International Webinar on

"Entropy theory and its application in Hydrologic Engineering" Date and Time: May 28, 2020, Thursday, 17.00 Hrs (IST) Expert: Professor Vijay P Singh, Texas A & M University, USA

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Entropy Theory and its Application in Hydrologic Engineering

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Grand Challenges of 21st Century

- Food security
- Water security
- Energy security
- Health security
- Climate security
- Environmental security
- Ecosystem sustainability
- Water-energy-food-environment nexus
- Survival of humanity is at risk without ensuring the above.



Environmental and Water Resources

Engineering

- Planning, design, operation, and management of water resources systems
- Water resources systems for
 - drainage
 - flood control
 - irrigation
 - water supply
 - hydropower
 - river training
 - navigation,
 - recreation, and others



Hydrologic Engineering

- For planning, design, operation, and management of environmental and water resources systems
- Some key Questions
 - What is the peak discharge for a given rainfall event?
 - How often does a discharge of a given magnitude occur?
 - What is the volume of discharge resulting from a rainfall event and how is it distributed in time?
 - How much and at what rate does rain water infiltrate into the ground?
 - How is the infiltrated water distributed into the vadose zone?
 - What are the space-time characteristics of droughts?
 - What should be the space-time monitoring of hydrologic data?

Hydrologic Engineering

- Some key Questions
 - What is the rate of groundwater depletion?
 - What is the rate groundwater recharge?
 - What is the velocity distribution in open channel flow?
 - What is the concentration of sediment in open channel flow?
 - What is the sediment discharge of a river?
 - What is the pollutant discharge of a river?
 - What is the optimal design of a canal?
 - What is the reliability of a water supply system?



Application of Hydrology

- Rainfall-runoff modeling
 - Watershed management
 - Drainage design
 - Pavement design
- Flow frequency analysis
 - Dam and reservoir design
 - Irrigation management
 - Environmental management



Application of Hydrology (contd.)

- Velocity Distribution
 - Flow modeling
 - Scour modeling
 - Bed profiles
- Sediment Concentration and Sediment Discharge
 - Environmental pollution
 - Bed forms
 - Sedimentation



Application of Hydrology (contd.)

- Hydraulic Geometry
 - River training
 - Restoration
- Optimal Canal Design
 - Irrigation
 - Drainage
- Water Distribution System Design
 - Design a water supply system
 - Reliability of a water distribution system



Hydrologic Engineering Landscape

- Methods of Solution
 - Empirical
 - Information theoretic
 - Probabilistic and stochastic
 - Physical



Development of a Unifying Theory

- Entropy Theory
 - Entropy: a measure of disorder, chaos, uncertainty, surprise, or information
 - Information reduces uncertainty; more information means less uncertainty
 - Uncertainty increases the need for information; more uncertainty means more information is needed.



Entropy, Information and Uncertainty

- Concept of information
 - Closely linked with the concept of uncertainty or surprise
- Assume a random variable $X = x_i$
 - $p_i = 1$ ($p_j = 0, j \neq i$) No surprise about occurrence of event $X = x_i$.
 - If p_i is very low, say 0.01 and if actually x_i occurs, then there is a great deal of surprise as to its occurrence and our anticipation of it is highly uncertain.
 - The information content of observing x_i or the anticipatory uncertainty of x_i prior to the observation is a decreasing function of the probability p(x_i)



Entropy, Information and Uncertainty

- Information is gained only if there is uncertainty about an event.
- Uncertainty suggests that the event may take on different values.
- The value that occurs with a higher probability conveys less information and vice versa.
- Shannon (1948) argued that entropy is the expected value of the probabilities of alternative values that an event may take on.
- The information gained is indirectly measured as the amount of reduction of uncertainty or of entropy.



