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Notes on the Asymptotic Linearity Theorems

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The present article provides three lemmas that initiate the generalization of the theory of additive correlation involving the Asymptotic Linearity Theorems, which were constructed for a study of the correlation between structure and properties in molecules having many identical moieties. The new tools provided here also help to pave the way to linking the above theory with a theoretical framework developed for the asymptotic analysis of certain chemical kinetic network systems.

In previous publications of the present authors, we provided the following Asymptotic Linearity Theorems (ALTs):

(i) the original version of the ALT [1,2],
(ii) the polynomial version of the ALT [2],
(iii) the special version of the ALT [3],
(iv) the practical version of the ALT [4],

which were developed for a study of the theoretical foundations for the correlation between structure and properties in molecules having many identical moieties. We have been concerned, in particular, with the applications of the ALTs and their related theorems to the additivity problems of:

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(a) the zero-point vibrational energies of hydrocarbons [5–11],
(b) the vibrational thermodynamic quantities of hydrocarbons (see [4] and references therein),
(c) the total pi-electron energies of alternant hydrocarbons [12–24].

While developing the above mentioned versions of the ALT, we have obtained new tools and insights with which it is possible to considerably generalize the theory of additive correlation involving the ALTs.

The main objective of the present note is to present some of these tools, which shall be given in the form of lemmas (lemmas 1, 2 and 3). The lemmas presented here consolidate and logically strengthen results which are scattered through [1–4]. We will use these stronger statements in subsequent work.

We first fix some notations. Let $(\{T, F\}, o_T)$ (or $\{T, F\}$ for short where no confusion arises) denote the topological space with the underlying set $\{T, F\}$ and the system of open sets $o_T = \{\emptyset, \{F\}, \{T, F\}\}$. Note that the topological space $(\{T, F\}, o_T)$ is not Hausdorff. Let $\mathbb{C}$ denote the field of complex numbers, and $\mathbb{R}$ the field of real numbers. Let $\boldsymbol{B}(X, \mathbb{K})$ denote the Banach space of all bounded linear functionals on a normed space X over the field of $\mathbb{K}$ ($= \mathbb{C}$ or $\mathbb{R}$), i.e., let $\boldsymbol{B}(X, \mathbb{K})$ denote the dual space of the normed space X.

LEMMA 1

Let $X = (X, \| \ \|)$ be a normed space over the field $\mathbb{K}$ ($= \mathbb{C}$ or $\mathbb{R}$) and let $\beta_n \in \boldsymbol{B}(X, \mathbb{K})$ be a sequence of bounded linear functionals on X. Let

$$X \xrightarrow{\pi} \{T, F\}$$

be a mapping defined by

$$\pi(\varphi) = \begin{cases} T & \text{if } \beta_n(\varphi) \text{ is convergent}, \\ F & \text{if } \beta_n(\varphi) \text{ is not convergent}. \end{cases} \tag{1}$$

Suppose that

$$\sup\{\|\beta_n\| : n \geqslant 1\} < \infty . \tag{2}$$

Then the following statements are true:
(a) π is continuous.
(b) For any subset X_0 of X, (I) implies (II):

(I) $\pi(X_0) = \{T\}$,
(II) $\pi(\bar{X}_0) = \{T\}$.

Proof

We first claim that statement (a) implies statement (b). Assume that statement

(a) is true. Let X_0 be any subset of X, and suppose we have (I). Noting the fact that $\{T\}$ is a singleton closed set in $\{T, F\}$, we have $\pi(\bar{X}_0) \subset \overline{\pi(X_0)} = \overline{\{T\}} = \{T\}$. On the other hand, clearly $\pi(\bar{X}_0) \supset \pi(X_0) = \{T\}$. Therefore, (II) is valid, and statement (b) is true.

Now one easily sees that the proof of lemma 1 is reduced to the proof of lemma 3(e), given in the sequel. □

The reader is referred to refs. [1,2] to recall that we proved the original version of the ALT in two steps by using

(i) the approach via the aspect of form, and
(ii) the approach via the aspect of general topology.

Note also that the first approach corresponds with statement (I) in lemma 1, and the second approach corresponds with the deduction of statement (II) from statement (I) by proving the continuity of mapping π from a real normed space to the topological space $\{T, F\}$. (Recall mapping π_β in ref. [2] and compare with mapping π in lemma 1.)

