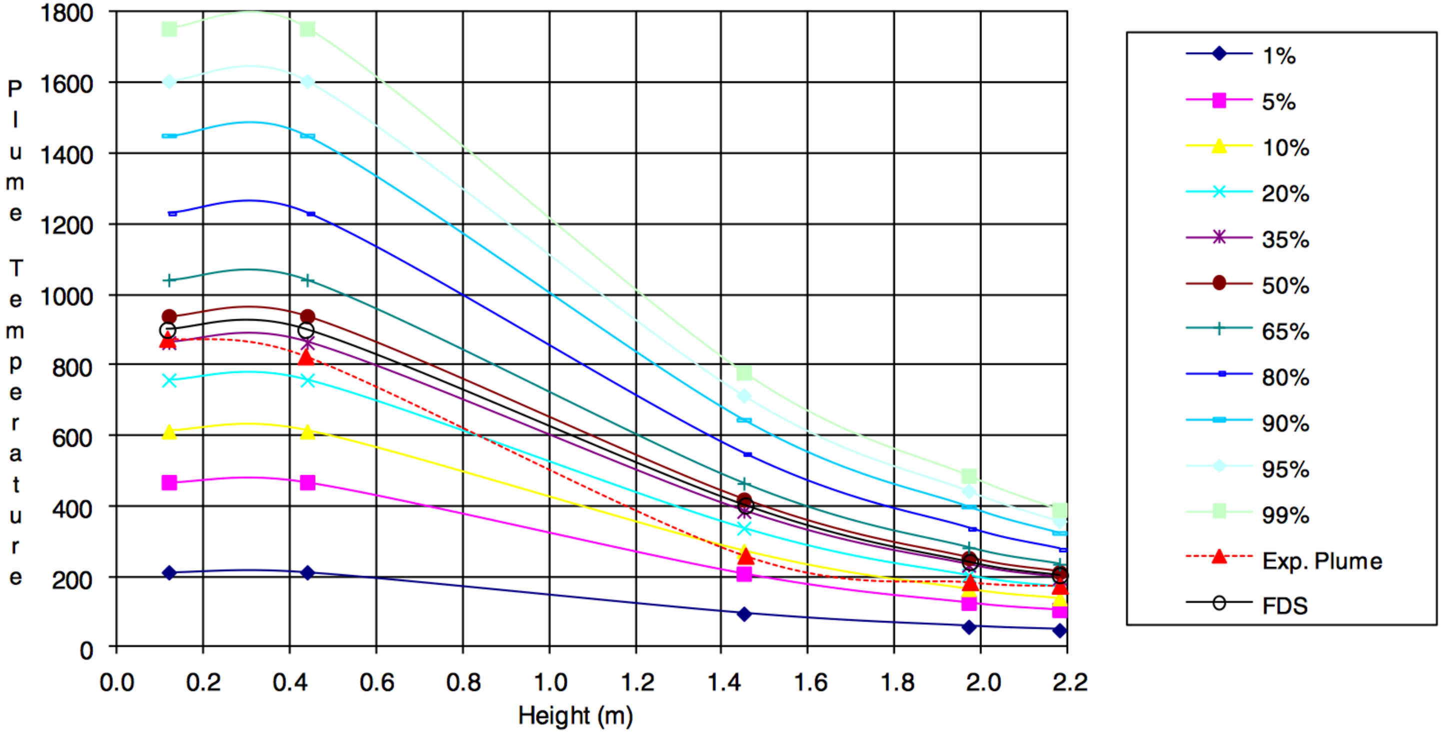
POINT SOURCE FIRE MODEL X LINE FIRE SOURCE MODEL



LINE FIRE PLUME TEMPERATURE

$$L_{\beta} = \left[L_{\alpha}\right]^{\beta}$$





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CHALLENGES AHEAD

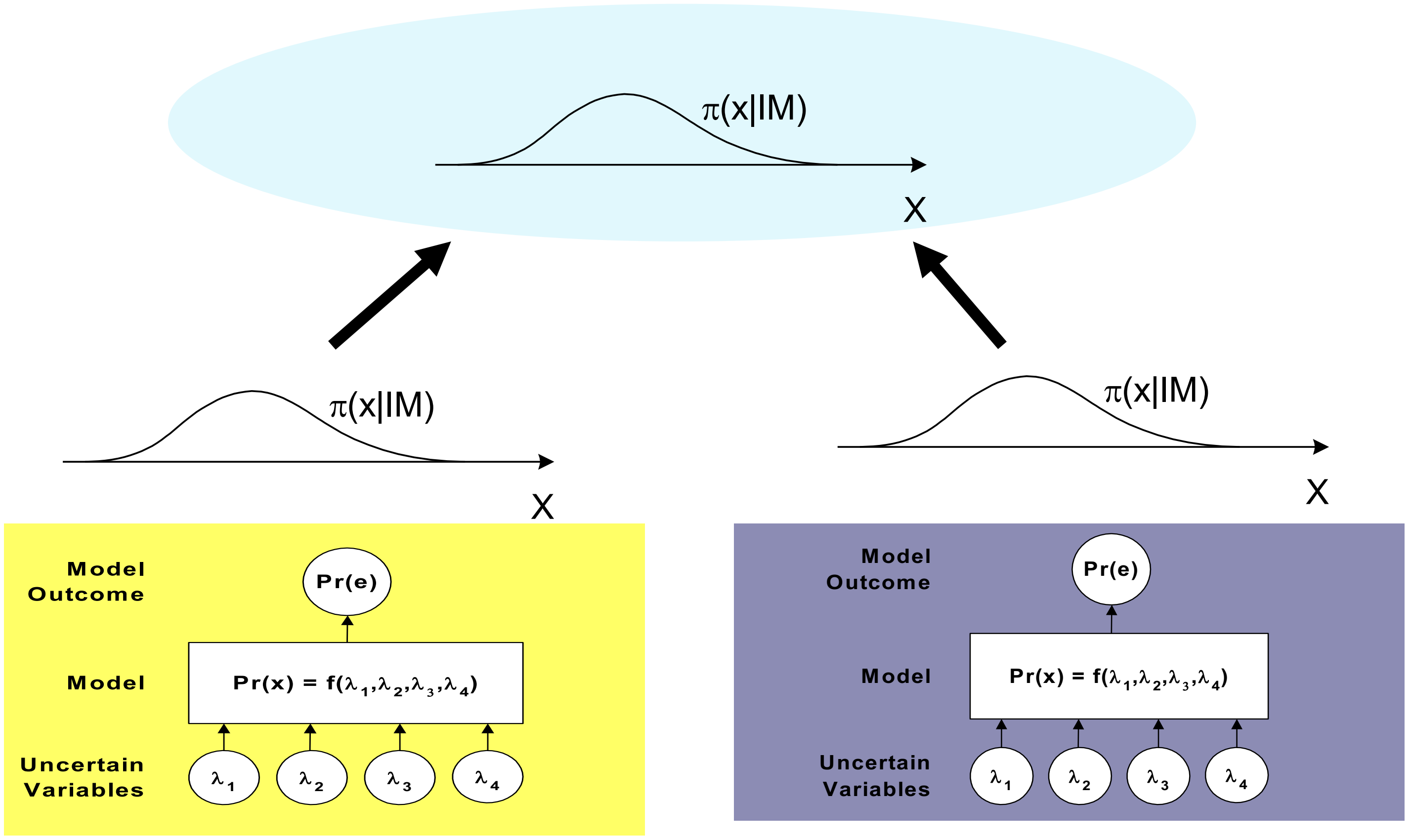
UNCERTAINTY IS UNCERTAINTY?

- Many believe that there is only one kind of uncertainty stemming from our lack of knowledge concerning reality

- "Let $p_0(n|t)$ be the true distribution of the number of events in [0,t], obtained by considering an infinite number of activities similar to the one considered" (T. Bjerga et al., 2014)

- When analyzing complex phenomena:
  - Epistemic – practically reducible (by collecting more data and increasing our knowledge of the phenomenon in question)
  - Aleatory – practically irreducible (due to level of modeling detail, limitation of resources, limitation in current state of the art)

ALTERNATIVE MODELS



Yellow Model/Assumption

Blue Model/Assumption

- Gaps in knowledge about relevant phenomena
- Approximations
- Quality of implementation
- This can lead to alternative assumptions on model structure giving raise to multiple models

