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CATEGORICAL SYSTEM THEORY AND THE PHENOMENOLOGICAL CALCULUS

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The mathematical theory of categories is used as a tool in the description of the structure and function of natural systems. The connections between the category of natural systems, with observables and dynamics, and the phenomenological calculus of response tensors, duality- and adjoint-invariance diagrams are established. The unified theory is applied to the analysis of hierarchies, pattern generation and the structure and dynamics of proteins.

1. Prologue. This essay serves as an introduction to the unification of categorical system theory (Louie, 1983) and the phenomenological calculus presented in a sequence of our previous papers (Richardson, 1980; Richardson *et al.*, 1982; Louie *et al.*, 1982; Louie and Richardson, 1983; Richardson and Louie, 1983). Henceforth the above references are respectively denoted L-83, R-80, R-L-S-82, L-R-S-82, L-R-83 and R-L-83. The basic definitions of category theory [treated in any one of the standard tests on the subject, e.g. Mac Lane (1971)] are assumed. The connections between categorical system theory and the phenomenological calculus are developed to a point where the biological examples considered in the above references can be analysed naturally. We shall also present an abstract description of the structure and dynamics of proteins. On the way, we meet duality-invariance diagrams (DIDs) and adjoint-invariance diagrams (AIDs), and there is a digression on the categorical system theory of hierarchies as well as one on Rosen's (1981) treatment of pattern generation.

2. The Category of Natural Systems. The thesis L-83 is an investigation of the structure and function of biological systems using the theory of categories. It examines the relationships which exist between different descriptions of natural systems through measurement of observables and dynamical interactions. Natural systems are treated formally as abstract mathematical objects in a category called **N**.

An **N**-object is a triple (S, F, D), where S is a set, F is a set of real-valued functions on S and D is a set of dynamics on S. The elements of S are the states and the elements of F are the observables of the natural system. An element of D, a dynamics, is a one-parameter group of bijections on

S, $T = \{T_t \in A(S)\colon t \in \mathbb{R}\}$. A dynamical response is initiated by the act of observation through a measuring instrument, while the change-of-state of a dynamics is itself an observable; thus there exists a *duality* between the static and dynamic, and hence structural and functional, aspects of a natural system.

An **N**-morphism $\phi \in \mathbf{N}((S, F, D), (S', F', D'))$ is a triple of functions $S \to S'$, $F \to F'$, $D \to D'$, linked by the following properties: (a) for all $f \in F$ and all $x, y \in S$, $f(x) = f(y)$ implies $(\phi f)(\phi x) = (\phi f)(\phi y)$; and (b) for every $T \in D$ and every $t \in \mathbb{R}$, the diagram

$$\begin{array}{ccc} S & \xrightarrow{\ \phi\ } & S' \\ {\scriptstyle T_t}\downarrow & & \downarrow{\scriptstyle (\phi T)_t} \\ S & \xrightarrow[\ \phi\ ]{} & S' \end{array} \tag{1}$$

commutes.

Property (a) says roughly that similar states are mapped to similar states, joining ϕ on the states and on the observables, and property (b) implies a compatibility of dynamics between systems, relating ϕ on the states and on the dynamics.

In L–83 the category **N** was constructed in two stages. A category **S**, consisting of objects (S, F) and morphisms $\phi\colon S \to S'$, $F \to F'$ with property (a), was first studied as a representation of the static aspects of systems with observables. Then duality dictated the alternate descriptions of the dynamic aspects, and the category **S** equipped with dynamics gave the category **N**.

The category **N** provides numerous biological implications ranging from cellular development and senescence to organismic sets as general living systems. These are discussed in L–83.

3. Phenomenological Connections. Our sequence of papers on the phenomenological calculus is a continuing exploration into the mathematical structures associated with the response tensor and description space, and their metaphorical interpretations in biological terms. A response tensor is a dyadic, a tensor of type (1, 1) over a real Hilbert space H [i.e. it is an element of $T^1_1(H)$], and is of the form

$$R = a^i u_i \tag{2}$$

(sum over i: the Einstein summation convention) for fixed $a^1, \ldots, a^m \in H^*$. The linear subspace

$$[a^1, \ldots, a^m] = [a^i] = \{a^i u_i\colon u_1, \ldots, u_m \in H\} \tag{3}$$

of $T^1_1(H)$ spanned by the response tensors is the description space. $[a^i]$ is a Hilbert space with the double inner product

$$\langle\langle a^i u_i, a^j v_j \rangle\rangle = \langle a^i, a^j \rangle^* \langle u_i, v_j \rangle = L^{ij} \langle u_i, v_j \rangle \tag{4}$$

(L-R-S-82). The set $\{a^i\}$ of constitutive parameters phenomenologically characterizes the system $[a^i]$ and forms a complete set of descriptions of the dynamic response of the system to the imposition of a set of forces (or more generally, causes) $\{u_i\}$.