Various Interpretations of Entropy

Measure of Uncertainty

Measure of Information

Measure of Randomness

Measure of Unbiasedness or Objectivity

Measure of Equality

Measure of Diversity

Measure of Lack of Concentration

Measure of Flexibility

Measure of Surprise

Measure of Complexity

Measure of Departure from Uniform Distribution

Measure of Interdependence

Measure of Dependence

Measure of Interactivity

Measure of Similarity



- Real Domain
 - Shannon Entropy
 - Tsallis Entropy
 - Exponential Entropy
 - Kapur Entropy
 - Renyi Entropy
 - Cross or relative Entropy (Kullback-Leibler entropy)

Types of Entropy

- Others
- Frequency Domain
 - Burg Entropy
 - Configurational Entropy
 - Relative Entropy



Development of Entropy Theory

Elements of Entropy Theory

- Definition of Entropy
- Principle of Maximum Entropy (POME)
- Principle of Minimum Cross-Entropy (POMCE)
- Theorem of Concentration

*Singh, V.P. (2013). Entropy Theory and its Application in Environmental and Water Engineering. 642 pp., John Wiley.

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Concept and Formulation of POMCE

- Building blocks of the entropy theory.
 - A powerful principle.
- Formulated by Kullback and Leibler (1951) and detailed in Kullback (1959).
- Consider a probability distribution Q = {q₁, q₂, ..., q_N} for a random variable X which takes on N values.
 - To derive the distribution $P = \{p_1, p_2, ..., p_N\}$ of X, one should minimize the distance between P and Q.
 - Closer the *P* and *Q*, greater will be the uncertainty.
 - POMCE is expressed as,

$$D(P,Q) = \sum_{i=1}^{N} p_i \ln \frac{p_i}{q_i}$$

where *D* is the cross-entropy or distance

(1)

Contd.

- If no prior distribution is available in the form of constraints and *Q* is chosen to be a uniform distribution,
 - Equation (1) takes the form,

$$D(P,Q) = \sum_{i=1}^{N} p_i \ln\left[\frac{p_i}{1/N}\right] = \ln N + \left(\sum_{i=1}^{N} p_i \ln p_i\right) = \ln N - H$$
(2)

where, *H* is the Shannon entropy.

$$H = -\sum_{i=1}^{N} p_i \ln p_i \tag{3}$$

- Minimizing D(P, Q) is equivalent to maximizing H.
- Since *D* is a convex function, its local and global minimum are same.
- A posterior distribution *P* is obtained by combining a prior *Q* with specified constraints.
 - Minimization of cross- entropy results asymptotically from Bayes' <u>theorem</u>.



Contd.

- POMCE involves two major concepts,
 - A prior probability distribution.
 - A measure of distance.
- POMCE is a measure between two probability distributions,
 - One related to the system to be characterized
 - Assumed to be unknown.
 - One related to the model chosen to describe the system.
 - Models to characterize a system,
 - Set of moments.
 - Mean and any symmetric part of the covariance matrix of the system called constraints.
- POMCE measure is obtained by minimizing the discrimination information with respect to the given prior distribution over all probabilistic descriptions of the system which concur with the given constraints.



EXAS A&M • One of the case is of root square sense as the measure of distance.

Properties of POMCE

- KL measure has the following properties,
 - The distance measure D(P, Q) is non-negative, $D(P, Q) \ge 0$
 - The distance measure D(P, Q) is asymmetric, $D(P,Q) \neq D(Q,P)$

NOTE: This is not a true distance between distributions, because it does not obey the triangle inequality and is not symmetric.



Examples POMCE

• Assuming first *Q* as uniform, show that then *P* as uniform.

Let *Q* be a uniform distribution: $q_i = 1/N$. Then one obtains, $D(P,Q) = \sum_{i=1}^{N} p_i \ln \frac{p_i}{1/N} = \ln N + \sum_{i=1}^{N} p_i \ln p_i = \ln N - H$ where *H* is the Shanhon entropy.

Now if *P* is uniform , then

$$D(Q, P) = \sum_{i=1}^{N} q_i \ln \frac{q_i}{1/N} = \ln N + \sum_{i=1}^{N} q_i \ln q_i$$

=> $D(P,Q) \neq D(Q,P)$ However, it turns out that the measure of, $W(P,Q) = D(P,Q) + D(Q,P) = \sum_{i=1}^{N} p_i \ln \frac{p_i}{q_i} + \sum_{i=1}^{N} q_i \ln \frac{q_i}{p_i} = \sum_{i=1}^{N} (p_i - q_i) \ln \frac{p_i}{q_i}$ is symmetric, i.e., W(P,Q) = W(Q,P).