The following lemma 2 is a specialized version of lemma 3. Note that if $\mathbb{K} = \mathbb{R}$ in lemma 1, then the validity of lemma 1 follows from lemma 2(e).

LEMMA 2

Let $X = (X, \| \ \|)$ be a normed space over the field $\mathbb{R}$, and let $\beta_n \in \boldsymbol{B}(X, \mathbb{R})$ be a sequence of bounded linear functionals on X. Let l^∞ denote the Banach space of all bounded sequences $\{a_n\}$ in $\mathbb{R}$ equipped with the norm given by $\|\{a_n\}\| = \sup\{|a_n| : n \geqslant 1\}$. Consider the following diagram:

$$\begin{tikzcd}
X \arrow[rr, "\pi"] \arrow[d, "\theta_1"'] & & \{T, F\} \\
& \mathbb{R}^2 \arrow[dr, "\eta_2"] & \\
l^\infty \arrow[ur, "\eta_1"] \arrow[rr, "\theta_2"'] & & \mathbb{R} \arrow[uu, "\theta_3"']
\end{tikzcd}$$

Diagram I

Here, π, θ_1, θ_2, and θ_3 are defined by

$$\pi(\varphi) = \begin{cases} T & \text{if } \beta_n(\varphi) \text{ is convergent}, \\ F & \text{if } \beta_n(\varphi) \text{ is not convergent}. \end{cases} \tag{3}$$

$$\eta_1(\{a_n\}) = (\limsup_{n\to\infty} a_n, \liminf_{n\to\infty} a_n). \tag{4}$$

$$\eta_2((x,y)) = x - y. \tag{5}$$

$$\theta_1(\varphi) = \{\beta_n(\varphi)\}. \tag{6}$$

$$\theta_2 = \eta_2 \circ \eta_1. \tag{7}$$

$$\theta_3(x) = \begin{cases} \boldsymbol{T} & \text{if } x = 0, \\ \boldsymbol{F} & \text{if } x \neq 0. \end{cases} \tag{8}$$

Then, the following statements are true.

(a) Diagram I is commutative.
(a)′ η_1 is continuous.
(a)″ η_2 is continuous.
(b) $\sup\{\|\beta_n\| : n \geqslant 1\} < \infty$ implies that θ_1 is continuous.
(c) θ_2 is continuous.
(d) θ_3 is continuous.
(e) $\sup\{\|\beta_n\| : n \geqslant 1\} < \infty$ implies that π is continuous.

Proof

(a): The triangular part of the diagram is commutative by the definition of θ_2. The rectangular part of the diagram is commutative, since $(\theta_3 \circ \theta_2 \circ \theta_1)(\varphi) = \boldsymbol{T}$ if and only if

$$\limsup_{n\to\infty} \beta_n(\varphi) - \liminf_{n\to\infty} \beta_n(\varphi) = 0, \tag{9}$$

i.e., if and only if $\pi(\varphi) = \boldsymbol{T}$. Therefore, the whole diagram is commutative.

(a)′: Note that the mapping $\{a_n\} \mapsto \limsup_{n\to\infty} a_n$ is Lipschitz continuous:

$$\begin{aligned} &|\limsup_{n\to\infty} a_n - \limsup_{n\to\infty} b_n| \\ &\quad \leqslant \limsup_{n\to\infty} |a_n - b_n| \\ &\quad \leqslant \lim_{n_0\to\infty} (\sup\{|a_n - b_n| : n \geqslant n_0\}) \\ &\quad \leqslant \sup\{|a_n - b_n| : n \geqslant 1\} \\ &\quad = \|\{a_n\} - \{b_n\}\|. \end{aligned} \tag{10}$$

Similarly, the mapping $\{a_n\} \mapsto \liminf_{n\to\infty} a_n$ is Lipschitz continuous:

$$
\begin{aligned}
&|\liminf_{n\to\infty} a_n - \liminf_{n\to\infty} b_n| \\
&\quad \leqslant \limsup_{n\to\infty} |a_n - b_n| \\
&\quad \leqslant \|\{a_n\} - \{b_n\}\| .
\end{aligned} \tag{11}
$$

The conclusion immediately follows.

(a)$''$: Evident.

