Information Theory and the Hydrological Sciences

"Models, Data, Uncertainty and Learning" Hoshin V Gupta (University of Arizona)

2016 Information Theory Workshop Schneefernerhaus, Garmisch-Partenkirchen, Germany, April 24-28

Information Theory & Hydrology

There have been a great many applications ... (Singh 1997)*

- O Derivation of Probability Distributions & Estimation of Pars
- O Flow Forecasting via Maximum Entropy Spectral Analysis
- Basin Geomorphology Characterization of Landscapes & River networks
- Design of Hydrological Networks for Data Collection
- Reliability of Water Distribution Systems
- Hydraulics
- O Water Quality Assessment & Design of Water Quality Networks

* Singh, V. P. (1997), The use of entropy in hydrology and water resources, Hydrological Processes, 11(6)

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Incomplete Review of the Hydro. Lit.

Amorocho & Espildor (WRR 1973) - Entropy In Assessment Of Uncertainty In Hydrologic Systems And Models

In modeling catchments, a wide choice exists among models of varying completeness and sophistication \rightarrow The concept of Entropy (via Transinformation) provides an objective criterion for model selection.

The Recent Revival ...

Amorocho & Espildor (WRR 1973) Entropy In Assessment Of Uncertainty In Hydrologic Systems And Models

Abebe & Price (HSJ 2003) Managing Uncertainty In Hyd. Models Using Complementary Models Gupta et al (HP 2008) **Reconciling Theory With Observations: Elements Of A Diagnostic Approach** To Model Evaluation Pokhrel and Gupta (WRR 2011) On The Ability To Infer Spatial Catchment Variability Using Streamflow Hydrographs Weijs et al (HESS 2010) Why Hydrological Predictions Should Be Evaluated Using Info. Theory Pan et al (JoH 2012) Scale Effects On Info Theory-based Measures Applied To Streamflow Patterns In Two Rural Watersheds Weijs et al (HESS 2013) Data Compression To Define Info Content Of Hydrological Time Series Gong et al (WRR 2013) Estimating Epistemic and Aleatory Uncertainties during Hydrologic Modeling: An Info. Theoretic Approach Weijs & van de Giesen (JoH 2013) An Information-theoretical Perspective On Weighted Ensemble Forecasts Nearing et al (JoH 2013) Information Loss In Approximately Bayesian Estimation Techniques: A Comparison Of Generative And Discriminative Approaches ... Weijs et al (HESS 2013) Data Compression To Define Info Content Of Hydrological Time Series Nearing et al (WRR 2013) An Approach To Quantifying The Efficiency Of A Bayesian Filter

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The Recent Revival ...

Gong et al (WRR 2014) Sharma & Mehrotra (WRR 2014)

Nearing & Gupta (WRR 2015) Gupta & Nearing (WRR 2015) Estimating Information Entropy For Hydrological Data: One-dim Case An Info Theoretic Alternative To Model A Natural System Using Obs Info Alone

The Quantity And Quality Of Information In Hydrologic Models

Using Models And Data To Learn: A Systems Theoretic Perspective On The Future Of Hydrological Sciences (WRR Debates)

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Some Themes Emerge

- Inherently Probabilistic Nature of Hydrological System Modeling
- Assessing Information Content of Data
- ♦ Improving Model Predictions
- ♦ Model Selection & Calibration
- Model Benchmarking "Best Achievable Performance"
- Assessing Power of Data Assimilation Strategies
- Evaluating & Improving Model Structures (Learning)



1 - Inherently Probabilistic Nature of Hydrological System Modeling

Singh (HP 1997): Environmental systems are inherently spatial and complex, and our <u>understanding is less than complete</u>. Many are either fully stochastic, or part-stochastic/ deterministic, due to randomness in:

- a) System Structure (geometry)
- b) System Dynamics
- c) Forcings (sources and sinks)
- d) Initial and Boundary Conditions

<u>A stochastic description is needed</u> \rightarrow the Principle of Maximum Entropy (POME) enables:

- 1) Development of such a description
- 2) Determination of the least-biased PDF of a random variable, subject to available information.
- 3) Suggests whether available information is adequate, and if not then additional information should be sought.