AS A&M • Measure of symmetric cross-entropy or W divergence (Lin, 1991).

Shannon Entropy: Discrete Random Variable

- Probability distribution
 - *N* outcomes (*x_i*, *i*=1, 2, ..., *N*) of a random variable *X* or a random experiment
- Shannon defined a measure *H* as a function of probabilities as

$$H(p_1, p_2, ..., p_N) = -\sum_{i=1}^N p_i \log p_i$$

- Satisfies a number of desiderata
- Logarithm is to the base of 2
 - Entropy is measured in bits



Shannon Entropy: Discrete Random Variable

• The gain function describing the information from an event as a log function:

$$\Delta I_i = -\log p_i , \sum_{i=1}^{N} p_i = 1$$

where ΔI_i is the gain in information from an event *i* which occurs with probability p_i , and *N* is the number of events. Thus, entropy is the expected value of the gain function and is also written as

$$H = \sum_{i=1}^{N} p_i \Delta p_i$$



Shannon Entropy





Shannon Entropy: Continuous Random Variable

 Let X be a random variable with probability density function f(x). Then, the Shannon entropy, denoted by H(x), of X or H(f) is:

$$H(X) = -\int_{a}^{b} f(x) \ln f(x) dx$$

• Logarithm is to the base of 2, and entropy is measured in bits. The base can also be *e* or 10.



Principle of Maximum Entropy (POME)

- In practice, it is common that some information is available on the random variable.
- Choose the probability distribution that is consistent with the given information.
- Choose the distribution that has the highest entropy.
- Principle of Maximum Entropy (Jaynes, 1957)



Principle of Maximum Entropy (POME) (Contd.)

- Principle of Maximum Entropy (Jaynes, 1957)
 - Assignment of probabilities which maximizes entropy subject to the given information.
- Laplace's principle of insufficient reason
 - All outcomes of an experiment should be considered equally likely unless there is information to the contrary.
- Entropy defines a kind of measure on the space of probability distributions.



Concentration Theorem

Spread of lower entropies around the maximum entropy values. For a random variable *X* with PDF f(x), the Shannon entropy, denoted by H(x), of *X* will be in the range:

 $H_{\max} - \Delta H \le H(x) \le H_{\max}$

where H_{max} is given by POME. For *N* observations and *n* probabilities, the concentration of these probabilities near the upper bound H_{max} is given by the theorem. Asymptotically, $2N\Delta H$ is distributed as χ^2 with *n*-*m*-1 degrees of freedom. *m*= number of constraints. Denoting the critical value of χ^2 for k=n-m-1 degrees of freedom at 95% significance level as *F*, ΔH is given in terms of the upper tail area 1-*F* (=0.05) as:

 $\chi_c^2(1-F) = 2N\Delta H$

One can compute H_{max} for a known PDF and the value of χ^2 for a given significance level (say, 5%) from χ^2 tables. Then, one computes the value of $2N\Delta H$ which yields ΔH . One then determines the range in which 95% of the values will lie and evaluates if the majority of realizations will follow the



Methodology for Application of Entropy Theory

- Define Shannon entropy.
- Specify constraints.
- Maximize entropy using POME.
- Use the method of Lagrange Multipliers.
- Determine Lagrange multipliers in terms of constraints.
- Probability distribution in terms of Constraints.
- Determine the maximum Shannon Entropy.
- Derive the desired result.



Specification of Constraints

Constraints

- Constraints should be simple.
- Constraints should be defined such that they are more or less preserved in the future.
- Constraints should be defined as far as possible in terms of the laws of mathematical physics-mass conservation, momentum conservation, and energy conservation-or constitutive laws.
- Total probability

$$C_0 = \int_a^b f(x) \, dx = 1$$

Constraints

$$C_n = \int_{a}^{b} g_r(x) f(x) dx = E[g_r(x)], r = 1, 2, 3, \dots, n$$

where g(x) is some function of x.



