Extended Characteristic Polynomial

Subjects: Others

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In the context of molecular topology it is well known the Characteristic Polynomial (ChP) for its important uses in relating the structure with molecular properties of hydrocarbons, as well as a high resolution discriminant for chemical structures. Also it is well known that, as any other topological based descriptor/function, the ChP is blind to the nature of the chemical element and of the chemical bond, both being treated as indistinguishable in the context of the chemical graphs theory. An extension of the Characteristic Polynomial (EChP) is proposed by relaxing the identity matrix and adjacency matrix to contain non-binary based values, by in the same time keeping the meaning of those matrices (identity as collecting information regarding the identity of the atoms in the molecule and adjacency as collecting information regarding the connectivity or bonds in the molecule) and their feature (of being symmetrical).

Keywords: characteristic polynomial ; molecular descriptors ; structure-property relationships

1. Extending the Characteristic Polynomial

The characteristic polynomial was firstly encountered (at that time so called 'secular equation') in conjunction with the movement of the planets by famous mathematicians: Euler (1743)[1], D'Alembert (1750)[2], Lagrange (1773)[3], Laplace (1775)[4], its theory and use was gradually refined by others: Fourier (1822)[5], Cauchy (1829)[6], Sylvester (1852)[7], Hermite (1857)[8], Weierstrass (1867)[9], Jordan (1872)[10], and Kronecker (Kronecker, 1890)[11].

Once the more general problem were identified as standing for any Hessian matrix by Sylvester (1880)[12] the characteristic polynomial found its use in the approximate treatment of the Schrödinger's equation (1926)[13] for the wavefunction (Hartree, 1928)[14], [15] and Fock (Fock, 1930)[16], [17] finding the same eigenvector-eigenvalue problem as in the Slater's treatment (1929)[18], revised later by Hartree & Hartree (1935)[19].

While the first reports relating to the use of the characteristic polynomial in relation with the chemical structure appears shortly after the discovery of wave-based treatment of microscopic level from Hückel (1931)[20], the roots of this extended version of the characteristic polynomial can be attributed to the assignment of the individual electronic energies (ε_i), as accounted for the first time by Coulson in 1937[21], 1940[22], and 1950[23].

The characteristic polynomial (ChP) is the natural construction of a polynomial in which the eigenvalues of the [Ad] are the roots of the ChP as it follows:

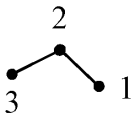
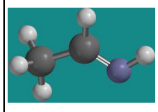
$$\lambda \text{ is an eigenvalue of } [Ad] \leftrightarrow \text{it exists } [v] \neq 0 \text{ eigenvector such that } \lambda\cdot[v] = [Ad]\cdot[v] \rightarrow$$

$$(\lambda\cdot[Id]-[Ad])\cdot[v] = 0; \text{ since } v \neq 0 \rightarrow [\lambda\cdot Id - Ad] \text{ is singular} \rightarrow \det([\lambda\cdot Id - Ad]) = 0$$

The characteristic polynomial ChP is a polynomial in λ of degree the number of atoms, $ChP(\lambda) = \det([\lambda\cdot Id - Ad])$.

As introduced in (Joița & Jäntschi, 2017)[24], the Extended Characteristic Polynomial (EChP) of a chemical structure is defined similarly (see Table 1) with the Characteristic Polynomial (ChP) of its associated topology (T).

Table 1. Topology, Chemistry and Geometry for Ethanimine ($HN{=}CH{-}CH_3$)