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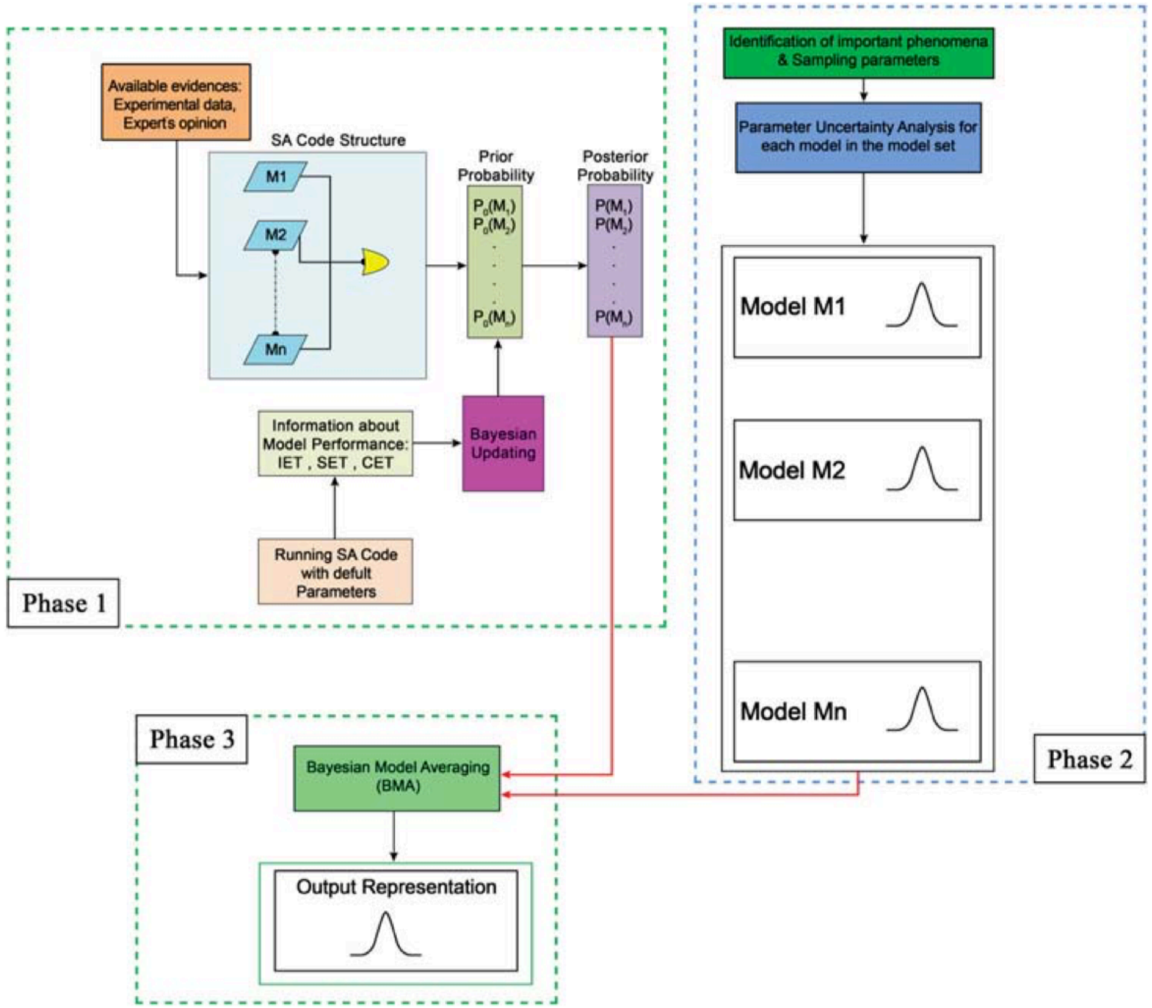
SUBMODELS UNCERTAINTY – COMPUTATIONAL CODE



- Model uncertainty in severe accident analysis:
  - Probability of best model based on Bayesian additive error model
  - Use of performance data
  - Multiple independent submodels
  - Model uncertainty due to multiple submodels via BMA

Hoseyni and Pourgol-Mohammad, 2016

DEPENDENCY AMONG MODELS

- Models are likely to share some common theoretical principles as they are representations of the same reality
- Models may be subject to same common implementation procedures such as mathematical approximations and numerical techniques
- Models may have been conceptualized and implemented by individuals sharing the same basic training and knowledge
- As a result of sharing similar modeling processes, models might have common structural elements such as similarities in form and common sets of parameters
  - They would then share, to some degree, available information sources and some of their inputs