Maximization of entropy

Method of Lagrange multipliers:

Lagrangian function *L* can be expressed as:

$$\mathcal{L} = -\int_{a}^{b} f(x) ln f(x) dx - (\lambda_0 - 1) \int_{a}^{b} f(x) dx - \sum_{i=2}^{n} \lambda_i [g_i(x) f(x) dx - \overline{g_i(x)}]$$

Applying the Euler-Lagrange calculus of variation for differentiating L with respect to f(x), noting f as variable and x as parameter, and equating the derivative to zero, one gets:

$$f(x) = \exp[\lambda_0 + \lambda_1 g_1(x) + \lambda_2 g_2(x) + \ldots + \lambda_n g_n(x)]$$

The next step is to determine the Lagrange multipliers.



Determination of Lagrange Multipliers

• Use of f(x) determined earlier in the specified constraints leads to:

$$\lambda_{0} = \ln \int_{a}^{b} \exp[-\sum_{r=1}^{n} \lambda_{r} g_{r}(x)] dx, \ r = 1, 2, ..., n$$
$$C_{r} = \int_{a}^{b} g_{r}(x) \exp[-\sum_{r=1}^{n} \lambda_{r} g_{r}(x)] dx, \ r = 1, 2, ..., n$$

and

• Differentiate the zeroth Lagrange multiplier with respect to other Lagrange multipliers: $\partial \lambda_0$

$$\frac{\partial \lambda_0}{\partial \lambda_r} = -C_r, r = 1, 2, \dots, n$$

• Express the zeroth Lagrange multiplier as

$$\lambda_0 = \lambda_0(\lambda_1, \lambda_2, ..., \lambda_n)$$

and then take the derivatives.

- Equate the derivatives determined in the above two ways.
- Obtain a set of equations leading to the expression of the Lagrange multipliers in terms of constraints.



Hydrologic Problems

- 1. Physical
 - Physical law in the form of a flux-concentration relation
 - A hypothesis on the CDF of flux or concentration
 - Examples: Rainfall-runoff modeling, infiltration, soil moisture movement, velocity distribution, hydraulic geometry, channel cross-section, sediment concentration and discharge, sediment yield, river bed profile, and rating curve

Statistical

- Empirical
- Examples: Frequency analysis, parameter estimation, network evaluation and design, flow forecasting, spatial analysis, grain size distribution, complexity analysis, and clustering

Mixed

AS A&N

- Partly empirical and partly physical
- Examples: Geomorphic relations for elevation, slope, and fall; and reliability of water distribution systems; hydraulic geometry

Flux-Concentration Relation

Fundamental Assumption

- Let *X* be flux and *h* be the associated concentration. In many problems the time-averaged flux can be considered as a random variable. For example, in open channel flow, time averaged velocity at a given crosssection can be considered as a random variable.
- If *X* is space-averaged, it can be considered as a random variable. For example, space-averaged infiltration capacity rate can be considered as a random variable.
- Space-averaged soil moisture can be considered as a random variable.



Fundamental Hypothesis

Let *X* be flux and *Y* be the associated concentration. The CDF of *X* can be expressed as

$$F(x) = \alpha_0 + \alpha_1 (\frac{y}{D})^{\alpha_2}$$

where α_o and α_i are parameters and α_2 is exponent, and D is the maximum value of y. Here x is a specific value of X and y is a specific value of Y. Often, $\alpha_o = 0$ or 1, and $\alpha_i = 1$ or -1, and $\alpha_2 = 1$. As an example, the CDF of velocity of flow in open channels is often considered with $\alpha_o = 0$, $\alpha_i = \alpha_2 = 1$ and is written as

$$F(u) = \frac{y}{D}$$

Parameters α_0 , α_1 , and α_2 need to be determined empirically from data. From a sampling standpoint, all values of y are equally likely to be sampled. This is a simple hypothesis but is not entirely unrealistic.



