Improving Model Identification:

Reconciling Theory with Observations & The Problem of Sufficient Statistics

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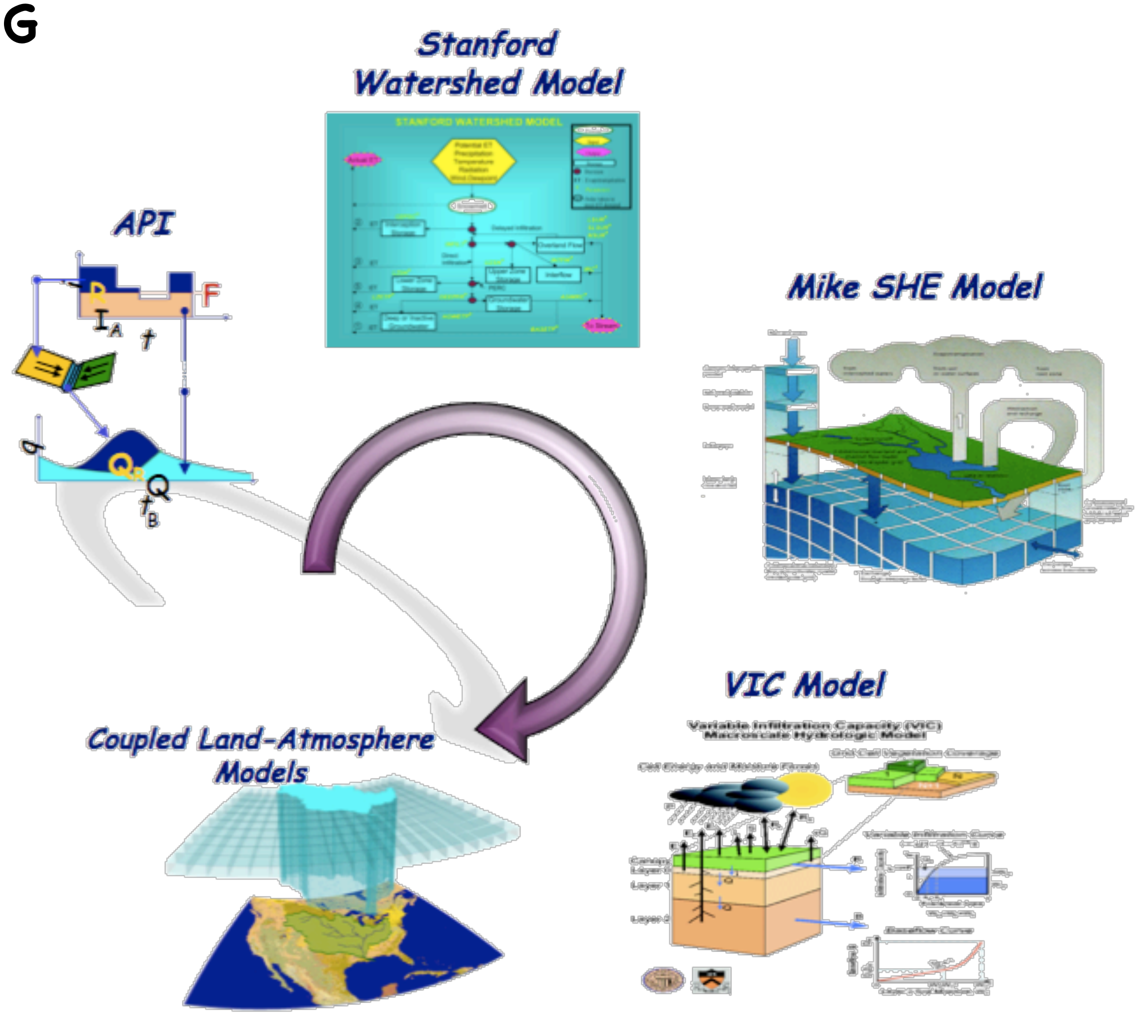
University of Arizona

Session HS1.6 on
Metrics and the Use of Data in Hydrology to support Model Structure Improvement

EGU Meeting

Vienna, Austria

FIVE DECADES OF COMPUTER-BASED HYDROLOGIC MODELING



FIVE DECADES OF COMPUTER-BASED HYDROLOGIC M

MANY REPORTS OF DIFFICULTIES IN MODEL IDENTIFICATION

"A true optimum set of (parameter) values was not found *in over 2 years of full-time work concentrated on one watershed,* although many apparent optimum sets were readily obtained."

VOL. 12 NO. 3 WATER ... EARCH JUNE 1976

Parameter Optimiza... for Watershed Models

P. R. JOHNSTON[1] AND D. H. PILGRIM

School of Civil Engineering, University of New South Wales, Kensington, N. S. W., Australia

A detailed search for the optimum values of the parameters of the Boughton model is described. The Simplex and Davidon optimization methods were used. Rapid initial reductions in the objective function were readily achieved, but the solutions approached several widely different apparent optima. Alternate use of different optimization methods and numerical and algebraic studies enabled considerable further progress to be made in the search. Much information was obtained on various aspects of parameter optimization. These include interdependence and indifference of parameters, the form of the response surface and the occurrence of discontinuities, the required length of the 'warm-up' period for different types of stores, and the effects of using different types of objective functions. As typical stores were analyzed and the only basic assumption involved was that the data contained errors, the findings should apply to most watershed models.

Two broad approaches have been used in assigning values to the parameters of mathematical rainfall-runoff models for appl...ion to given watersheds. In the first, values are estimated from available knowledge of processes or from measurements of physical properties of the watershed, it being

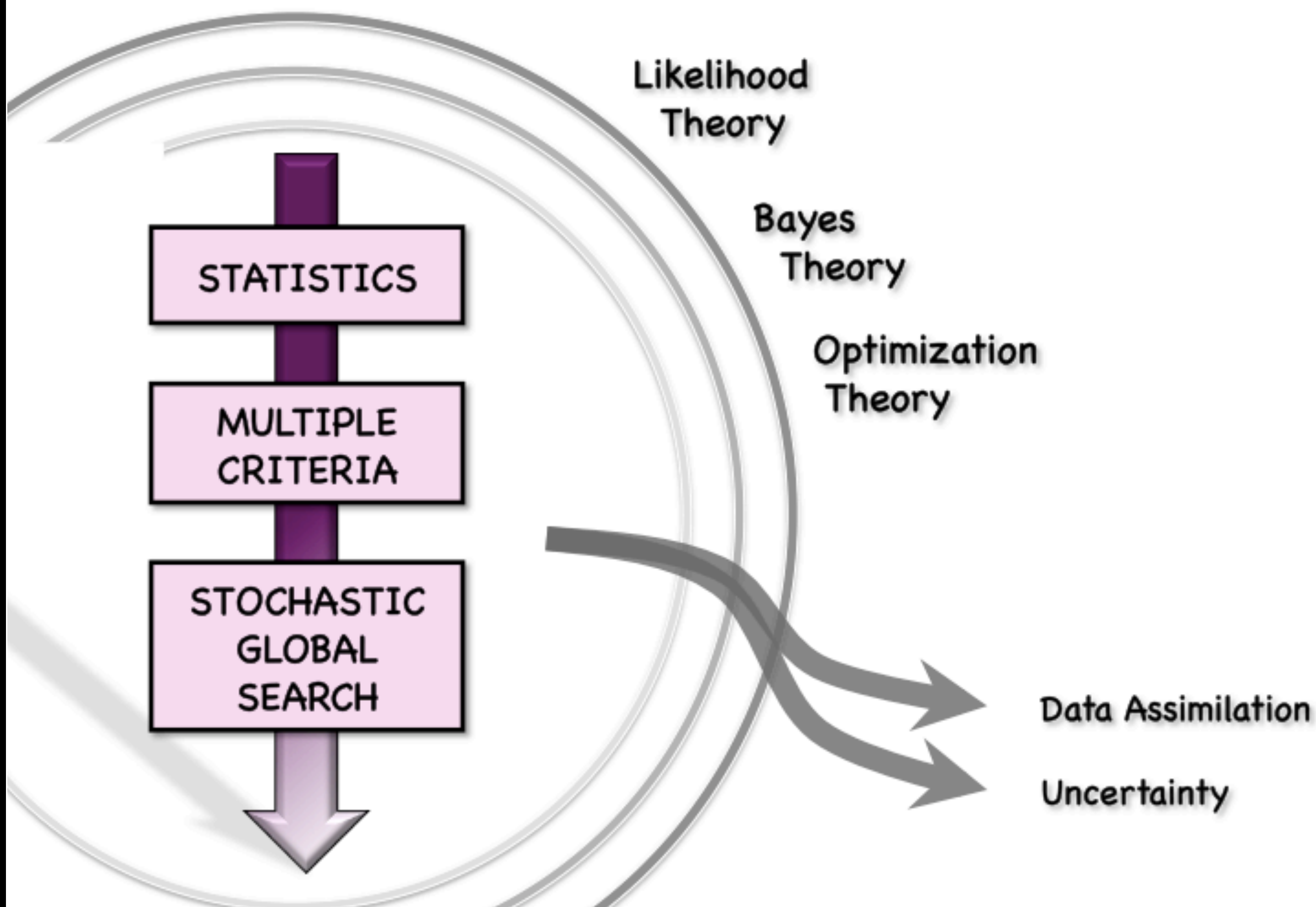
model, most of the findings are generally applicable to watershed models, since typical moisture stores were analyzed. A more detailed description of the study has been given by *Johnston and Pilgrim* [1973].

