

ENTROPY AND ENERGY OF SUBSTRUCTURES OBTAINED BY VERTEX CUTTING IN REGULAR TREES

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The entropy (a quantitative measure of disorder in a system) and informational energy (informational "disorder") of substructures obtained by cutting the vertex in regular trees was investigated and is presented. In a regular tree every vertex has the same number of children and leafs had no children at all. The information energy was defined as $\text{Energy} = \sum p_i^2$, where p_i = the probability of apparition of a substructure of i size. The entropy was defined as $\text{Entropy} = -\sum p_i \cdot \log_2 p_i$, where p_i has the signification described above. Regarding the entropy the following remarks can be done: (a) the entropy decrease with ramification; (b) the entropy increase with increasing of the number of levels; and (c) the decreasing with ramification is more accentuate compared with the increasing of the number of levels. Regarding the information energy a decrease with the decrease of ramification and with the increase of number of levels was observed.

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VERTEX CUTTING IN REGULAR TREES**

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Having a regular b-tree with Y levels (Figure 1) the removal of a arbitrary vertex from the tree will generate from one (when removal are applied to a leaf) to two (when removal are applied to the root), and to three (when removal are applied to a inside node) sub-graphs.

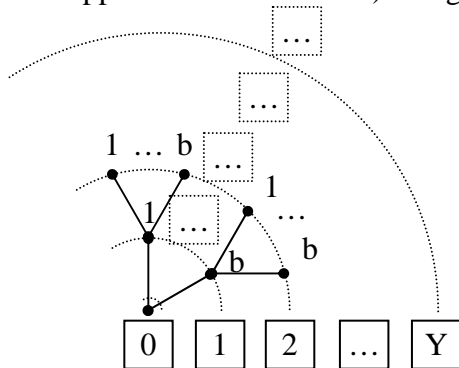


Figure 1. A b-Tree with Y levels, $T(b, Y)$

By removing once at the time every vertex from the tree, it is possible to evaluate the number of sub-graphs by size which may be obtained.

Somebody may say that systematically removing of every vertex is not a usual procedure for a given practical problem. Indeed, but usually in a real application an issue may be the removal of one vertex when the specification of which one vertex is to be removed is unknown. One example may be then having a network topology like a tree (let us say a Regional Internet Registry providing Internet resource allocations). In these cases assessing of the impact when a node is removed it is an important issue for projecting the network. Then we will move from complete characterization of a set (the set of all sub-graphs obtained by removing of an arbitrary vertex of a tree) to an issue of probability (obtaining of the appearance probability of a set of a given size). In terms of the entire structure (the tree), even the appearance probability of a set of a given size may not be a relevant information and we may want to obtain a global

parameter which to characterize the tree under the given circumstances (removal of one vertex).

Two parameters are often used for characterization of the mess: the information entropy (or Shannon's entropy [¹], a measure of the uncertainty associated with a random variable) and information energy (Onicescu's energy [²], a supplement and a complement of the Shannon's entropy, a formula obtained complementing to 1 the Simpson's measure of diversity [³]). Both measures proved to be very useful for characterizing physical and chemical processes [⁴].

¹ Claude E. SHANNON, A Mathematical Theory of Communication, Bell System Technical Journal, 1948, 27:379-423, 623-656.

² Octav ONICESCU, Energie informationelle, Comptes Rendus de la Academie des Sciences Paris Ser. A, 1966, 263:841-841.

³ E. H. SIMPSON, Measurement of Diversity, Nature 1949, 163(4148):688-688.

⁴ Sorana D. BOLBOACĂ, Elena M. PICĂ, Claudia V. CIMPOIU, LORENTZ JÄNTSCHI, Statistical Assessment of Solvent Mixture Models Used for Separation of Biological Active Compounds, Molecules, 2008, 13(8):1617-1639.

Let us define these two measures of information. Let be X a discrete variable taking the values $\{x_1, \dots, x_n\}$ and $p(\cdot)$ the probability mass function (gives the probability that a discrete random variable is exactly equal to a value).

The Shannon's entropy $H(X)$ is given by (where logarithm is taken to base 2 to give a value in bits):

$$H(X) = - \sum_{1 \leq i \leq n} p(x_i) \log_2(p(x_i)) \quad (\text{eq1})$$

The Onicescu's energy $E(X)$ is given by:

$$E(X) = \sum_{1 \leq i \leq n} p^2(x_i) \quad (\text{eq2})$$

Let us recall the structure from figure 1. The following formula (NSSP) describes completely the number of substructures (coefficients of the X variable) by sizes (powers of the X variable):

$$\text{NSSP}(T(b, Y)) = \sum_{k=1}^Y b^k \left(X^{\frac{b^{Y+1-k}-1}{b-1}} + X^{\frac{b^{Y+1}-b^{Y+1-k}}{b-1}} \right) + \frac{b^{Y+1}-1}{b-1} X^0 \quad (\text{eq3})$$

The formula (eq3) give the complete description of the substructures counts and sizes for any $Y, b > 0$. The following table (Table 1)

gives the substructures and sizes for some particular cases of trees. Note that the coefficient of X^0 counts the total number of vertices in the original structure.