Applications: A sample





Hydrologic Problems for Modeling

1. Entropy Maximization: Application of POME

- Frequency Analysis and Parameter estimation
- Network Evaluation and Design
- Spatial Analysis
- Geomorphologic Analysis
- Grain size distribution
- 2. Coupling with Theory of Minimum Energy Dissipation Rate
 - . Hydraulic geometry



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3. Coupling with Flux-Concentration Relation

- Infiltration
- Soil moisture movement in vadose zone
- Rainfall-runoff relation
- Rating curve
- Flow duration curve
- Hydraulic geometry
- Erosion and Sediment transport
- Debris flow
- Longitudinal river profile
- Velocity distribution
- Sediment concentration



Contd.

Methodology for Application of Entropy Theory

- Definition of entropy: Shannon, Tsallis, or others
- Specification of constraints
- Formulation of fundamental hypotheses: physical/hydraulic
- Maximization of Shannon Entropy: POME
- Lagrange Multipliers
- Determination of Lagrange Multipliers in terms of constraints
- Entropy Distribution in terms of Constraints
- Maximum Shannon Entropy
- Derivation of the desired result



Infiltration Equations

- Infiltration: The rate of entry of water at the soil surface
 - Potential infiltration rate
 - Actual infiltration rate
 - Steady infiltration rate
 - Cumulative infiltration rate
 - Maximum soil moisture retention
 - Soil porosity



Constraints on Infiltration

Total probability constraint

$$\int_{a}^{b} f(I) dI = 1$$

• Moment constraints

$$\int_{-\infty}^{b} g_{r}(I) f(I) dI = \overline{g_{r}(I)}, r = 1, 2, ..., n$$

where $g_r(I)$, r = 1, 2, ..., n, represent some functions of infiltration rate I, n denotes the number of constraints, and is the expectation of $g_r(I)$. If r=1, it would correspond to the mean infiltration rate; likewise, for r=2, it would denote the variance of I.



Maximization of the Shannon Entropy

- Method of Lagrange multipliers
 - Entropy-based probability distribution of infiltration rate

$$f(I) = \exp \left[-\lambda_0 - \sum_{r=1}^n \lambda_r g_r(I)\right]$$

- Lagrange Multipliers
- Determination of Lagrange Multipliers in terms of constraints
- Entropy Distribution in terms of Constraints
- Maximum Shannon Entropy
- In general, *n*=1.



Derivation of Infiltration Equations

- Horton equation (1938)
- Kostiakov equation (1932)
- Generalized Kostiakov equation
- Smith-Parlange equation (1972)
- Philip two-term equation (1957)
- Green-Ampt equation (1911)
- Overton overton equation (1964)
- Holtan equation (1961)
- Singh-Yu equation (1990)



Horton Equation

- Steady or constant rate denoted as I_c and Initial infiltration rate denoted as I_o
- Fundamental hypothesis: Let *i* be the excess infiltration rate, *J* the excess cumulative infiltration, and *S* the maximum excess soil moisture retention. The cumulative probability distribution function *F*(*i*) is defined as

$$F(i) = 1 - \frac{J}{S}$$

- Constraint: Total probability constraint
- Probability distribution of the Horton equation: Uniform

$$f(I) = \frac{1}{I_0 - I_c}$$



Horton Equation (Contd.)

• Entropy of the Horton equation

 $H(I) = \ln (I_0 - I_c)$

Horton equation

$$I(t) = I_c + (I_0 - I_c) \exp((-t/k))$$

• Physical interpretation of *k*

$$k = \frac{S}{(I_0 - I_c)}$$



Horton Equation

• Robertsdale loamy sand (Entropy 2.28 Napiers)





Horton Equation (Robertsdale loamy sand (S=0.8S)





Conclusions

- There are two fundamental issues: (1) Hypothesis on fluxconcentration, and (2) specification of constraints based on laws of physics.
- The use of entropy theory leads to explicit expressions of flux in terms of concentration or time, as the case may be.
- Parameters in the derived relations seem to have physical meaning.
- Entropy theory provides a probabilistic description and makes a statement on uncertainty. This has important implications for sampling and model reliability.



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THANK YOU