The Boughton model (Figure 1) was selected for use in the ... on a daily basis and is thus suitable

FIVE DECADES OF COMPUTER-BASED HYDROLOGIC

MANY REPORTS OF DIFFICULTIES IN MODEL

MANY ATTEMPTS TO IMPROVE MODEL IDENTIFICATION



FIVE DECADES OF COMPUTER-BASED HYDROLOGIC

MANY REPORTS OF DIFFICULTIES IN MODEL

MANY ATTEMPTS TO IMPROVE MODEL IDENTIFICATION

NOW RECOGNIZED BY "NSF" AS A "GRAND CHALLENGE"

White Paper

GRAND CHALLENGES OF THE FUTURE FOR ENVIRONMENTAL MODELING

Report of the NSF Project (Award # 0630367)
May 2006 - May 2008

DRAFT

M B Beck

Warnell School of Forestry and Natural Resources
University of Georgia, Athens, Georgia 30602-2152

October, 2008

Beck et al (2008)

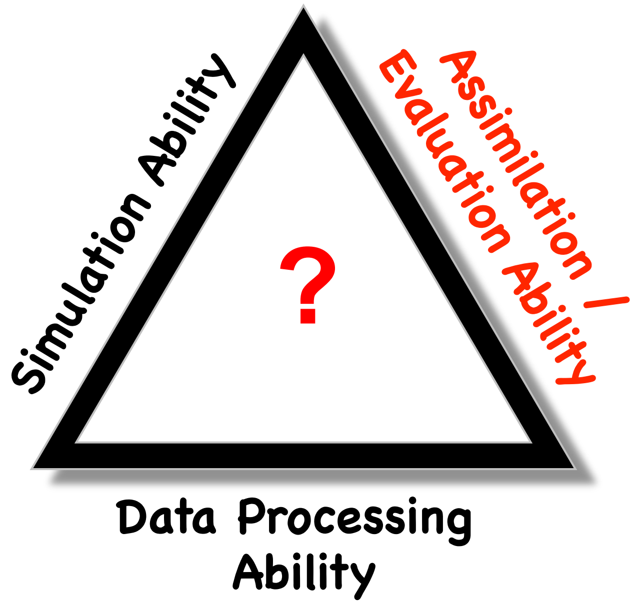
We do a poor job at reconciling complex models with field data. How do we improve this?

Challenge # 7:

Under the expectatio… sive expansion in the scop… olume of field observations generat… he Environmental Observatories, couple… d integrated with the prospect of equally… assive expansion in data processing and sc… ntific visualization enabled by the future environmental cyber-infrastructure, what radically novel procedures and algorithms are needed to rectify the chronic, historical deficit of the past four decades in engaging complex models (VHOMs) systematically and successfully with field data for the purposes of learning and discovery and, thereby, enhancing the growth of environmental knowledge?

THE PROBLEM

INCREASING MODEL COMPLEXITY



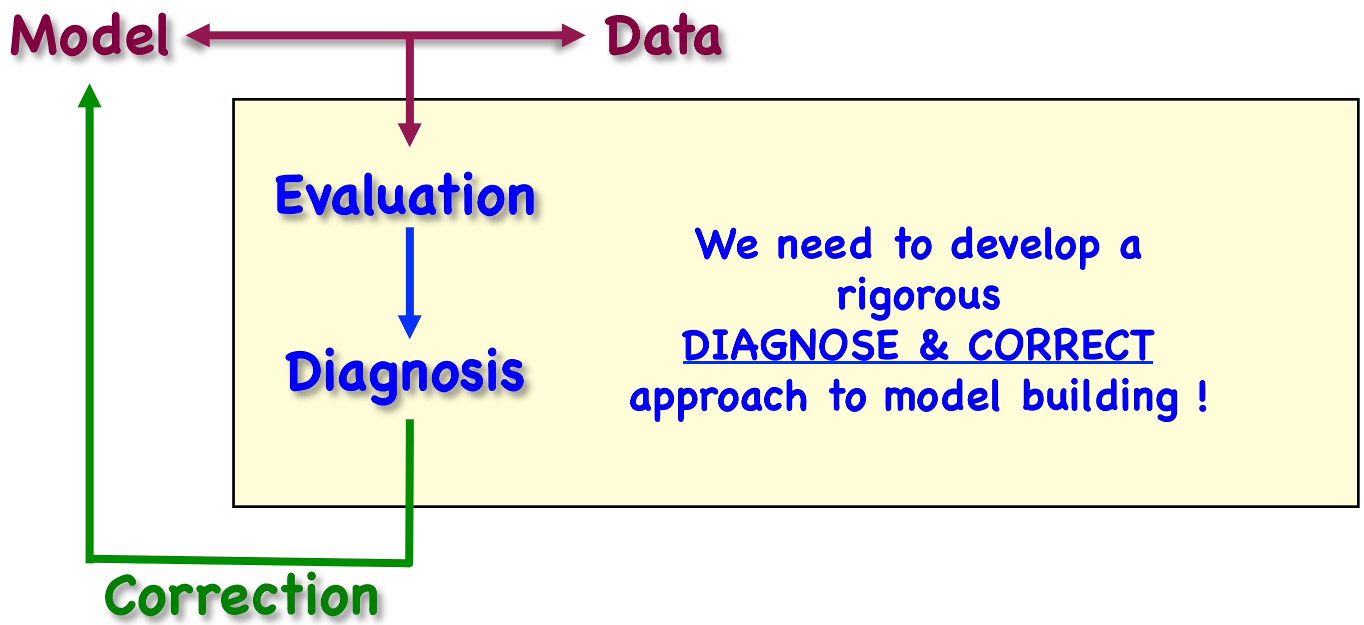
INCREASING COMPUTATIONAL POWER

INCREASING DATA AVAILABILITY

THE SOLUTION

WE NEED A THEORY OF DIAGNOSTIC EVALUATION

The theory should enable us to link what we “see” in the data to what is “right” and “wrong” with our models.



BLUEPRINT FOR SUCH A THEORY

HYDROLOGICAL PROCESSES
Hydrol. Process. (2008)
Published online in Wiley InterScience
(www.interscience.wiley.com) DOI: 10.1002/hyp.6989

Reconciling theory with observations: elements of a diagnostic approach to model evaluation

Hoshin V. Gupta,[1]* Thorsten Wagener[2] and Yuqiong Liu[1]

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[2] *Department of Civil and Environmental Engineering, Pennsylvania State University, University Park, PA 16802*

This paper discusses the need for a well-cons
has clear and compelling diagnostic power. Th
'Predictions in Ungaged Basins' initiative and
initiative, among others. It is suggested that r
observational data are inadequate in the face c
environmental science, and steps are proposed
This paper presents the concept of a diagnostic
signature indices that measure theoretically rele
issue of degree of system complexity resolvable
facilitate uncertainty analysis, and can be readily
in ungaged basins. Copyright © 2008 John Wil

KEY WORDS model identification; information;

Received 26 June 2007; Accepted 15 December

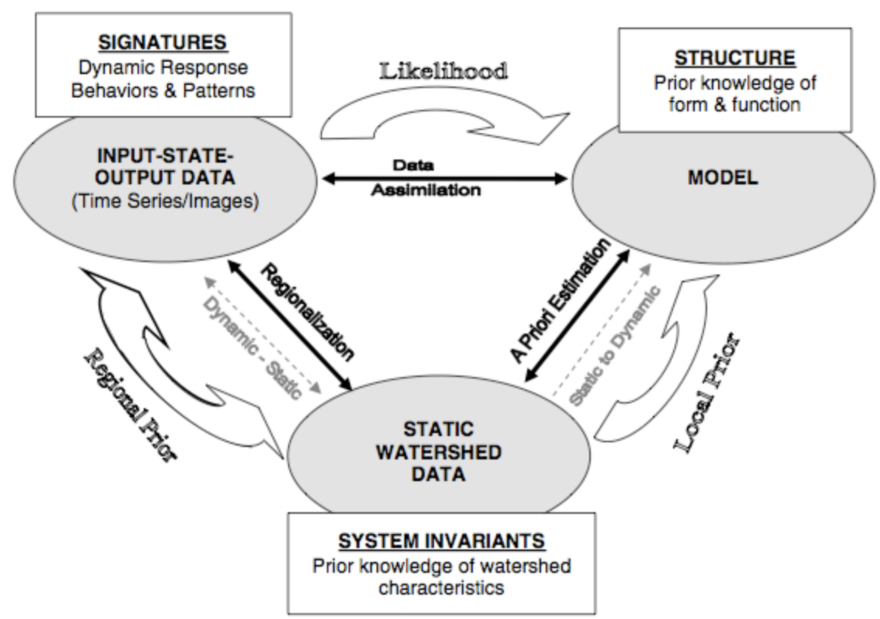
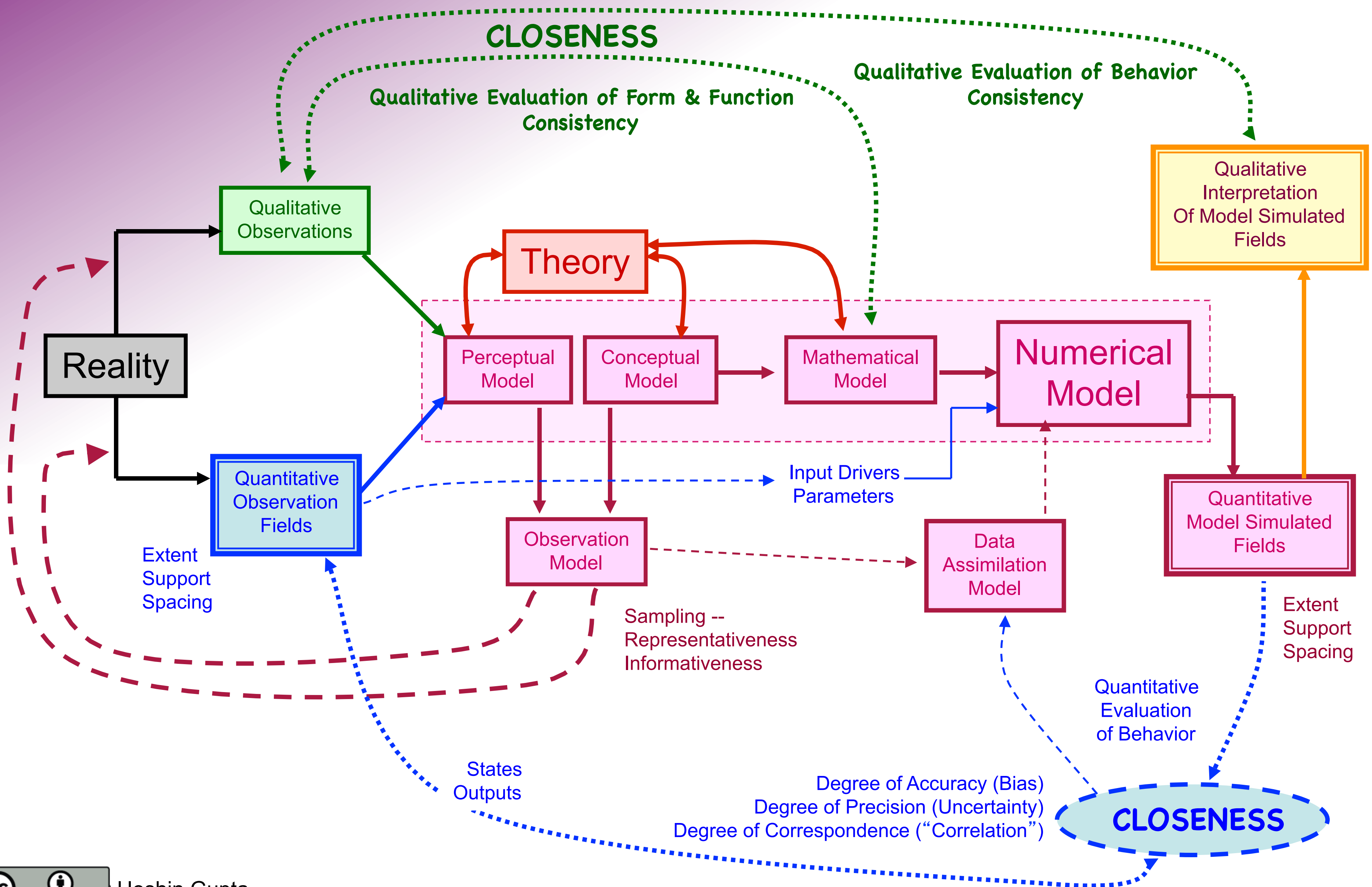
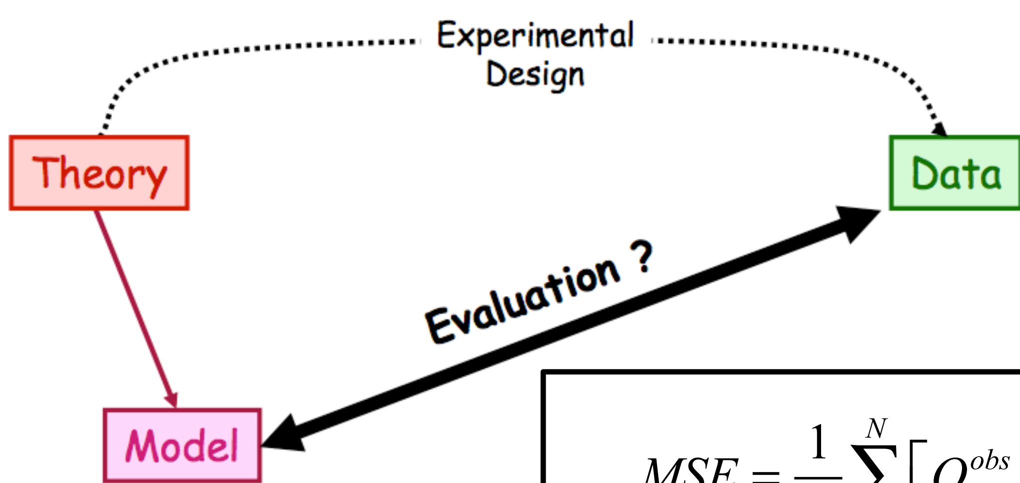