Polynomial	Structure	Example	Identity (I)	Connectivity (C)
ChP ← |λ·[Id]-[Ad]|	Graph		[Id] 1 2 3 1 1 0 0 2 0 1 0 3 0 0 1	[Ad] 1 2 3 1 0 1 0 2 1 0 1 3 0 1 0
EChP ← |λ·I-C|	Molecule		"A" 1 2 3 1 a_N 0 0 2 0 a_C 0 3 0 0 a_C "B" 1 2 3 1 b_N 0 0 2 0 b_C 0 3 0 0 b_C "C" 1 2 3 1 1 0 0 2 0 1 0 3 0 0 1 "D" 1 2 3 1 d_N 0 0 2 0 d_C 0 3 0 0 d_C "E" 1 2 3 1 e_N 0 0 2 0 e_C 0 3 0 0 e_C "F" 1 2 3 1 f_N 0 0 2 0 f_C 0 3 0 0 f_C "G" 1 2 3 1 g_N 0 0 2 0 g_C 0 3 0 0 g_C "H" 1 2 3 1 1 0 0 2 0 1 0 3 0 0 3 "I" 1 2 3 1 i_1 0 0 2 0 i_2 0 3 0 0 i_3 "J" 1 2 3 1 j_1 0 0 2 0 j_2 0 3 0 0 j_3 "K" 1 2 3 1 k_1 0 0 2 0 k_2 0 3 0 0 k_3 "L" 1 2 3 1 l_1 0 0 2 0 l_2 0 3 0 0 l_3	"t" 1 2 3 1 0 1 0 2 1 0 1 3 0 1 0 "g" 1 2 3 1 0 g_{12} 0 2 g_{12} 0 g_{23} 3 0 g_{23} 0 "c" 1 2 3 1 0 0.5 0 2 0.5 0 1 3 0 1 0 "b" 1 2 3 1 0 b_{12} 0 2 b_{12} 0 b_{23} 3 0 b_{23} 0 "T" 1 2 3 1 0 1 ½ 2 1 0 1 3 ½ 1 0 "G" 1 2 3 1 0 g_{12} g_{13} 2 g_{12} 0 g_{23} 3 g_{13} g_{23} 0 "C" 1 2 3 1 0 ½ $^2/_3$ 2 ½ 0 1 3 $^2/_3$ 1 0 "B" 1 2 3 1 0 b_{12} B_{13} 2 b_{12} 0 b_{23} 3 B_{13} b_{23} 0

Legend for replacement values:

a_C = 12/294; a_N = 14/294; b_C = 3915/3915; b_N = 77.355/3915; d_C = 2267/30000; d_N = 1495/30000; e_C = 2.55/4.00; e_N = 3.04/4.00; f_C = 1086.2/1312.0; f_N = 1402/1312; g_C = 3915/3915; g_N = 63.15/3915; i_1 = -0.738; i_2 = 0.497; i_3 = -0.756; j_1 = -0.593; j_2 = 0.090; j_3 = -0.653; k_1 = -0.628; k_2 = 0.097; k_3 = -0.734; l_1 = 0.0; l_2 = 0.0; l_3 = 0.0; g_{12} = 1/1.290; g_{13} = 1/2.451; g_{23} = 1/1.496; b_{12} = 1/1.869; b_{23} = 1/0.905; B_{13} = 1/(1/1.869+1/0.905).

2. Extended Characteristic Polynomial

A natural extension of ChP is to store in the identity matrix (instead of unity) non-unity values accounting for different atoms (and then the [Id] matrix is replaced by a generic matrix, $[I_p]$, having more than one alternative to be filled with values), as well as to store in the adjacency matrix (instead of unity) non-unity values accounting for different bonds (and then the [Ad] matrix is replaced by a generic matrix, $[C_q]$, having more than one alternative to be filled with values). Then the extended characteristic polynomial is defined by EChP(λ; p, q) = det($[\lambda \cdot I_p - C_q]$).

The proposed alternatives for identifying the atoms are p ∈ {"A", "B", "C", "D", "E", "F", "G", "H" "I", "J", "K", "L"}, being exemplified in Table 1 and having the following meanings: Atomic mass ("A"), Boiling point ("B"), Count ("C"), Density ("D"), Electronegativity ("E"), First ionization potential ("F"), Melting point ("G"), Hydrogen connections ("H"), Electrostatic charge ("I"), Mulliken charge ("J"), Natural charge ("K"), and Spin ("L").

The proposed alternatives for identifying the bonds are q ∈ {"t", "g", "c", "b", "T", "G", "C", "B"}, being exemplified in Table 1 and having the following meanings: being derived of adjacencies ({"t", "g", "c", "b"}) and on distances {"T", "G", "C", "B"}, as classical topological measures ("t" and "T"), inverses of geometrical distances ("g" and "G"), inverses of conventional bond orders ("c" and "C"), and inverses of Mulliken bond orders ("b" and "B").

It should be noted that all proposed alternatives keep the symmetry alive in both identity (I_p) and connectivity (C_q) replacements of identity matrix ([Id]) and adjacency matrix ([Ad]), keeping thus the Hessian property of their linear combination.