(b): It is easy to see that θ_1 is linear. Hence, it suffices to verify that θ_1 is bounded. Assume that $\sup\{\|\beta_n\|: n \geqslant 1\} < \infty$, and let $\varphi \in X$, then we have

$$
\begin{aligned}
\|\theta_1(\varphi)\| &= \|\{\beta_n(\varphi)\}\| \\
&= \sup\{|\beta_n(\varphi)|: n \geqslant 1\} \\
&\leqslant (\sup\{\|\beta_n\|: n \geqslant 1\})\|\varphi\| ,
\end{aligned} \tag{12}
$$

which shows that θ_1 is bounded.

(c): By (a)$'$, (a)$''$, and the definition of θ_2, statement (c) is true.

(d): Inverse images of $\emptyset$, $\{\boldsymbol{F}\}$, and $\{\boldsymbol{T}, \boldsymbol{F}\}$ under θ_3 are, respectively, $\emptyset, \mathbb{R} \setminus \{0\}$, and $\mathbb{R}$, which are all open sets in $\mathbb{R} = (\mathbb{R}, |\ |)$. Hence, θ_3 is continuous.

(e): By (a), (b), (c), and (d), statement (e) is true. □

The reader is referred to ref. [2] to recall that we considered the following diagram to prove the original version of the ALT:

$$
\begin{tikzcd}
X \arrow[rr, "\pi_\beta"] \arrow[dr, "f_\beta"'] & & \{\boldsymbol{T}, \boldsymbol{F}\} \\
& \mathbb{R}^2 \arrow[ur, "f_\Delta"'] &
\end{tikzcd}
$$

Diagram II

where $\pi_\beta, f_\beta, f_\Delta$ are respectively corresponding with π, $\eta_1 \circ \theta_1$, and $\theta_3 \circ \eta_2$ in diagram I of lemma 1.

LEMMA 3

Let $X = (X, \|\ \|)$ be a normed space over the field $\mathbb{K}$ ($= \mathbb{C}$ or $\mathbb{R}$), and let $\beta_n \in \boldsymbol{B}(X, \mathbb{K})$ be a sequence of bounded linear functionals on X. Let l^∞ denote the Banach space of all bounded sequences $\{a_n\}$ in $\mathbb{K}$, equipped with the norm given by $\|\{a_n\}\| = \sup\{|a_n|: n \geqslant 1\}$. Consider the following diagram:

$$
\begin{tikzcd}
X \arrow[r, "\pi"] \arrow[d, "\theta_1"'] & \{T, F\} \\
l^\infty \arrow[r, "\theta_2"'] & \mathbb{R} \arrow[u, "\theta_3"']
\end{tikzcd}
$$

Diagram III

Here, π, θ_1, θ_2, and θ_3 are defined by

$$\cdot\ \pi(\varphi) = \begin{cases} \boldsymbol{T} & \text{if } \beta_n(\varphi) \text{ is convergent}, \\ \boldsymbol{F} & \text{if } \beta_n(\varphi) \text{ is not convergent}. \end{cases} \tag{13}$$

$$\cdot\ \theta_1(\varphi) = \{\beta_n(\varphi)\}. \tag{14}$$

$$\cdot\ \theta_2(\{a_n\}) = \lim_{n_0 \to \infty} \sup\{|a_m - a_n| : m, n \geqslant n_0\}. \tag{15}$$

$$\cdot\ \theta_3(x) = \begin{cases} \boldsymbol{T} & \text{if } x = 0, \\ \boldsymbol{F} & \text{if } x \neq 0. \end{cases} \tag{16}$$

Then, the following statements are true.

(a) Diagram III is commutative.
(b) $\sup\{\|\beta_n\| : n \geqslant 1\} < \infty$ implies that θ_1 is continuous.
(c) θ_2 is continuous.
(d) θ_3 is continuous.
(e) $\sup\{\|\beta_n\| : n \geqslant 1\} < \infty$ implies that π is continuous.

Proof

(a): Note that $(\theta_3 \circ \theta_2 \circ \theta_1)(\varphi) = \boldsymbol{T}$ if and only if $\beta_n(\varphi)$ is Cauchy. Since $\mathbb{K}$ is complete, statement (a) is clearly true.