Figure 6. The three kinds of information used to constrain the predictive model

The Model Building & Evaluation Process

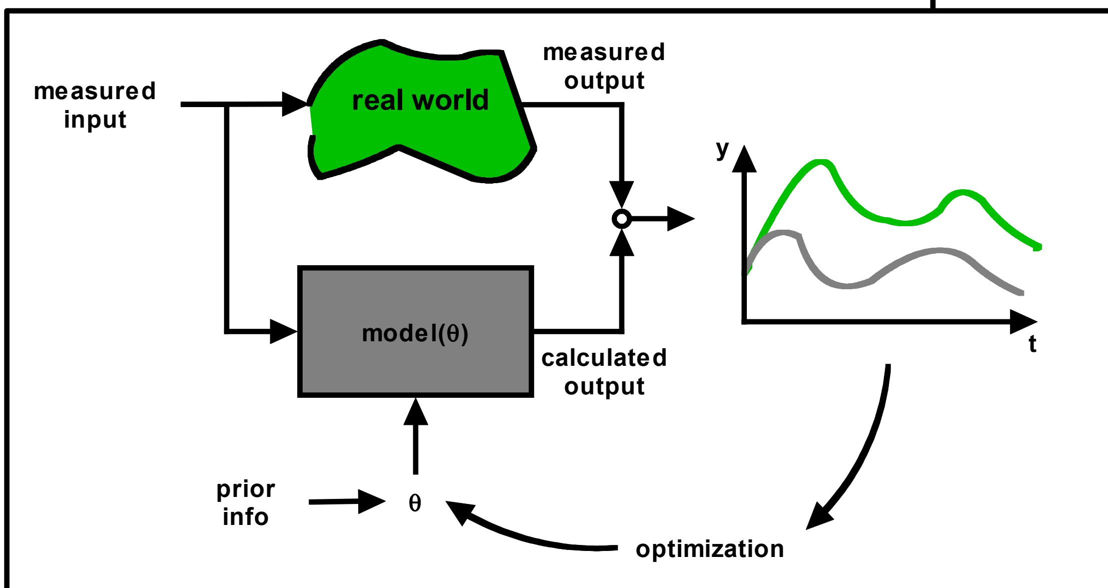


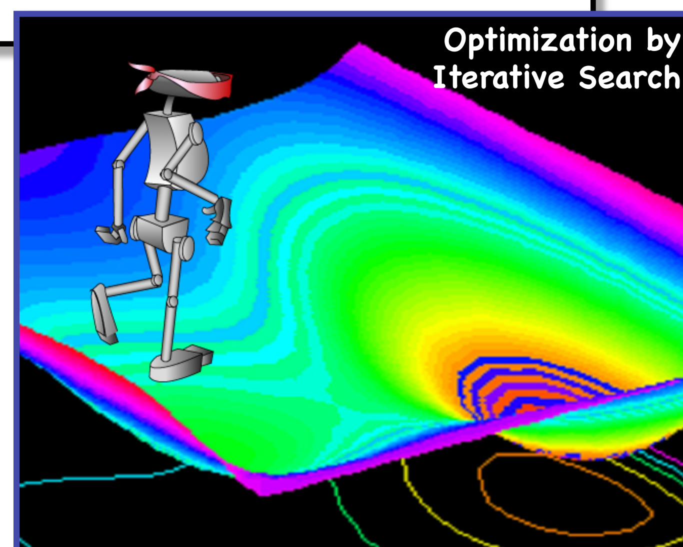
NEO-CLASSICAL APPROACH TO MODEL EVALUATION



Matching the data point-for-point

$$MSE = \frac{1}{N}\sum_{t=1}^{N}\left[Q_t^{obs} - Q_t^{m}(\theta)\right]^2$$





BUT … 'MSE' DECOMPOSES* INTO THREE STATISTICS OF MODEL PERFORMANCE

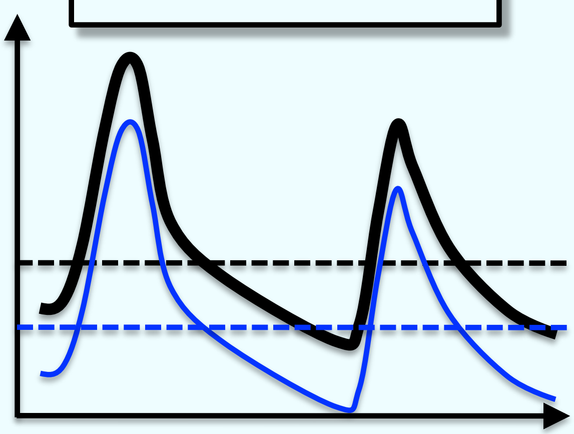
$$MSE = \frac{1}{N}\sum_{t=1}^{N}\left[Q_t^{obs} - Q_t^{\mathrm{m}}(\theta)\right]^2$$

$$MSE = \left(\mu_{\mathrm{m}} - \mu_{obs}\right)^2 + \left(\sigma_{\mathrm{m}} - \sigma_{obs}\right)^2 + 2\sigma_{\mathrm{m}}\sigma_{obs}(1-r)$$

MSE = $\mathcal{F}$(**Mean Error**) + $\mathcal{F}$(**Variability Error**) + $\mathcal{F}$(**Linear Correlation**)