HEAT RELEASE RATE

- Heat Release Rate (HRR) in an enclosure fire:

$$Q = Q_o e^{\left(\frac{t}{\tau_g}\right)} \qquad\qquad Q = Q_p \left(\frac{t}{\tau_g}\right)^2$$

- Copulas based quantification:
  - Likelihood function in terms of the Frank´s copula

$$\bar{L}(Q_1, Q_2|Q) = \log_\alpha\left[1 + \frac{\left(\alpha^{F_1(Q_1|Q)} - 1\right)\left(\alpha^{F_2(Q_2|Q)} - 1\right)}{\alpha - 1}\right]$$

  - Assuming multiplicative error:

$$f_i(Q_i|Q) = \frac{1}{\sqrt{2\pi}\sigma_i Q_i} e^{-\frac{1}{2}\left(\frac{\ln Q_i - (\ln Q + \ln b_i)}{\sigma_i}\right)^2}$$

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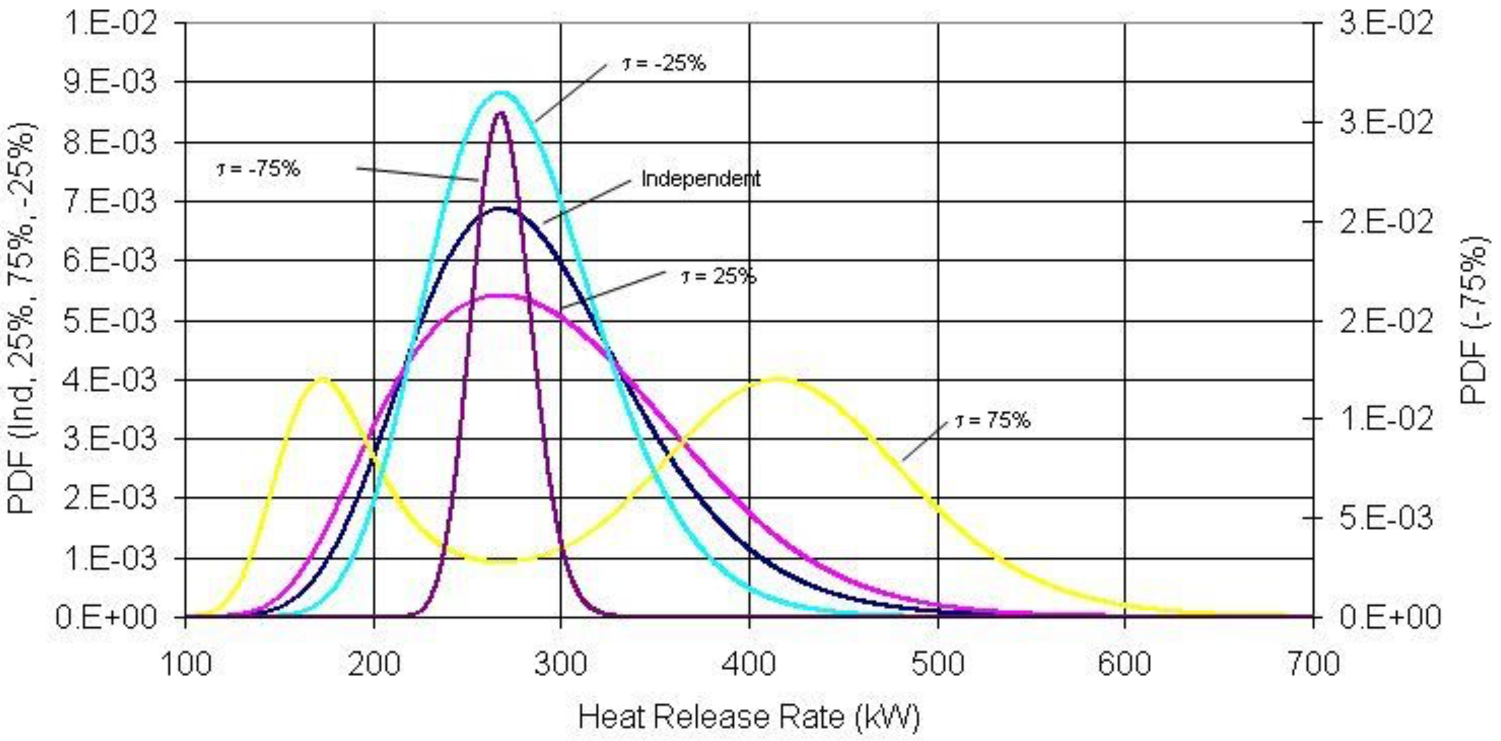
MODEL UNCERTAINTY IN HEAT RELEASE RATE