In this way it brings a model and its modeler closer.

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2 - Assessing Information Content of Data

Pan et al (JoH 2008): "<u>Information Content</u>" of precipitation time series is higher than streamflow, but the "<u>Complexity</u>" is higher for the latter \rightarrow watersheds act as filters of precipitation info, which results in the observed additional complexity. <u>Temporal effects of information</u> are important and must be considered in model evaluation and comparison.

Weijs et al (HESS 2013): <u>Data Compression</u> can be used to <u>Quantify Info Content</u> of hydrological time series \rightarrow "How much can potentially be learned using a data set"). This requires first answering:

- (a) Information about what?
- (b) What is the current state of knowledge/belief about that?

Quantification is closely linked to problems of (i) Separating Aleatoric and Epistemic uncertainties (ii) Quantifying Best Achievable Model Performance.

Gong et al (WRR 2014): Discusses <u>how to estimate Entropy</u> of hydrologic (rainfall and runoff data) while dealing with practical problems of the (a) Zero Effect (discrete-continuous hybrid distributions), (b) Bin-Width Selection, (c) Finite Precision of Measurements, and (d) Skewness in the PDF.

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3 - Improving Model Predictions

Abebe & Price (HSJ 2003): Data-driven (ANN) approach based in Mutual Information can be used to model the prediction errors of a conceptual model, and added on top to improve the forecasts.

Weijs & van de Giesen (JoH 2013): Present method for <u>Weighting Ensemble Forecasts</u>, based on an extension of POME, <u>to ensure that no more information is added to the</u> <u>ensemble than is present in the forecast</u>. Demonstrate that all other methods result in weights that add either too little or too much (i.e. fictitious) information to the ensemble.

4 - Model Selection & Calibration

Amorocho & Espildor (WRR 1973): In modeling catchments, a wide choice exists among models of varying completeness and sophistication \rightarrow The concept of Entropy (via Transinformation) provides an objective criterion for model selection.

Weijs et al (HESS 2010): All models should be explicitly probabilistic, and all hydrological predictions should be evaluated using Information Theory.

In practice, <u>all Deterministic Forecasts are interpreted as uncertain</u> by the user.

Models should be calibrated using information-theoretical scores, to:

- a) Maximize the information they provide
- b) Extract all information from the observations
- c) Avoid learning from information that is not there.

5 - Model Benchmarking: Best Achievable Performance

Gong et al (WRR 2013): Suggests a way to <u>quantify "Best Achievable Performance"</u> for a model via data-driven modeling, thereby characterizing Model Structure Adequacy.

Presents way to <u>estimate Model Adequacy</u> in terms of its Aleatory Uncertainty (that cannot be diminished) and its Epistemic Uncertainty (that can be resolved by improving the model).

Sharma & Mehrotra (WRR 2014): Propose an Info Theoretic approach to <u>model natural</u> <u>systems using observational information alone</u>, as an alternative to empirical or semiempirical approaches.

Test their approach using synthetically generated data sets from known linear, nonlinear, and high-dimensional dynamic yet chaotic systems

6 – Assessing Power of Data Assimilation Strategies

Nearing et al (JoH 2013): Uses Shannon's theory to measure the information assimilated into models from observations and to characterize:

- (a) <u>Missing</u> Information
- (b) <u>Used</u> Information
- (c) <u>Bad</u> Information.

Shows that discriminative modeling (regression) to be more efficient than generative modeling (data assimilation) in extracting info from obs (so better suited for many practical problems).

Nearing et al (WRR 2013): Uses metrics based on Discrete Shannon Entropy to quantify how much of the uncertainty in a Posterior PDF is due to:

- (a) Observation operator
- (b) Observation error
- (c) Approximations of Bayes' Law.

Makes possible to analyze the efficiency of a proposed observation system and data assimilation strategy (e.g., EnKF does not use all of the info in soil moisture observations).

7 - Evaluating & Improving Model Structures (Learning)

Gupta et al (HP 2008): Info Theory can be used to <u>characterize "system-relevant"</u> <u>information</u> in a data set (signature properties), and to develop a "<u>Diagnostic Evaluation</u>" approach to reconciling environmental theory/models with observations.