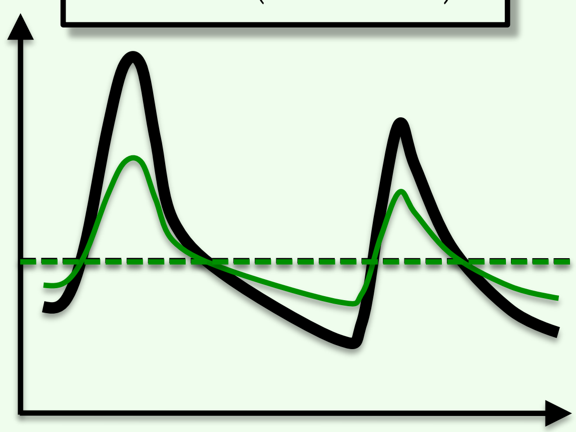
Water Balance

$$\Delta\mu = \left(\mu_{\mathrm{m}} - \mu_{obs}\right)$$



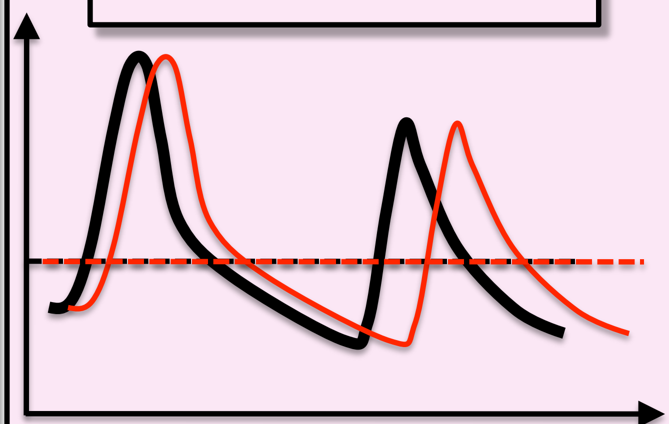
Variability

$$\Delta\sigma = \left(\sigma_{\mathrm{m}} - \sigma_{obs}\right)$$



Timing & Shape

$$r$$

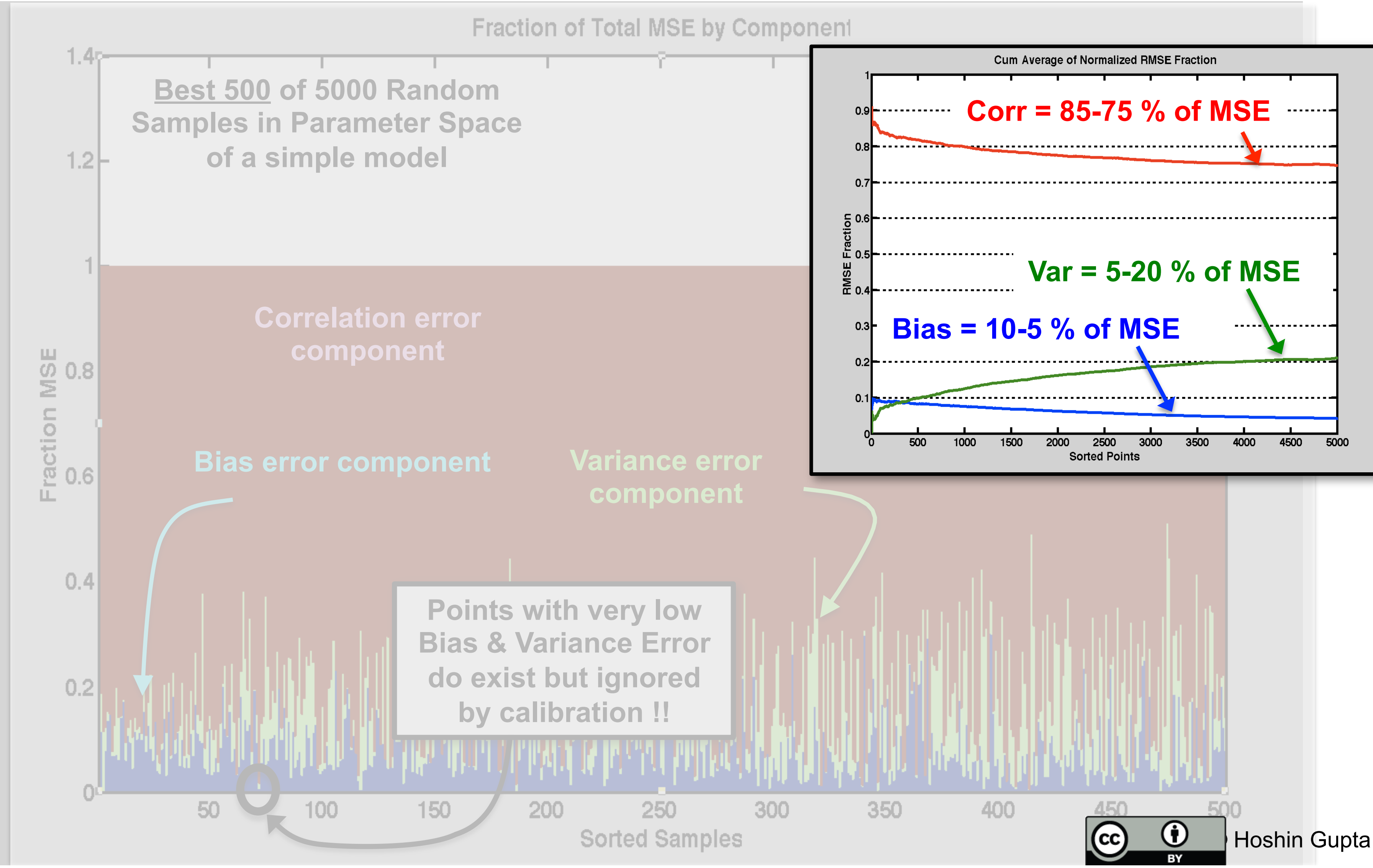


* **Decomposition of the Mean Squared Error & NSE Performance Criteria: Implications for Improving Hydrological Modeling**
Gupta, H.V., H. Kling, Y.K. Yilmaz & G.F. Martinez-Baquero, *Manuscript submitted to Journal of Hydrology*, 2009.

 Hoshin Gupta

PROBLEM 1. CORRELATION COMPONENT DOMINATES

$$MSE = \mathcal{F}(\text{Bias Error}) + \mathcal{F}(\text{Var Error}) + \mathcal{F}(\text{Corr Error})$$



PROBLEM 2.
MODEL PERFORMANCE WILL BE SIGNIFICANTLY OVER-ESTIMATED

$$MSE = \left(\mu_{\mathrm{m}} - \mu_{obs}\right)^2 + \left(\sigma_{\mathrm{m}} - \sigma_{obs}\right)^2 + 2\sigma_{\mathrm{m}}\sigma_{obs}(1-r)$$

IDEAL

If we ensure $\mu_m = \mu_{obs}$ and $\sigma_m = \sigma_{obs}$ the expected 'best' value for *MSE* is:

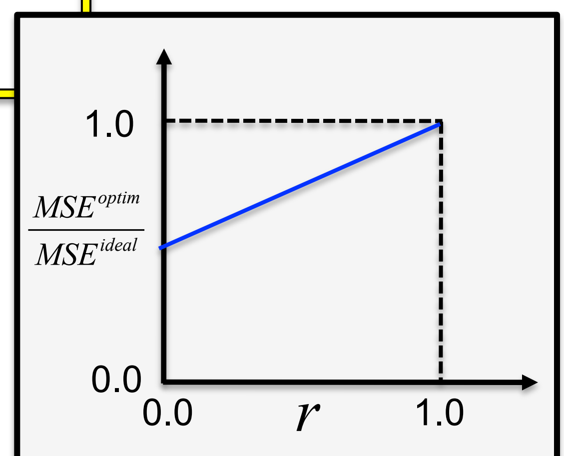
$$\frac{MSE_{ideal}}{\sigma^2_{obs}} = 2\left(1 - r_{ideal}\right)$$

OPTIMIZED

But if we optimize on *MSE* <u>without</u> constraining μ_m & σ_m we will get:

$$\frac{MSE_{optim}}{\sigma^2_{obs}} = \left(1 - r^2_{optim}\right)$$

$$MSE^{optim} \approx \left(\frac{1+r}{2}\right) MSE^{ideal}$$



$$\boxed{MSE_{optim} < MSE_{ideal}}$$

assumes $r_{ideal} \sim r_{optim}$

PROBLEM 3.
VARIABILITY WILL BE UNDER-ESTIMATED

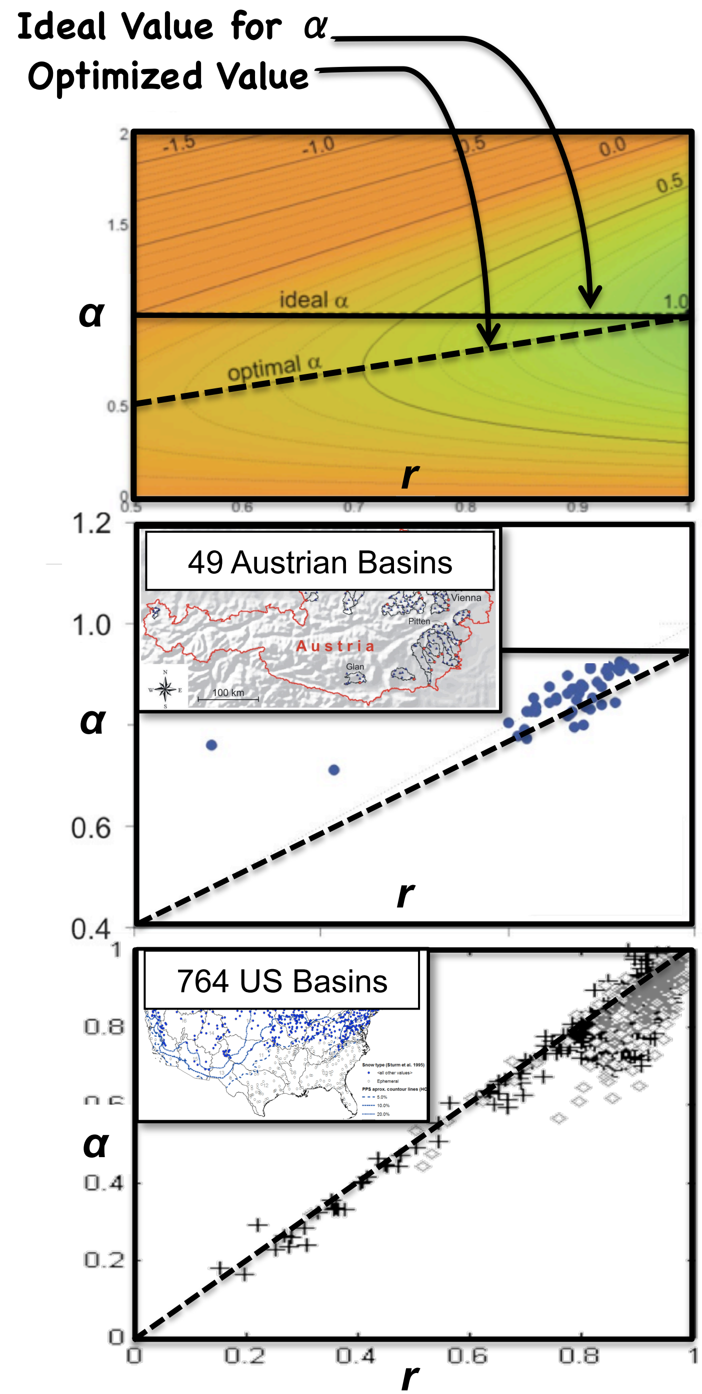
'Optimal' MSE is achieved when:

$$\sigma_m = r \bullet \sigma_{obs}$$

In other words:

$$\alpha = \frac{\sigma_m}{\sigma_{obs}} = r < 1.0$$

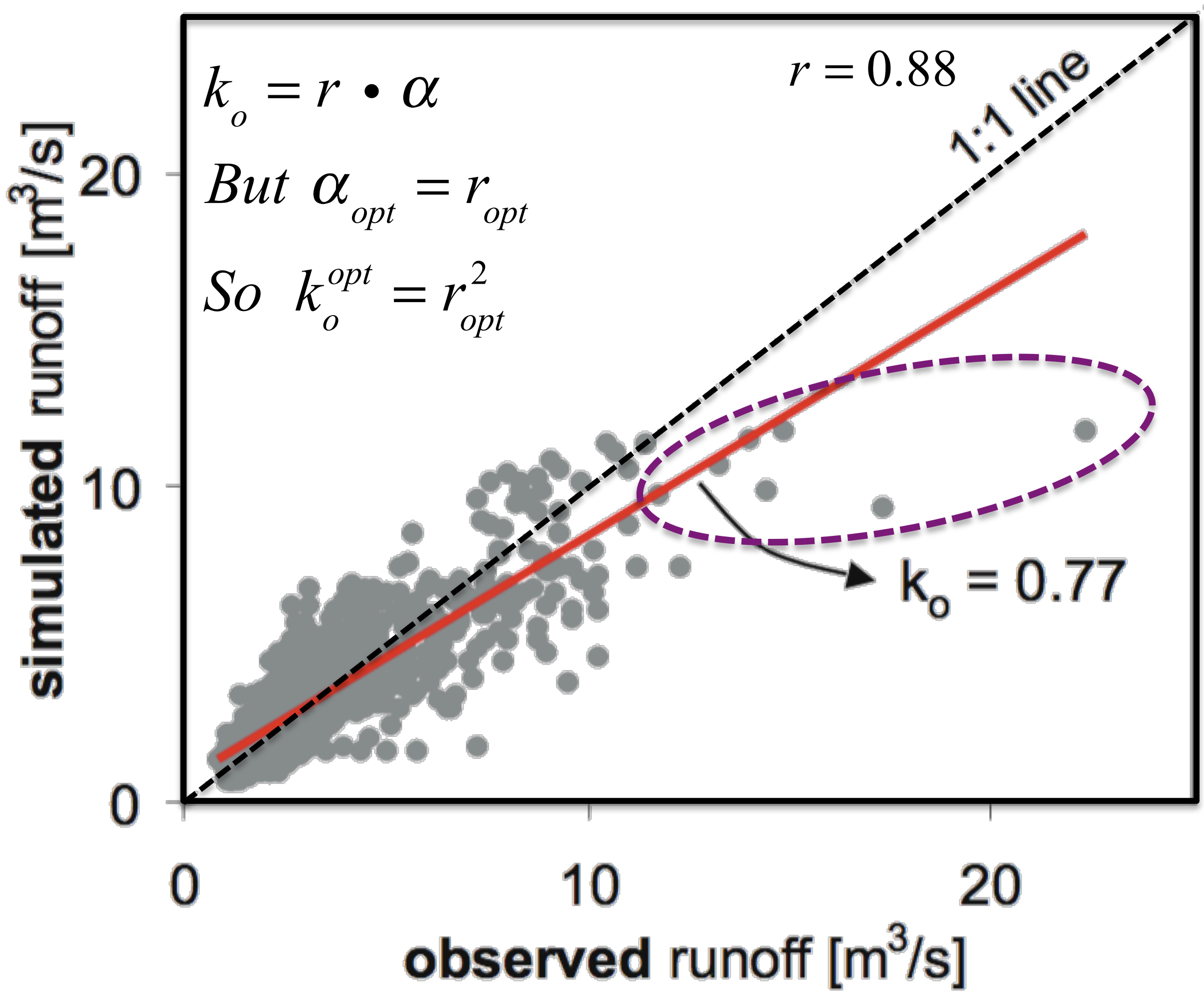
'Optimal' model will <u>underestimate</u> the observed variability of the data



PROBLEM 4.
PEAK FLOWS WILL BE UNDERESTIMATED

THIS IS IN SPITE OF THE FACT THAT 'MSE' IS SUPPOSED TO GIVE BETTER FIT TO THE LARGE VALUES !!!

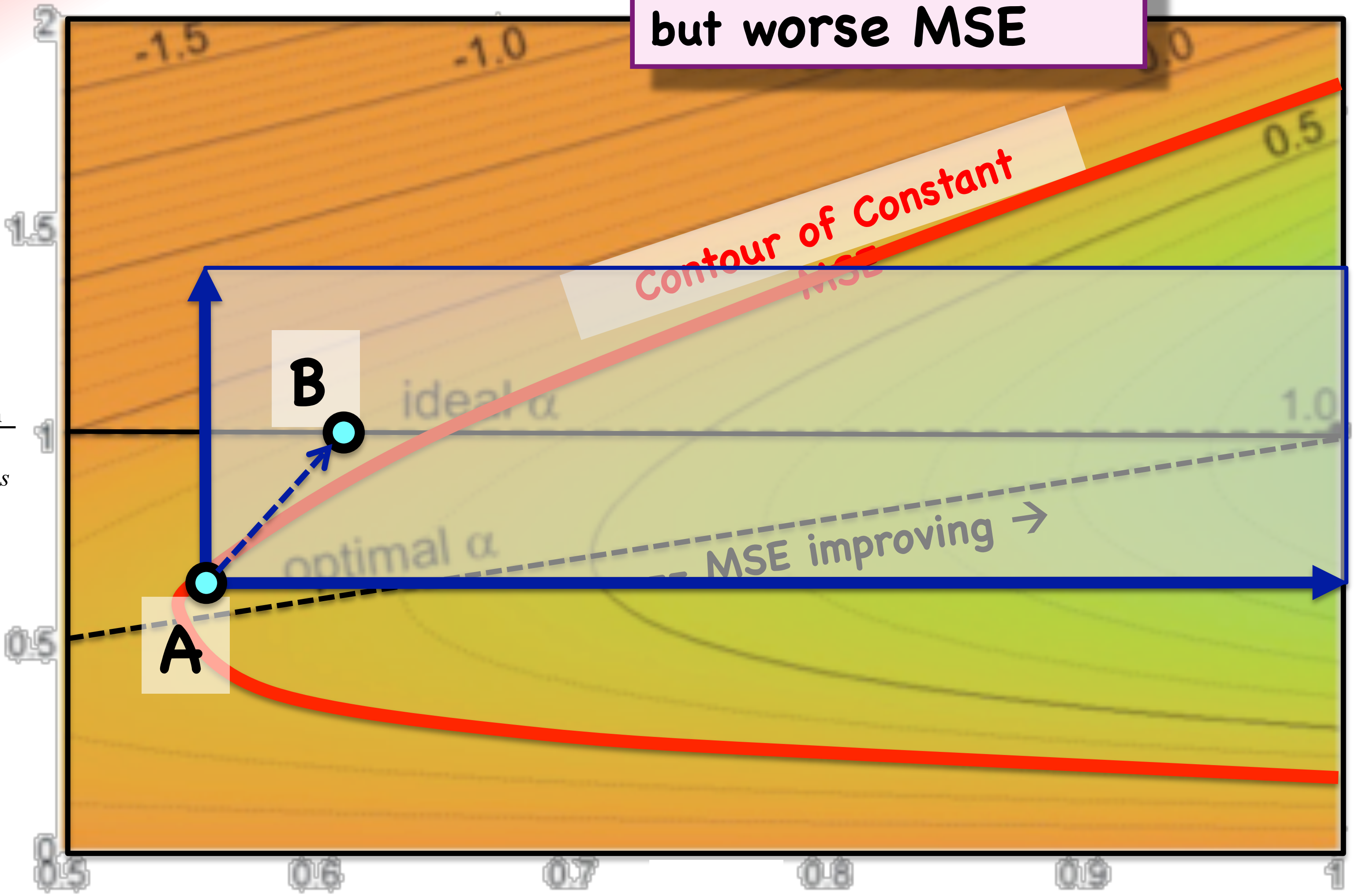
regression against observed runoff



PROBLEM 5.
MODEL RESULT CAN BE BETTER FOR WORSE VALUE OF 'MSE'