- At t = 200s, we have Q_1 = 193 kW and Q_2 = 347 kW



ACCOUNTING FOR THE UNKNOWN AND UNEXPECTED (I)

- What if our models are out of touch with reality

- The possibility that due to some unforeseen conditions (upset events) the real value could fall totally out of the rage of model predictions

- Events associated with changes in natural, socio-economic, and political systems:
  - Wars
  - Sudden change of governments
  - Climate change
  - ….

ACCOUNTING FOR THE UNKNOWN AND UNEXPECTED (II)

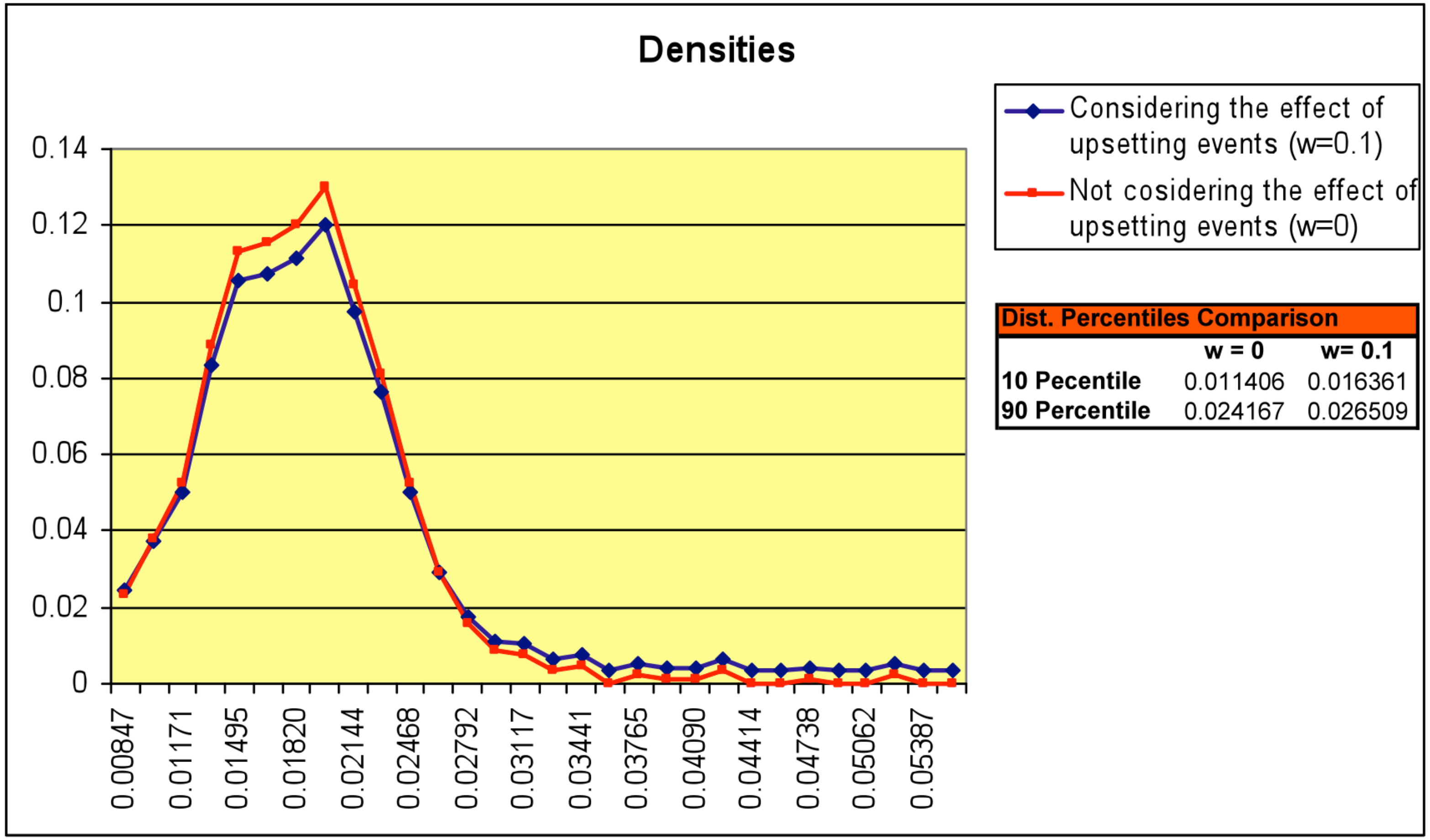
$$\pi'(p^{True} \mid p^{Estimate}, E) = (1-w) * \pi(p^{True} \mid p^{Estimate}, E) + w * g(p^{True})$$