Also it should be noted that any value greater than 1 as entry in any of identity (I_p) and connectivity (C_q) matrices is dangerous to the computations of the associated characteristic polynomial (any number greater than 1 easily diverges producing huge numbers when is risen at a natural power), and as such, proportion (from 0 to 1, or from -1 to 1) scales

must be used whenever is possible to keep at reasonably low level the evaluations for the extended version of the characteristic polynomial.

A series of constant values has been used for a group of atomic properties ({"A", "B", "D", "E", "F", "G", "H"}) by keeping the track between chemical elements through their atomic number (Z) as listed in Table 2.

Table 2. List of the atomic numbers associating atomic properties with chemical elements

Z	0	1	2	3	4	5	6	7	8	9
0	0	1	2	3	4	5	6	7	8	9
1	10	11	12	13	14	15	16	17	18	19
2	20	21	22	23	24	25	26	27	28	29
3	30	31	32	33	34	35	36	37	38	39
4	40	41	42	43	44	45	46	47	48	49
5	50	51	52	53	54	55	56	57	58	59
6	60	61	62	63	64	65	66	67	68	69
7	70	71	72	73	74	75	76	77	78	79
8	80	81	82	83	84	85	86	87	88	89
9	90	91	92	93	94	95	96	97	98	99
10	100	101	102	103	104	105	106	107	108	109

In the first element of the list (line 0 column 0 in Table 2) it has been kept the scale of the atomic property - the value to be used to divide all other values when are to be used as atomic property descriptors.

Following tables (from Table 3 to Table 9) lists the constants used for each chemical element.

Table 3. Atomic masses

"A"	0	1	2	3	4	5	6	7	8	9
0	294	1	4	6.9	9	10.8	12	14	16	19
1	20.2	23	24.3	27	28.1	31	32.1	35.5	40	39.1
2	40.1	45	47.9	50.9	52	54.9	55.9	58.9	58.7	63.6
3	65.4	69.7	72.6	74.9	79	79.9	83.8	85.5	87.6	88.9
4	91.2	92.9	95.9	98	101.1	102.9	106.4	107.9	112.4	114.8
5	118.7	121.8	127.6	126.9	131.4	132.9	137.3	138.9	140.1	140.9
6	144.2	144.9	150.4	152	157.3	158.9	162.5	164.9	167.3	168.9
7	173.1	175	178.5	181	183.8	186.2	190.2	192.2	195.1	197
8	200.6	204.4	207.2	209	209	210	222	0	0	0
9	0	0	0	0	0	0	0	0	0	0
10	0	0	0	0	0	0	0	0	0	0

Table 4. Boiling points

"B"	0	1	2	3	4	5	6	7	8	9
0	3915.0	20.271	4.222	1603	2742	4200	3915	77.355	90.188	85.03
1	27.104	1156.09	1363	2743	3538	553.7	717.8	239.11	87.302	1032
2	1757	3109	3560	3680	2944	2334	3134	3200	3003	2835
3	1180	2673	3106	887	958	332	119.93	961	1650	3203
4	4650	5017	4912	4538	4423	3968	3236	2435	1040	2345
5	2875	1908	1261	457.4	165.051	944	2118	3737	3716	3403
6	3347	3273.15	2173.15	1870.15	3506.15	3314.15	2835.15	2993.15	2783.15	2000.15
7	1739.15	3588.15	5673.15	5698.15	5933.15	5900.15	5300.15	4800.15	4100.15	3080.15
8	630.15	1730.15	2013.15	1833.15	1235.15	610.15	211.15	950.15	2010.15	3473.15
9	5063.15	273.15	4091.15	4175.15	3508.15	2880.15	0	0	0	0
10	0	0	0	0	0	0	0	0	0	0

Table 5. Densities

"D"	0	1	2	3	4	5	6	7	8	9
0	30000	88	214	535	1848	2460	2267	1026	1495	1700
1	1444	968	1738	2700	2330	1823	1960	2030	1616	856
2	1550	2985	4507	6110	7140	7470	7874	8900	8908	8920
3	7140	5904	5323	5727	4819	4050	2155	1532	2630	4472
4	6511	8570	10280	11500	12370	12450	12023	10490	8650	7310
5	7310	6697	6240	4940	3640	1879	3510	6146	6689	6640
6	6800	7264	7353	5244	7901	8219	8551	8795	9066	9321
7	6570	9841	13310	16650	19250	21020	22610	22650	21090	19300
8	14190	11850	11340	9780	9196	6400	4400	2900	5000	10070
9	11724	15370	19050	20450	19816	13780	13510	14780	15100	13500
10	8840	9000	8000	9840	17000	21600	23200	27200	28600	28200