Table 1. Substructures by removal of an arbitrary vertex for some regular trees

b	Y	Formula	Comments
1	1	$2X^0+2X^1$	A graph with two vertices and one edge
1	>1	$(Y+1)X^0+2X(X^Y-1)/(X-1)$	For b=1 tree degenerates in a path
>1	1	$(b+1)X^0+b(X+X^b)$	For Y=1 tree degenerates in a star
b	2	$(b^2+b+1)X^0+b(X^{b+1}+X^{b^2})+b^2(X+X^{b^2+b})$	Powers of X's may be repeated in the series

Recalling

$$\text{NSSP}(T(b, Y)) = \sum_{k=1}^Y b^k \left(X^{\frac{b^{Y+1-k}-1}{b-1}} + X^{\frac{b^{Y+1}-b^{Y+1-k}}{b-1}} \right) + \frac{b^{Y+1}-1}{b-1} X^0 \quad (\text{eq3})$$

We may want to find roots of:

$$b^{Y+1-k_1} - 1 = b^{Y+1} - b^{Y+1-k_2} \quad \text{i.e.} \quad 1 + b^{k_2-k_1} = b^{k_2} + b^{k_2-(Y+1)} \quad (\text{eq4})$$

Excluding $b=1$, since b , Y , k_1 , and k_2 are natural not null numbers, and natural too are 1 and b^{k_2} the equality (eq4) can be satisfied only for $b^{k_2-k_1} = b^{k_2-(Y+1)}$ which implies that the only solutions of (eq5) is for $k_1=Y+1$ (implying as consequence $b=1$). The conclusion that can be drawn from here is that for $b>1$ all terms inside the sum from (eq3) are distinct.

Since the problem of sub-graphs sizes occurrences (n_o) was solved in the general case for $b>1$ (no repeats in terms of eq3) we are able to calculate it for a given Y and a given b (note that the problem can be extended to any b less or equal to a given value and for a Y less or equal to a given value):

$$n_o \left(\frac{b^{Y+1-k} - 1}{b-1} \right) = \text{coef} \left(X^{\frac{b^{Y+1-k} - 1}{b-1}} \right) = n_o \left(\frac{b^{Y+1} - b^{Y+1-k}}{b-1} \right) = \text{coef} \left(X^{\frac{b^{Y+1} - b^{Y+1-k}}{b-1}} \right)$$

(eq5)

It follows that probabilities are given by:

$$p \left(\frac{b^{Y+1-k} - 1}{b-1} \right) = p \left(\frac{b^{Y+1} - b^{Y+1-k}}{b-1} \right) = \frac{b^k}{2 \sum_{k=1}^Y b^k} = \frac{b^k (b-1)}{2(b^Y - 1)}$$

(eq6)

Replacing of (eq6) into (eq1) and (eq2) is now only a matter of calculation:

$$H(T(b, Y)) = -2 \sum_{k=1}^Y \frac{b^k (b-1)}{2(b^Y - 1)} \log_2 \left(\frac{b^k (b-1)}{2(b^Y - 1)} \right) = \sum_{k=1}^Y \frac{b^k (b-1)}{(b^Y - 1)} \log_2 \left(\frac{2(b^Y - 1)}{b^k (b-1)} \right)$$

(eq7)

$$E(T(b, Y)) = 2 \sum_{k=1}^Y \frac{b^{2k} (b-1)^2}{4(b^Y - 1)^2} = \frac{b^2}{2} \frac{b^Y + 1}{b^Y - 1} \frac{b-1}{b+1}$$

(eq8)

where $H(T(b,Y))$ is the Shannon's entropy and $E(T(b,Y))$ is the Onicescu's energy of removal of a vertex from a $T(b,Y)$ tree, when $b>1$.

For $b=1$ (path) a entry from Table 1 can help us to obtain the values for $H(T(1,Y))=H(P(Y))$ and $E(T(1,Y))=E(P(Y))$:

$$H(P(Y)) = - \sum_{k=1}^Y \frac{2}{2Y} \log_2 \left(\frac{2}{2Y} \right) = - \sum_{k=1}^Y \frac{1}{Y} \log_2 \left(\frac{1}{Y} \right) = \log_2 Y \quad (\text{eq9})$$

$$E(P(Y)) = \sum_{k=1}^Y \left(\frac{2}{2Y} \right)^2 = \frac{1}{Y} \quad (\text{eq10})$$