$$NSE = 1 - \frac{MSE}{\sigma_{obs}^2}$$

Point 'B' has better 'r' and 'α' but worse MSE



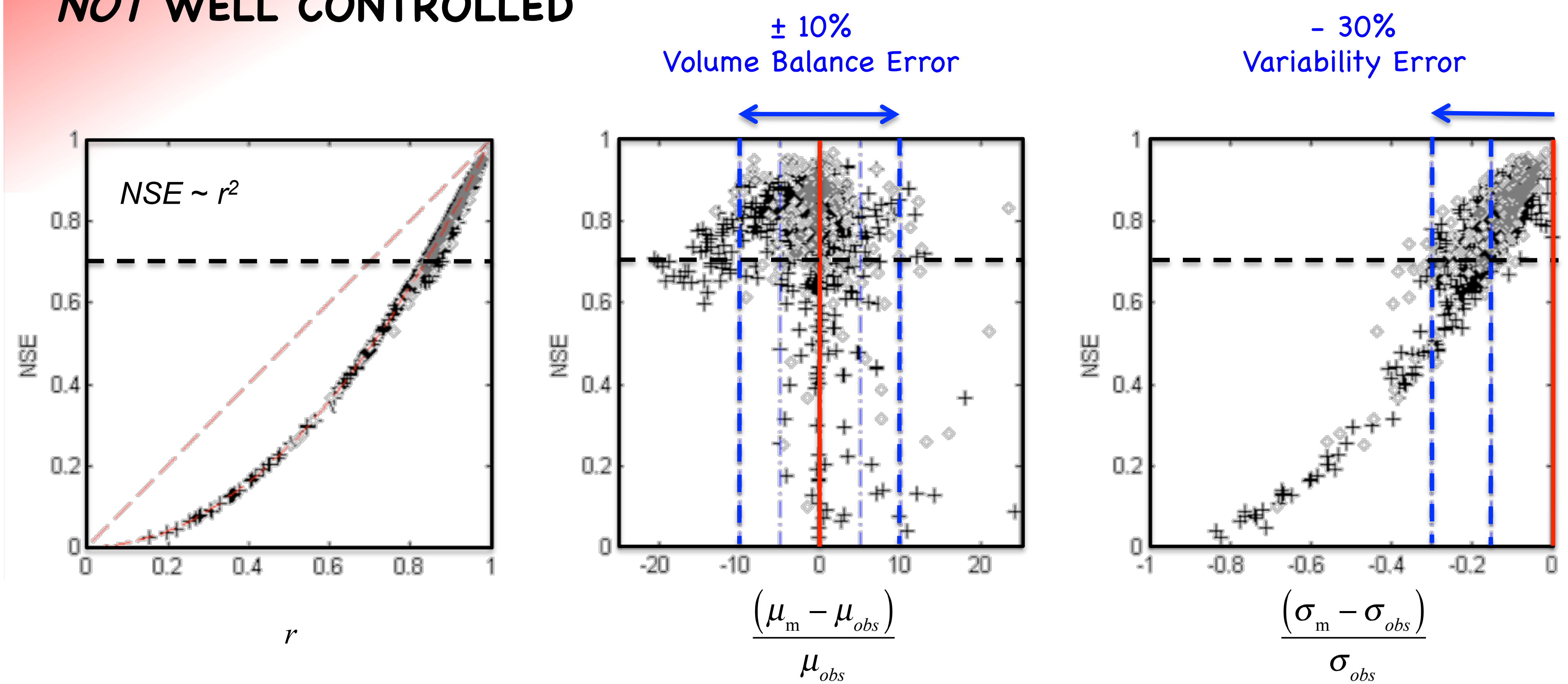
$$\alpha = \frac{\sigma_m}{\sigma_{obs}}$$

r

OVERALL PROBLEM

COMBINED EFFECT IS *NOT* WELL CONTROLLED

$$NSE = 1 - \frac{MSE}{\sigma^2_{obs}}$$



Water Balance Model
764 Catchments in Continental USA
Calibrated using NSE measure and SCE optimization algorithm

* **A Continental Scale Diagnostic Evaluation of the 'abcd' Monthly Water Balance Model for the Conterminous US**
G.F. Martinez-Baquero & H.V. Gupta, *Manuscript in preparation*, 2009.

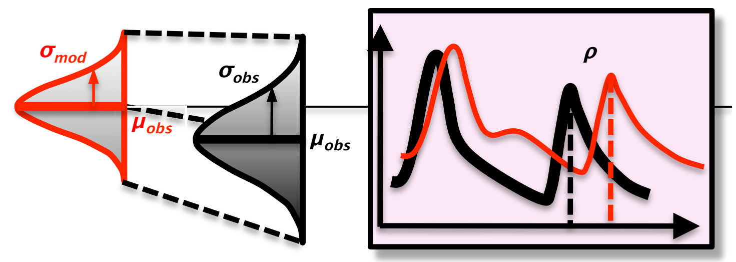
WHAT CAN WE LEARN FROM THIS?

$$MSE = \frac{1}{N}\sum_{t=1}^{N}\left[Q_t^{obs} - Q_t^{m}(\theta)\right]^2$$

$$MSE = \Delta\mu^2 + \Delta\sigma^2 + 2\sigma_{m}\sigma_{obs}(1-\rho)$$

1. Optimization using *MSE* is equivalent to trying to match *THREE* statistical properties of the data

   Data Mean (1st moment) – μ_{obs}
   Data Variance (2nd moment) – σ^2_{obs}
   Data Correlation structure – r



2. Two are properties of the data PDF, and the third is a property of the spatial &/or temporal correlation structure

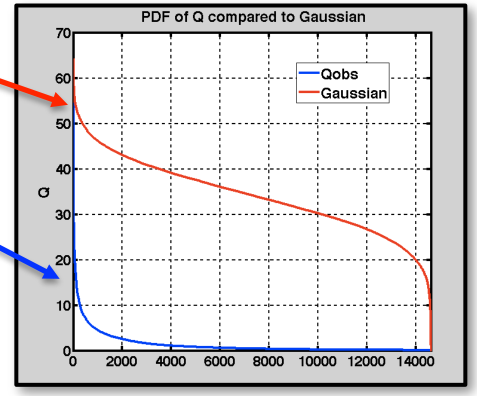
3. These are combined in a way that emphasizes certain aspects of system behavior … at the expense of others

4. For catchment modeling this can result in *poor Water Balance and under-estimation of Variability* – both being important system behaviors we wish to reproduce

BUT… WHY ONLY *THESE* THREE PROPERTIES ?

Gaussian CDF (symmetrical)

Typical CDF of Streamflow (highly skewed)



1. Data *PDF's* are very rarely Gaussian !
2. The Model should also reproduce <u>*other*</u> statistical properties of the data – particularly ones with hydrological significance !
3. *Linear correlation 'r'* aggregates different kinds of information about *spatio-temporal correlation structure* into ONE measure

THIS IS AN INEFFICIENT WAY TO EXTRACT INFORMATION !

THE CHALLENGE OF MODEL EVALUATION

TO DEVELOP

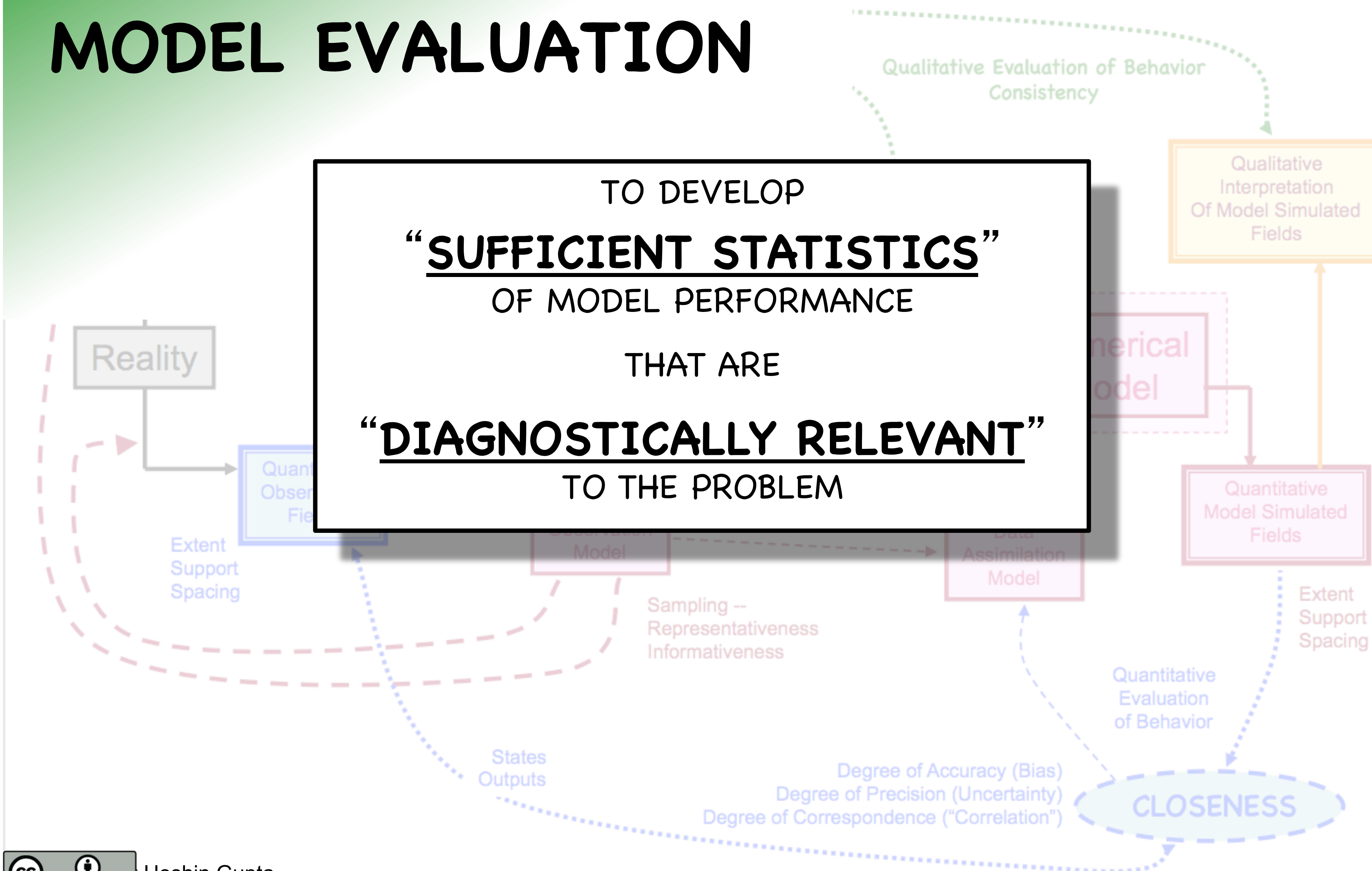
"**SUFFICIENT STATISTICS**"