Table 6. Electronegativities

"E"	0	1	2	3	4	5	6	7	8	9
0	4.0	2.2	5.5	0.98	1.57	2.04	2.55	3.04	3.44	3.98
1	4.84	0.93	1.31	1.61	1.9	2.19	2.58	3.16	3.2	0.82
2	1	1.36	1.54	1.63	1.66	1.55	1.83	1.88	1.91	1.9
3	1.65	1.81	2.01	2.18	2.55	2.96	2.7	0.82	0.95	1.22
4	1.33	1.6	2.16	1.9	2.2	2.28	2.2	1.93	1.69	1.78
5	1.96	2.05	2.1	2.66	2.2	0.79	0.89	1.1	1.12	1.13
6	1.14	1.13	1.17	1.2	1.2	1.2	1.22	1.23	1.24	1.25
7	1.1	1.27	1.3	1.5	2.36	1.9	2.2	2.2	2.28	2.54
8	2	2.04	2.33	2.02	2	2.2	2.06	0	0	0
9	0	0	0	0	0	0	0	0	0	0
10	0	0	0	0	0	0	0	0	0	0

Table 7. First ionization potentials

"G"	0	1	2	3	4	5	6	7	8	9
0	3915.0	13.99	0.95	453.65	1560	2349	3915	63.15	54.36	53.48
1	24.56	370.994	923	933.47	1687	317	388.36	171.6	83.81	336.7
2	1115	1814	1941	2183	2180	1519	1811	1768	1728	1357.77
3	692.68	302.915	1211.4	887	494	265.8	115.78	312.45	1050	1799
4	2128	2750	2896	2430	2607	2237	1828.05	1234.93	594.22	429.749
5	505.08	903.78	722.66	386.85	161.4	301.7	1000	1193	1068	1208
6	1297	1441	1350	1095	1586	1629	1685	1747	1802	1818
7	1097	1963	2503	3269	3680	3453	3327	2683	2045	1338
8	234	577	600	545	527	575	202	0	0	0
9	0	0	0	0	0	0	0	0	0	0
10	0	0	0	0	0	0	0	0	0	0

Table 8. Melting points

"G"	0	1	2	3	4	5	6	7	8	9
0	3915.0	13.99	0.95	453.65	1560	2349	3915	63.15	54.36	53.48
1	24.56	370.994	923	933.47	1687	317	388.36	171.6	83.81	336.7
2	1115	1814	1941	2183	2180	1519	1811	1768	1728	1357.77
3	692.68	302.915	1211.4	887	494	265.8	115.78	312.45	1050	1799
4	2128	2750	2896	2430	2607	2237	1828.05	1234.93	594.22	429.749
5	505.08	903.78	722.66	386.85	161.4	301.7	1000	1193	1068	1208
6	1297	1441	1350	1095	1586	1629	1685	1747	1802	1818
7	1097	1963	2503	3269	3680	3453	3327	2683	2045	1338
8	234	577	600	545	527	575	202	0	0	0
9	0	0	0	0	0	0	0	0	0	0
10	0	0	0	0	0	0	0	0	0	0

Table 9. Valences (to be used for Hydrogen connections)

"H"	0	1	2	3	4	5	6	7	8	9
0	0	1	0	1	2	3	4	3	2	1
1	0	1	2	3	4	3	2	1	0	1
2	2	3	4	5	6	7	3	2	2	2
3	2	3	4	3	2	1	0	1	2	3
4	4	5	6	4	3	3	2	1	2	3
5	4	5	4	1	0	1	2	3	3	3
6	3	3	3	3	3	3	3	3	3	3
7	3	3	4	5	6	5	4	4	4	3
8	2	3	4	3	2	1	0	1	2	3
9	4	5	6	5	4	3	3	3	3	3
10	3	3	3	3	3	3	3	3	3	2

The valences (Table 9) are to be used to calculate the number of attached Hydrogen atoms based on the bonds and their orders (by subtracting the sum of the bond orders form the valence), while the counts ("C" property) is trivial - always 1. For the remaining atomic properties ({"I", "J", "K", "L"}), those are molecule-dependent and are expected to be provided from energy calculations on the molecule. As can be observed excepting Hydrogen connections ("H", valences listed in Table 9) the rest of the atomic properties ({"A", "B", "C", "D", "E", "F", "G"}) are molecule-independent.