Nearing & Gupta (WRR 2015): Quantify intuition that "<u>models provide information</u>". Demonstrate that dynamical models use induction to assimilate and store information from hypotheses and data. Show how this stored information can be directly measured.

Gupta & Nearing (WRR 2015): A perspective based in Info Theory can improve our ability to learn from the juxtaposition of models and data.

Build upon the "Step-wise Characterization of Model Structure" proposed by Gupta et al (WRR 2012 - Towards A Comprehensive Assessment Of Model Structural Adequacy).

Argue that we <u>should give more emphasis to Process Modeling & System Architecture</u> (i.e., incorporating knowledge from Physics) rather than on improving (what are generally semiempirical) System Parameterization Equations and on Parameter Estimation.



Dynamical Environmental Systems Models

Working Definition

A Dynamical Environmental Systems Model (DESM) is a <u>simplified</u> <u>representation</u> of the structure & function of a dynamical system that:

- Enables (a) Reasoning within an idealized framework
 (b) Testable predictions under new circumstances.
- 2. By Encoding (a) Knowledge of Physics (conservation, thermodynamics)
 (b) Knowledge of System Geometry & Material Properties

(c) Knowledge of What we Know that we Do Not Know



Why Simplified?

- a) Knowledge is Incomplete & Uncertain
- b) Real system is Infinite Dimensional
- c) Need to "compute" in Finite Time using Finite Resources

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We Use DESM for Scientific Investigation

Intuitively

We understand that "Models" & "Data" codify Knowledge about the World ... in the form of <u>Information</u>





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But ... Information Can Be

GOOD BAD MIXED (Partially Good & Bad)

Dealing with this is a MAJOR CHALLENGE to ESTIMATION THEORY



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Nearing GS, HV Gupta and W Crow (2013), Information Loss in Approximately Bayesian Data Assimilation: A Comparison of Generative and Discriminative Approaches to Estimating Agricultural Yield, Journal of Hydrology, 507, pp. 163-173

Nearing GS, HV Gupta, WT Crow and Wei G (2013), An Approach to Quantifying the Efficiency of a Bayesian Filter, Water Resources Research, 49, 1–10, doi:10.1002/wrcr.20177

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How do DESM's Encode Information ? As a Hierarchical Sequence of Decisions

- 1. Control Volume, Physics, Processes to Include, System Geometry & Material Properties
- 2. Scale, Dimension & 3D Spatial Structure
- 3. Process Relationships
- 4. Uncertainty

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5. Solution Methodology

 H^{CL}

HSA

 H^{PP}

HUN



Step Two – System Architecture

Information About:

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2. Scale, Dimension and *3D* Spatial Structure of the *State-Space* (elements), to enable finite computation

Question: What is a sufficiently complex, <u>finite dimensional</u>, spatially organized representation of sub-system architecture?



Step Three – Process Parameterization

Information About:

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3. Process Relationships via *Equations*, that account for Sub-Element Process & Material Heterogeneity

Question: What mathematical forms to use for the Process Parameterization equations, at the architectural scale of interest?





Step Five – Solution Procedure

Information About:

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5. Procedure for 'Solving' the resulting Mathematical Model

Question: How to Integrate (in space & time) the resulting system of (stochastic) differential equations?



Result: A Computational Model

- \rightarrow Practical manifestation of the Overall System Hypothesis H^{OS}
- → Structured hierarchy of Conservation Law, System Architecture, Process Parameterization, and Uncertainty Hypotheses $H^{OS} = \{H^{UN} | H^{PP} | H^{SA} | H^{CL}\}$

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Information is Added at Each Step (Uncertainty is Changed)

2 1. Conservation Laws <u>restrict possible U-X-Y</u> <u>trajectories</u>

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- 2. System Architecture (a) <u>further restricts</u> <u>trajectories</u> & (b) <u>determines spatial variability</u>
 - 3. Process Parameterization (a) <u>further restricts</u> <u>trajectories</u> & (b) <u>introduces "tunable" parameters</u>
 - 4. Specification of Uncertainty <u>characterizes</u> and quantifies "known unknowns"
 - 5. Solution Procedure <u>converts Model Info & Input</u> <u>Info into specific (uncertain) X-Y trajectories</u>











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What Can Go Wrong?