OF MODEL PERFORMANCE

THAT ARE

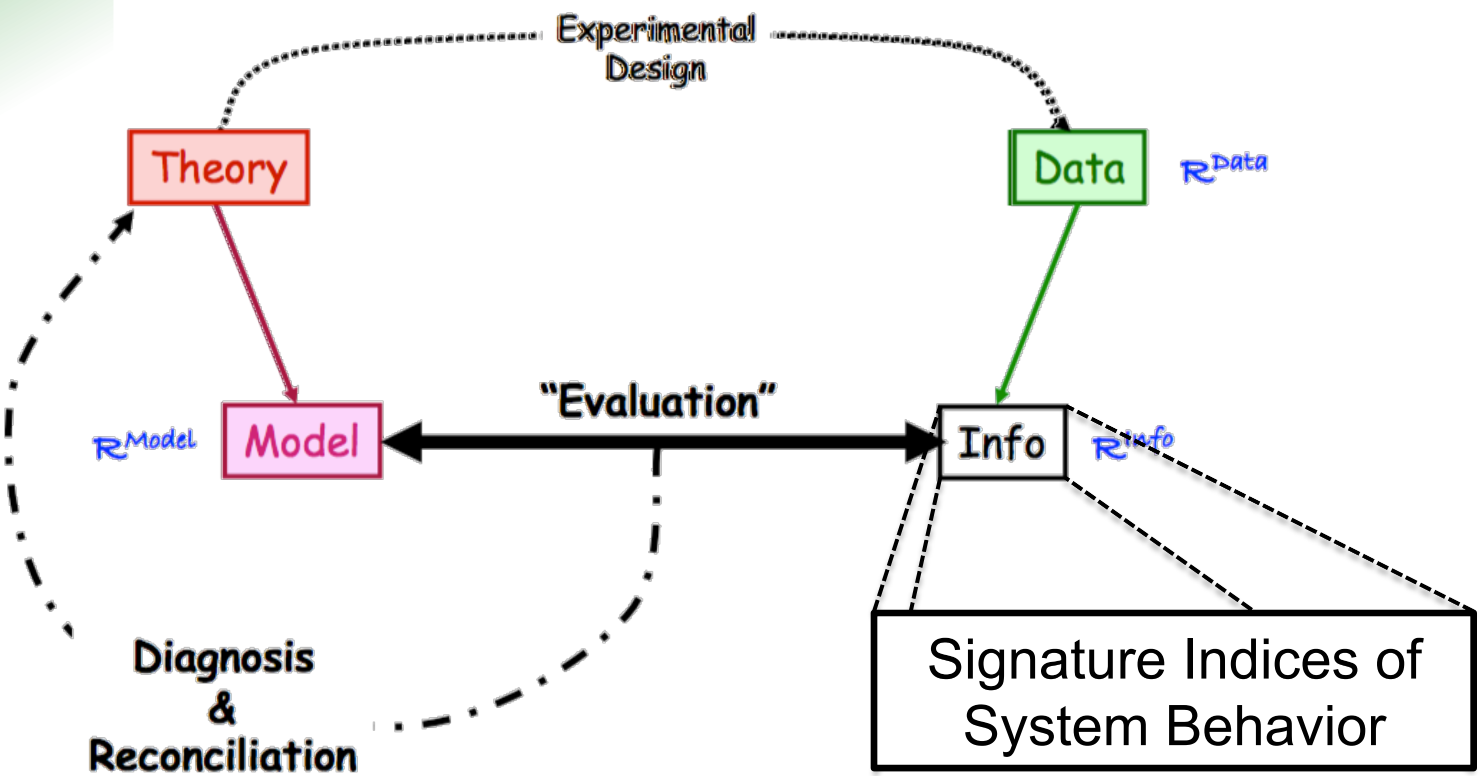
"**DIAGNOSTICALLY RELEVANT**"

TO THE PROBLEM



DIAGNOSTIC APPROACH TO MODEL EVALUATION

DATA IS NOT INFORMATION !!!

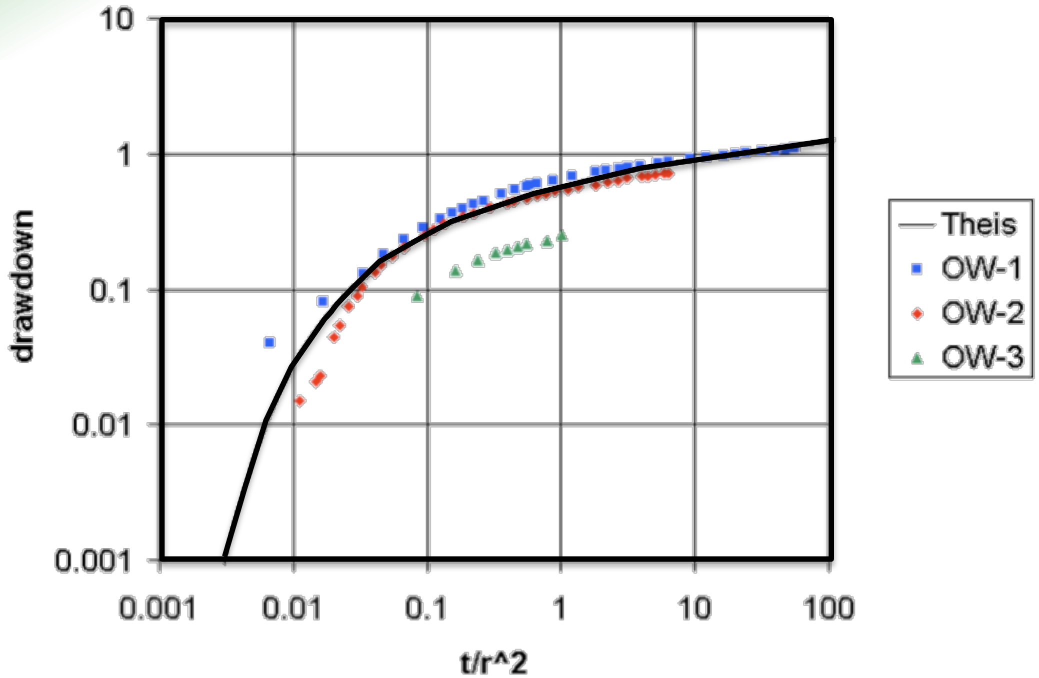


MODEL REFERENCED PATTERNS SHOULD BE RECONCILED WITH DATA REFERENCED PATTERNS

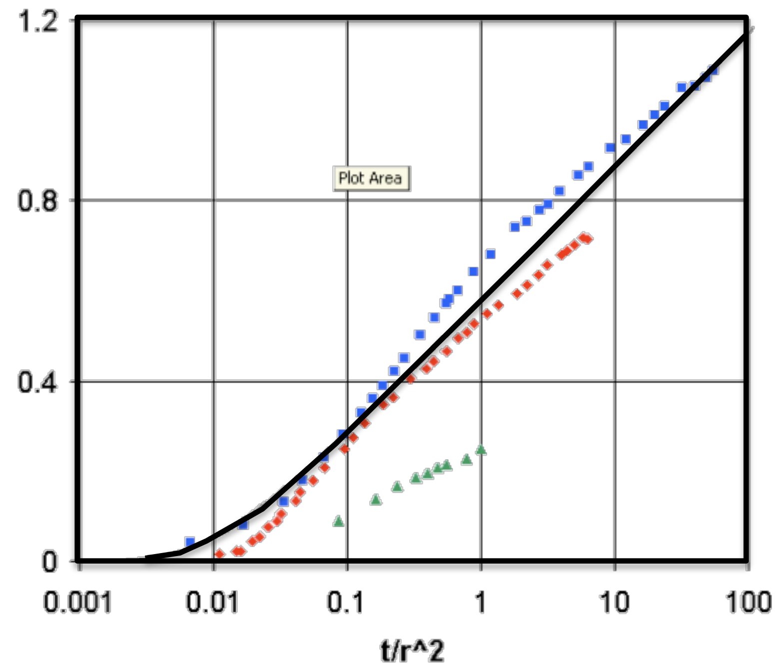
WHAT CONSTITUTES A SIGNATURE BEHAVIOR ?

Aquifer Well Test Analysis

Matching the Theis type curve to observed drawdown on log-log plot



Matching the Theis type curve to observed drawdown on semi-log plot



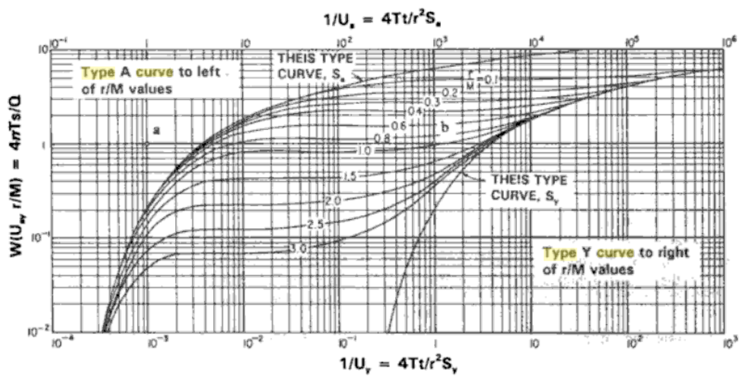
$$D = \frac{Q}{4\pi T} W(u) \quad where \quad u = \frac{r^2 S}{4Tt}$$