Where:

- "w" : relative frequency of "upset event"
- $\pi(p^{True} \mid p^{Estimate}, E)$: posterior distribution of default probability in the absence of upsetting events
- $g(p^{True})$: distribution of default probability in the case of occurrence of upset events
  - Uniform, non-informative

Kazemi, R; Mosleh, A. "Improving Default Risk Prediction Using Bayesian Model Uncertainty Techniques", Risk Analysis, v.12, n.11, 2012

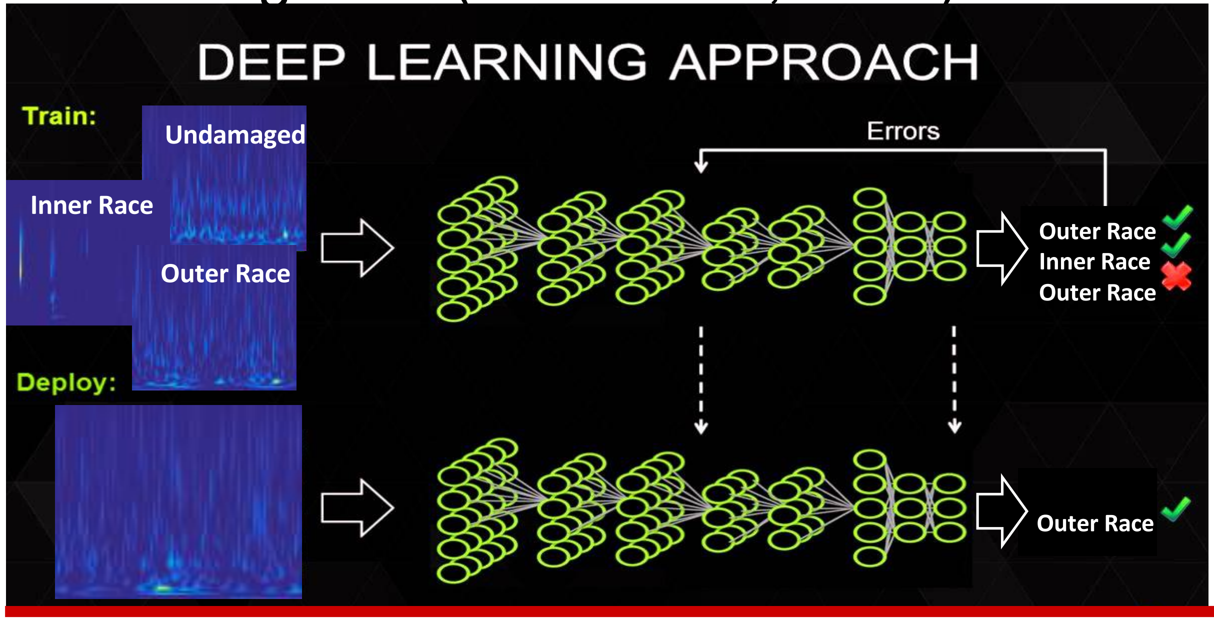
Example: Default Probability Uncertainty Distribution for 2006 (with Effect of Upset Events)