As exemplified also in Table 1, the connectivities are to be calculated as follows:

- "t" as adjacency matrix ([Ad]) provides;
- "T" as topological distance matrix ([Di]) provides, inversed ($[C_T]_{i,j} = 1/[Di]_{i,j}$ for $i \neq j$, 0 otherwise);
- "G" as geometrical distance matrix ([Dxyz]) provides, inversed ($[C_G]_{i,j} = 1/[Dxyz]_{i,j}$ for $i \neq j$, 0 otherwise);
- "g" as dot product of geometrical distances ([Dxyz]) and adjacency ([Ad]) matrices ($[C_g]_{i,j} = [Dxyz]_{i,j}[Ad]_{i,j}$);
- "C" and "B" construct first an replacement for adjacency matrix by replacing the values of 1 with the inverse of the bond order ("C" as classical bond orders and "B" as Mulliken bond orders) and calculate a distance matrix ([DC], [DB]) by using this new adjacency matrix, finally inversing those values ($[C_C]_{i,j} = 1/[DC]_{i,j}$ for $i \neq j$, 0 otherwise; $[C_B]_{i,j} = 1/[DB]_{i,j}$ for $i \neq j$, 0 otherwise);
- "c" and "b" as dot products of previously calculated [DC] and [DB] matrices with adjacency ($[C_c]_{i,j} = [C_C]_{i,j}[Ad]_{i,j}$; $[C_b]_{i,j} = [C_B]_{i,j} \cdot [Ad]_{i,j}$).

Parameterized by the atomic property (p ∈ {"A", "B", "C", "D", "E", "F", "G", "H" "I", "J", "K", "L"}) and by the connectivity (q ∈ {"t", "g", "c", "b", "T", "G", "C", "B"}) the extended characteristic polynomial become a family of polynomial functions (EChP(λ; p,q)).

3. Practical use of the Characteristic Polynomial extension

It has previously shown in (Bolboacă & Jäntschi)[25] how the classical characteristic polynomial can be used to link the chemical structure with measured properties and activities of the molecules build up from hydrocarbons.

In the same manner the EChP(λ; p, q) may serve to link the chemical structure with measured properties and activities of the molecules build up from any chemical elements.

One strategy is to evaluate the EChP(λ; p, q) polynomial in a series of evenly spaced points from -1 to 1. For three digits rational arguments (λ = -1.000, -0.999, …, -0.001, 0.000, 0.001, …, 0.999, 1.000) are 2001 evaluation points.

By multiplying with the number of alternatives from identity (I_p) and connectivity (C_q) choices (p and q), the number of individuals in the EChP family is 2001·12·8 = 192096. Three linearization operations can be applied ("I", "R", "L") through the functions $f_I(x) = x$, $f_R(x) = 1/x$ and $f_L(x) = \ln(x)$ increasing the number of individuals in the EChP family to 576288. To keep the track of each individual, the naming convention is: $L_1L_2L_3C_0D_1D_2D_3$ where L_1 ∈ {"I", "R", "L"} for linearization, L_2 ∈ {"A", "B", "C", "D", "E", "F", "G", "H" "I", "J", "K", "L"} for identity, and L_3 ∈ {"t", "g", "c", "b", "T", "G", "C", "B"} for connectivity with the correspondences above given, while C is "N" for λ < 0, "0" for λ = 0, and "P" for λ > 0, and $D_1D_2D_3$ is the group of (3) digits from the evaluating value of λ (varying from "000" to "999").

In (Joița & Jäntschi, 2017)[24] paper is given an application of the use of EChP for a series of C_{20} fullerene congeners obtained by replacing in a patterned manner carbon atoms with nitrogen and boron. The obtained results revealed good EChP explanatory capabilities of the structure-property relationship for the area ($r^2_{adj} = 0.994$) and for the volume ($r^2_{adj} = 0.946$) of the series of 46 C_{20} fullerene congeners.

It should be noted that the constants give in Tables 3 to 9 to be used as scaling factors for the atomic properties (as opposite to the atomic properties itself, which were taken from measured or published data) are more or less arbitrary and can be subject to debate, but the principle of constructing EChP is sound. Further studies are necessary to construct a

best fit for the scaling factors (eventually made by parameterizing them).

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