First let us consider the special Hilbert space $H = \mathbb{R}^n$ with the standard inner product, and let S be an open subset of $\mathbb{R}^n$. A linear functional a: $\mathbb{R}^n \to \mathbb{R}$ ($a \in H^*$) is in particular a real-valued function, i.e. an observable, on the state space S. So the set of constitutive parameters (or 'coordinate vectors') $\{a^i\}$ of the description space $[a^i]$ can be taken as the set of observables on S; i.e. $F = \{a^i\}$.

A vector field u: $S \to \mathbb{R}^n$ defining an autonomous differential equation

$$\frac{\mathrm{d}x}{\mathrm{d}t} = u(x) \tag{5}$$

gives rise to a C^1 (continuously differentiable)-dynamics T, where $T_t(x) = y_x(t)$ is the unique solution to (5) satisfying $T_0(x) = y_x(0) = x$. It is interesting to note that the converse also holds; namely, given a C^1-dynamics T: $S \times \mathbb{R} \to S$ (where S and $\mathbb{R}$ have the usual topology), there is associated with it a vector field and hence an autonomous differential equation. Define u: $S \to \mathbb{R}^n$ by

$$u(x) = \frac{\mathrm{d}}{\mathrm{d}t} T_t(x) \Big|_{t=0} . \tag{6}$$

Then for $x \in S$ $u(x)$ is a vector in $\mathbb{R}^n$ which we can think of as the tangent vector to the T-trajectory $y_x(\mathbb{R}) = \{T_t(x): t \in \mathbb{R}\}$ at $t = 0$. And it is clear that y_x is the unique solution to the autonomous differential equation (5) satisfying the initial condition $y_x(0) = x$. Thus this establishes a correspondence between vector fields u and C^1-dynamics T on S. The collection of m-tuples of components ('forces') $\{u_i\}$ defining response tensors $\boldsymbol{R} = a^i u_i$ can then be interpreted as C^1-dynamics on the phase space S through this correspondence. This family of C^1-dynamics on S is then considered as the set D for the natural system (S, F, D).

So we have shown that a description space over $H = \mathbb{R}^n$ is in fact a special kind of natural system fully equipped with its sets of observables and dynamics. This 'embedding' $[a^i] \to (S, F, D)$ is quite remarkable in that even the physical interpretation of the different corresponding entities coincides. The set of constitutive parameters $\{a^i\}$ of a description space and the set of observables F of a natural system are both indicators of the *complexity* of the system, and the former set is actually what we observe on a physical system. The connection $u \leftrightarrow T$ between H and D is even more transparent: a force vector field is the time derivative of a dynamics [in the sense of equation (6)] in classical physics.

Instead of the Euclidean inner product space $H = (\mathbb{R}^n, \cdot)$ we could have used a general Hilbert space and all of the above discussions would still go through. Since every Hilbert space is isomorphic to $l^2(A)$ for some set A (Rudin, 1974, Section 4.19) and $l^2(A) = L^2(\mu)$, where μ is the counting measure on A, it is without loss of generality to let $H = L^2(\mu)$ for some measure μ in the definition of description space. Under this formulation we would have incorporated into the setting the 'time-dependence' of the causes $u(t) \in L^2(\mu)$ and the 'cause-dependence' of the constitutive parameters $a(u) \in L^2(\mu)^* = L^2(\mu)$. These are discussed in R–L–S–82 and L–R–S–82.

The description space $[a^i]$ is in fact more than an **N**-object: it is an **N**-object with *linear structure*. The category of description spaces **R** bears the same relationship to **N** as that of **Vect** to **Ens**, where **Vect** is the category of vector spaces and linear transformations and **Ens** is the category of sets and functions. A **Vect**-morphism, a linear transformation, is an **Ens**-morphism which preserves the linear structure of vector spaces. Similarly, an **R**-morphism is an **N**-morphism which preserves the linear structure of description spaces:

$$\phi \in \mathbf{R}([a^i], [b^j]) \text{ if } \phi \in \mathbf{N}([a^i], [b^j])$$

and

$$\phi(a^i u_i) = \phi(a^i) u_i. \tag{7}$$

Note that the linearity condition (7) is a restriction of ϕ on the observables $\{a^i\}$ and ϕ is uniquely determined by the m images $\{\phi(a^i)\}$. This is analogous to the situation in **Vect**, where a linear transformation is uniquely determined by its action on a basis of the domain vector space. In L–R–83 the latter is represented by the adjointness of the 'free functor' $\hat{\mathbf{F}}$: **Ens** → **Vect** and the 'forgetful functor' $\hat{\mathbf{G}}$: **Vect** → **Ens**:

$$\mathbf{Ens}(A, \hat{\mathbf{G}}B) \cong \mathbf{Vect}(\hat{\mathbf{F}}A, B). \tag{8}$$

We now have the adjointness

$$\mathbf{N}([a^i], \hat{\mathbf{G}}[b^j]) \cong \mathbf{R}(\hat{\mathbf{F}}[a^i], [b^j]), \tag{9}$$

where $\hat{\mathbf{F}}$: **N** → **R** is the functor which sends '$[a^i]$ considered as a natural system' to '$[a^i]$ considered as a description space', and $\hat{\mathbf{G}}$: **R** → **N** is the 'amnesic functor' which forgets the linear structure of a description space but retains its observable-dynamics equipment.