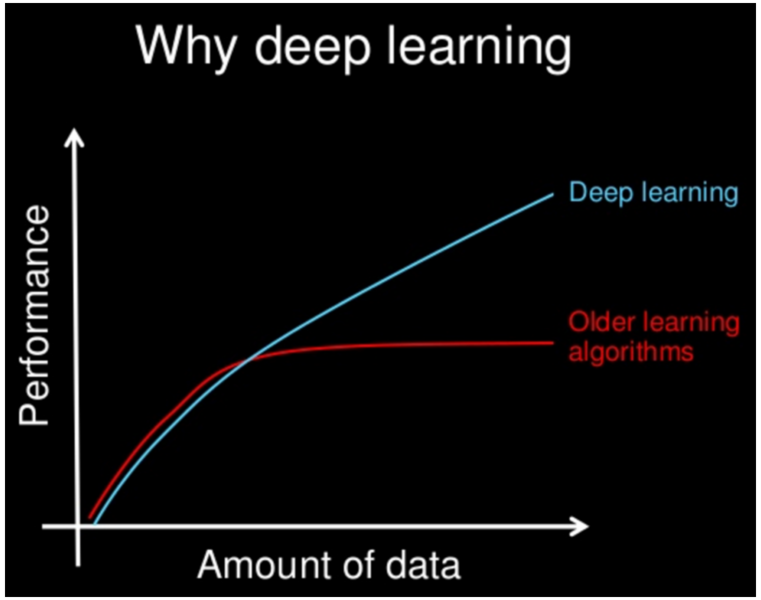


Dist. Percentiles Comparison		
	w = 0	**w= 0.1**
10 Pecentile	0.011406	0.016361
90 Percentile	0.024167	0.026509

DEEP LEARNING BASED PHM

- Deep learning has attracted tremendous attention from researchers in fields such as physics, biology, and manufacturing, to name a few (Baldi et al., 2014; Anjos et al., 2015; Bergmann et al., 2014)
- It has recently been introduced in reliability
  - Diagnosis (Droguett et al., 2017; Zhou et al., 2017)
  - Prognosis (Babu et al., 2016)





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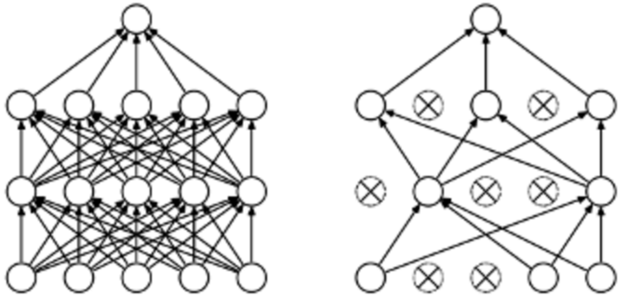
DRAWBACKS OF STANDARD DEEP LEARNING

- Compute point estimates
- Deep NNs make overly confident decisions about the correct class, prediction or action
- Deep NNs are prone to overfitting
- No uncertainty quantification
  - Serious limitation for decision making in critical applications such as safety, medical

BAYESIAN NEURAL NETWORKS AND DROPOUT

- Not **scalable** for modern applications and massive data sets

- Dropout:
  - Empirical technique used to avoid overfitting
  - It multiplies hidden activations by Bernoulli distributed random variables which take the value 1 with probability p and 0 otherwise
  - Randomly "drop out" hidden units and their connections during training time to prevents hidden units from co-adapting too much



(a) Standard Neural Net (b) After applying dropout.

Dropout Neural Net Model. **Left**: A standard neural net with 2 hidden layers. **Right**: An example of a thinned net produced by applying dropout to the network on the left. Crossed units have been dropped.

Srivastava, Hinton, Krizhevsky, Sutskever, Salakhutdinov.
Dropout: A Simple Way to Prevent Neural Networks from Overfitting,
J. Machine Learning Research (2014)

BAYESIAN DEEP LEARNING WITH MC DROPOUT*

- Requires applying dropout at every weight layer at test time

- For input *x** the predictive distribution for output *y** is:

$$q(y^* \mid x^*) = \int p(y^* \mid x^*, \omega) \cdot q(\omega) d\omega$$

- MC Dropout averages over *N* forward passes through the network at test time

- MC Dropout corresponds to model averaging
  - Results in estimation of the model output uncertainty
  - Model uncertainty and parameter uncertainty are comingled

*Y. Gal, Z. Ghahramani. Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning. Proceedings of the 33rd International Conference on Machine Learning, New York, NY, USA, 2016

CONCLUSIONS (I)

- Risk assessments are often model-based
- Not taking into account model uncertainty can underestimate the amount of uncertainty
- Understanding the fundamentals is a must
  - Research efforts are needed to explore fundamentals
  - Help in developing better quantification methods

CONCLUSIONS (II)

- Operationalization of model uncertainty poses various challenges:
  - Multiple and dependent models
  - Time varying dependences
  - Effective ways to disentangle model and parameter uncertainties
  - Submodels, computer codes
  - Bayesian approaches are usually too expensive
  - Explore other alternatives for model uncertainty representation (e.g., evidence theory)

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THANK YOU!