- 1. Problem Becomes Over-Constrained Due to <u>Hypotheses that are Unjustifiably Strong</u>
 - a) Neglect Heterogeneity that is important
 - b) Over-simplify the System Architecture
 - c) Incorrect Process Equations forms
 - d) Deterministic Process Parameterizations (instead of Stochastic)

2. Problem Becomes Under-Constrained

Due to Lack of Knowledge

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- a) Do not know Process Physics at the scale of system elements
- b) Do not know Heterogeneity of Material Properties and Geometry at scale of system elements
- c) Do not know (& account for) Heterogeneity of Material Properties and Geometry <u>at scales smaller than the system elements</u>

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What Can Go Wrong?

1. Problem Becomes Over-Constrained Due to <u>Hypotheses that are Unjustifiably Strong</u>

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Usually some Combination of Both

2. Problem Becomes Under-Constrained Due to Lack of Knowledge

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What is A Maximum-Entropy Parameterization ?

1. A Flux Parameterization must have the general form $Y_{t} = K_{t}^{xy} \cdot X_{t}$ where X_{t} is the <u>gradient</u> to be dispersed and K_{t}^{xy} is the <u>conductivity</u> of the medium



Basic Principle of Thermodynamics

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- 2. Condition $0 \le Y_t \le X_t$ must hold to preserve <u>mass balance</u>, implying that

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$$0 \le K_t^{xy} \le 1$$

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1	What is A Maximum-Entropy Parameterization ?50
2	1. A Flux Parameterization must have the general form $Y_{t} = K_{t}^{xy} \cdot X_{t}$ where X_{t} is the <u>gradient</u> to be dispersed and K_{t}^{xy} is the <u>conductivity</u> of the medium
3	2. Condition $0 \le Y_t \le X_t$ must hold to preserve mass balance, implying that $0 \le K_t^{xy} \le 1$
4	3. K_t^{xy} is a monotonic non-decreasing or constant function of X_t
	Consistent with physical principle that
	Larger gradients → Larger fluxes



What is A Maximum-Entropy Parameterization? 1 1. A Flux Parameterization must have the general form $Y_t = K_t^{xy} \cdot X_t$ where X_t is the <u>gradient</u> to be dispersed and K_t^{xy} is the <u>conductivity</u> of the medium 2 3 2. Condition $0 \le Y_t \le X_t$ must hold to $0 \le K_t^{xy} \le 1$ preserve mass balance, implying that 4 3. K_t^{xy} is a monotonic non-decreasing K_t^{xy} or constant function of X_t 5 X_{\star} 4. K_t^{xy} is a Probabilistic $\overline{\left[K_{t}^{xy} \sim p\left(K_{t}^{xy} \mid X_{t}\right)\right]}$ function of X_t X_{t}

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The Result

Strategy to investigate System Architecture

Without the need to make Strong Assumptions Regarding Process Parameterizations (Equations)

> In Principle a similar approach could be used to investigate value of different Conservation Laws

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More Generally

Bring more "Honesty/Rigour" into the Model Building Process

 Build Into the Model Clarity Regarding What We Feel Certain/Uncertain About

2) Be Clear about "What is Known" versus "What is Hypothesis / Assumption"

"Maximum Entropy Approach" To Model Building

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l	Some Comments in Conclusion
	1. Models & Data codify Information about the world
2	2. Information implies Change in Uncertainty about Something
3	3. Models are <u>Hierarchical Assemblages of Hypotheses</u>
	 Conservation Laws Process Parameterization System Architecture Uncertainty
ł	4. Model Hypotheses can be:
	1. <u>Over-Constrained</u> by un-justifiably strong hypotheses
5	 2. <u>Under-Constrained</u> by lack of knowledge about a) Scale-dependence of process relationships b) Sub-element heterogeneity
5	5. System Architecture Inference can be done using Max-Entropy PP's
7	6. Process Parameterization Inference can be done by Application of Bayes' Law
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