(b): It is easy to see that θ_1 is linear. Hence, it suffices to verify that θ_1 is bounded. Assume that $\sup\{\|\beta_n\| : n \geqslant 1\} < \infty$, and let $\varphi \in X$, then we have

$$\begin{aligned} \|\theta_1(\varphi)\| &= \|\{\beta_n(\varphi)\}\| \\ &= \sup\{|\beta_n(\varphi)| : n \geqslant 1\} \\ &\leqslant (\sup\{\|\beta_n\| : n \geqslant 1\})\|\varphi\|, \end{aligned} \tag{17}$$

which shows that θ_1 is bounded.

The proofs of (d) and (e) proceed in the same way as in the proofs of (d) and (e) in lemma 1.

It remains to prove (c):

$$\begin{aligned}
&|\theta_2(\{a_n\}) - \theta_2(\{b_n\})| \\
&= \lim_{n_0 \to \infty} |\sup\{|a_m - a_n| : m, n \geqslant n_0\} - \sup\{|b_m - b_n| : m, n \geqslant n_0\}| \\
&\leqslant \lim_{n_0 \to \infty} \sup\{||a_m - a_n| - |b_m - b_n|| : m, n \geqslant n_0\} \\
&\leqslant \lim_{n_0 \to \infty} \sup\{|(a_m - b_m) + (b_n - a_n)| : m, n \geqslant n_0\} \\
&\leqslant \lim_{n_0 \to \infty} \sup\{|a_m - b_m| + |b_n - a_n| : m, n \geqslant n_0\} \\
&\leqslant \sup\{|a_m - b_m| + |a_n - b_n)| : m, n \geqslant 1\} \\
&\leqslant 2 \sup\{|a_n - b_n| : n \geqslant 1\} \\
&= 2\|\{a_n\} - \{b_n\}\| . \qquad (18)
\end{aligned}$$

Thus, θ_2 is Lipschitz continuous, and hence θ_2 is continuous. □

Through the theory of additive correlation using the approach via the aspect of form and general topology [1–4], one can infer that the additive relations, which empirical chemists initially investigated in the analysis of thermodynamic and spectroscopic data on organic compounds (cf. [5–9] and references therein), are physical or physicochemical manifestations of mathematical phenomena. One can also recognize that a molecular language alone is not sufficient in order to structurally elucidate the mechanism of this kind of manifestations. For this purpose, one needs to use both a molecular language and, so to speak, a meta-molecular language that complements the former as its logical and mathematical superstructure and is capable of unifying various additive relations, which had been separately investigated [1–4]. We wish to further extend our theoretical framework and the system of generic meta-molecular language for broader physical, physicochemical, and possibly other applications.

In order to generalize the theory of additive correlation involving the ALTs for a wider class of sequences of linear operators representing sequences of physicochemical network systems, one may take the following steps:

(i) Recall the approach via the aspect of form given in refs. [1–4], and extend the approach to include sequences of non-Hermitian matrices having repeating patterns along the diagonal. Take the following $N \times N$ matrix K_N as an example of such a sequence of non-Hermitian matrices:

$$K_N = \begin{pmatrix} -k & \kappa & & & & & \\ & -k & \kappa & & & \mathbf{0} & \\ & & -k & \ddots & & & \\ & & & \ddots & \ddots & & \\ & & & & -k & \kappa & \\ & \mathbf{0} & & & & -k & \kappa \\ \kappa & & & & & & -k \end{pmatrix}. \tag{19}$$

This is a specialized form of matrices used in ref. [25] for the analysis of certain dynamical systems of chemical kinetic equations.

(ii) Recall the approach via the aspect of general topology given in refs. [1–4], and extend the approach to be applicable to complex normed spaces as we extended lemma 2 to lemma 3 in this note.

In the present note, we confined ourselves to provide tools concerning the extension of the approach via the aspect of general topology. In Part IV of the series of papers [26–29], entitled "Structural Analysis of Certain Linear Operators Representing Chemical Network Systems via the Existence and Uniqueness Theorems of Spectral Resolution", the extension of the approach via the aspect of form is given, and the tools provided in the present note are further developed and linked with the theoretical frameworks in refs. [25–29] through the setting of the Banach space $\boldsymbol{B}(X, \mathcal{B})$ of all bounded linear operators from a normed space X to a Banach space $\mathcal{B}$ (cf. ref. [29] for details).

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