D = drawdown
Q = pumping rate
T = Transmissivity
u = dimensionless time

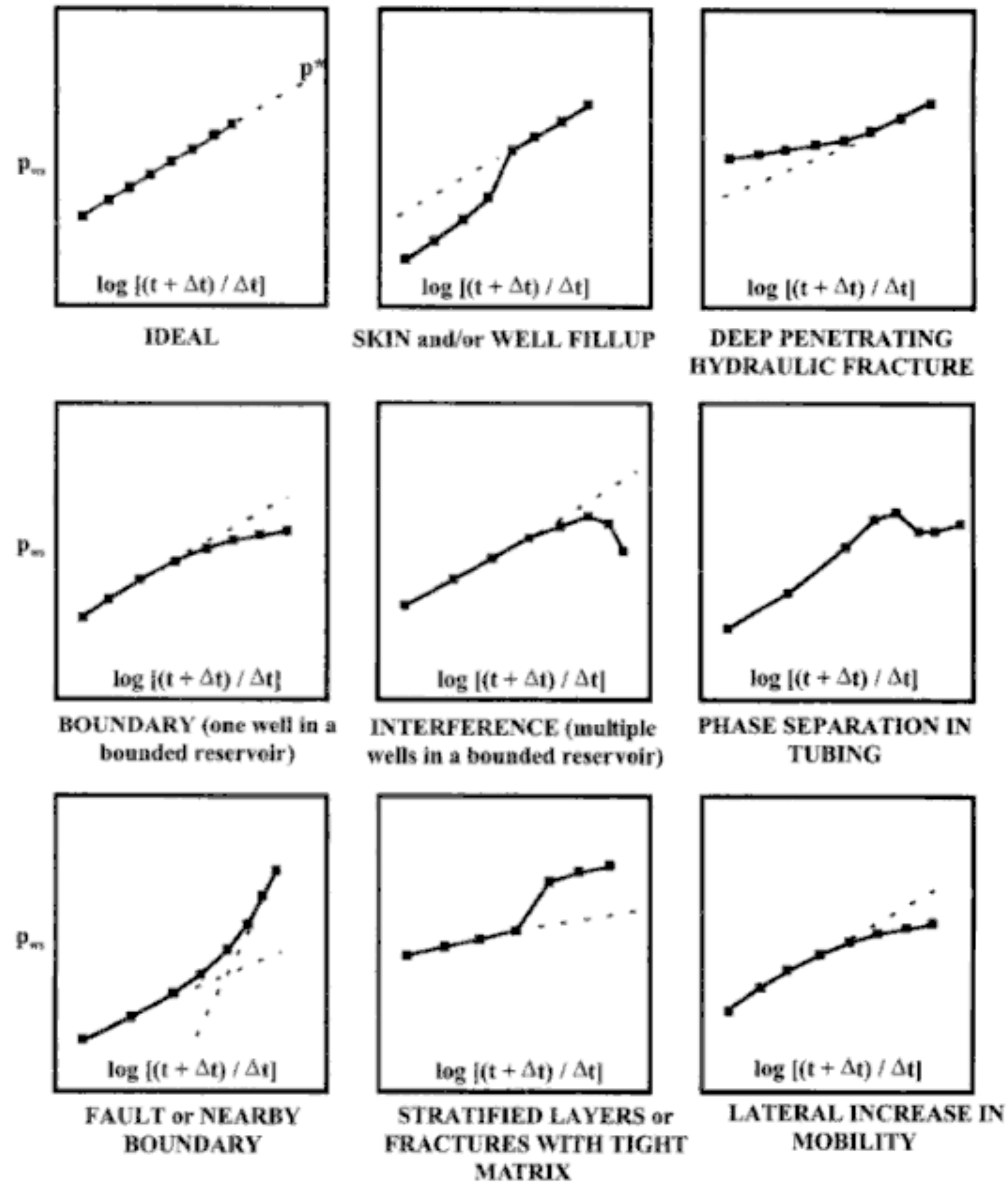
S = Storativity
r = distance from well
t = time

WHAT CONSTITUTES A SIGNATURE BEHAVIOR ?

Tests in Unconfined Aquifers



Example Build-up Curves Illustrating Various Effects



From Matthews & Russell [1]

IN CONCLUSION

THE PROBLEM OF INFERENCE (Reconciling Theory With Obs) ⟷ **PROBLEM OF DEVELOPING DIAGNOSTIC SUFFICIENT STATISTICS**

The MODELING problem:

To explicitly state

a) The Hypothesis to be tested
b) The Tests that will unambiguously challenge the hypothesis.

The OBSERVATIONAL problem:

To extract from the data, INFO that

a) Diagnostically characterizes system behavior
b) Supports or challenges the model hypothesis

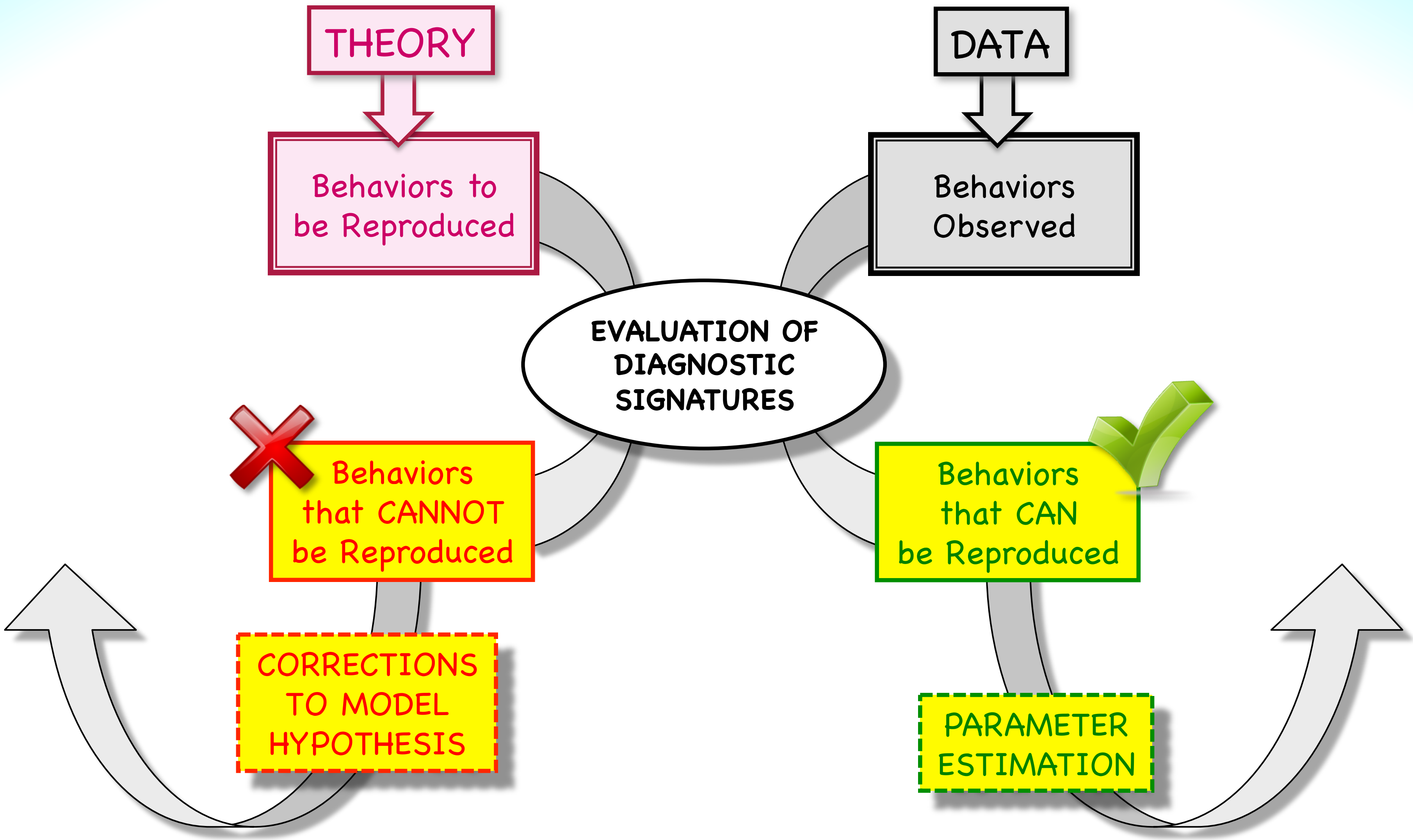
The RECONCILIATION problem is to:

a) Make robust inferences regarding which aspects of the model hypothesis are (are not) supported by the observations

b) Diagnostically guide improvements to the theory (model)

c) Suggest improvements in the acquisition of observations

MODEL REFERENCED PATTERNS ARE TO BE RECONCILED WITH DATA REFERENCED PATTERNS



Corrections to Model Hypothesis … WRR 2009

WATER RESOURCES RESEARCH, VOL. 45, W00B13, doi:10.1029/2007WR006749, 2009

Click Here for Full Article

Estimating the uncertain mathematical structure of a water balance model via Bayesian data assimilation

Nataliya Bulygina[1,2] and Hoshin Gupta[1]

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[1]
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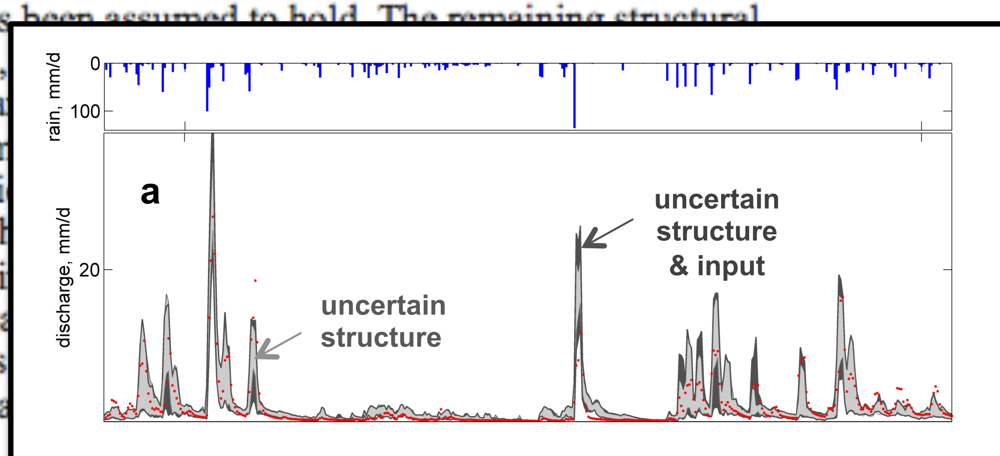
determined; that is, the system boundaries have been specified, the important state variables and input and output fluxes to be included have been selected, the major hydrological processes and geometries of their interconnections have been identified, and the continuity equation (mass balance) has
identification problem that remains, then,
dependence of the output on the inputs a
model can be constructed for making sim
input-state-output behavior. The conventi
some fixed (and possibly erroneous) math
We show instead how Bayesian data assi
(construct) the form of these mathematica
consistent with macroscale measurements
state variables. The resulting model has a

… Correcting the Model EQUATIONS …



Improving Model Identification:

Reconciling Theory with Observations & The Problem of Sufficient Statistics

Evaluation should enable us to link what we "see" in the data to what is "right" and "wrong" with our models.

This task will require the active collaboration of Process Scientists, Modelers & Systems Theorists.