4. Special **R**-*Morphisms.* It is shown in R–L–S–82 that if the coordinate vectors $\{a^i\}$ span a subspace of $(\mathbb{R}^n)^*$ of dimension $k(\leqslant n)$, then the description space $[a^1, \ldots, a^m]$ is of dimension kn (over $\mathbb{R}$). Now suppose the coordinate vectors $\{b^j\}$ of a second description space $[b^1, \ldots, b^l]$ also span a subspace of $(\mathbb{R}^n)^*$ of dimension k. Then $[b^1, \ldots, b^l]$ is again of dimension kn and so we would expect somehow that the two description spaces are 'isomorphic'.

Now what is an **R**-isomorphism? Clearly it has to be an **N**-isomorphism in the first place. So far we have neglected the double inner product on the description spaces. Recalling that a linear transformation between two inner product spaces of the same (finite) dimension is an isomorphism iff it preserves inner products, we shall say that an **R**-morphism ϕ *preserves double inner products* if for all response tensors $\boldsymbol{R}$ and $\boldsymbol{S}$,

$$\langle\langle \boldsymbol{R}, \boldsymbol{S}\rangle\rangle = \langle\langle \phi(\boldsymbol{R}), \phi(\boldsymbol{S})\rangle\rangle. \tag{10}$$

(Note the two double inner products appearing on the two sides of equation (10) are on different description spaces.) Then we shall say that two description spaces $[a^i]$ and $[b^i]$ of the same finite dimension are **R**-*isomorphic* if there is an **R**-morphism which is an **N**-isomorphism and preserves double inner products between the two spaces. So under this definition **R**-isomorphic description spaces are abstractly the same with respect to all of their mathematical structures.

Next, suppose $\phi \in \mathbf{R}([a^i], [b^j])$ is such that there exists an $\epsilon > 0$ and for every $\boldsymbol{R} \in [a^i]$, $\|\boldsymbol{R} - \phi(\boldsymbol{R})\| < \epsilon$. This condition can be roughly stated as $\|\boldsymbol{R}(a) - \boldsymbol{R}(b)\| < \epsilon$, in which the notation is self-explanatory. This leads us to the idea of the 'distance' between response tensors from different description spaces. It is intuitively clear that the closer two description spaces are to being 'identical', the smaller the norm $\|\boldsymbol{R}(a) - \boldsymbol{R}(b)\|$ will be. And conversely, the smaller the norm is, the more **R**-isomorphic the two spaces are. So while the condition $\|\boldsymbol{R}\| \geqslant 0$ describes the dissipation (i.e. aging) *within* a system (R–80), the condition $\|\boldsymbol{R}(a) - \boldsymbol{R}(b)\| \geqslant 0$ allows one to compare the extent of aging *between* two systems. The former depends on the constitution (i.e. structure) of a system itself and the latter depends on the morphisms (i.e. on how close they can get to being identities) between systems.

There is, moreover, an alternate description of the inter-system comparison of aging. As usual, **R**-monomorphisms give rise to a partial order on the **R**-objects, where an **R**-monomorphism is some natural analogue of an injective linear transformation and an **N**-monomorphism. Thus $\|\boldsymbol{R}(a) - \boldsymbol{R}(b)\|$ gives an indication of how close two systems are in age while $\boldsymbol{R}(a) \leqslant \boldsymbol{R}(b)$ gives an ordering, a directionality to aging. This bears a remarkable resemblance to the aspects of *simultaneity* and *temporal succession* in the concept of time discussed in Rosen (1982). Perhaps this is not too surprising. After all, although aging and time are distinct concepts, they do share a lot of characteristics in common. In particular, they are both clocks—aging is an intrinsic clock and time is an extrinsic clock—for natural systems.

5. Categorical Hierarchies. There is a categorical definition of 'structure' but here we shall only take the term intuitively. Let us consider the idea that '**R** is a category of **N**-objects with linear structure' in more detail. The adjoint isomorphism (9) can be paraphrased into

$$\begin{array}{c}[a^i]\in\mathbf{R}\\ \hat{\mathbf{F}}\ \Big\uparrow\Big\downarrow\ \hat{\mathbf{G}}\\ (S,F,D)\in\mathbf{N}\end{array} \tag{11}$$

representing the concept that **R** is one step up the *hierarchy* on **N**. The category **N**, in turn, can be further 'decomposed', and we eventually obtain

$$\begin{array}{c}[a^i]\in\mathbf{R}\\ \uparrow\downarrow\\ (S,F,D)\in\mathbf{N}\\ \uparrow\downarrow\\ (S,F)\in\mathbf{S}\\ \uparrow\downarrow\\ S\in\mathbf{Ens}\end{array} \tag{12}$$

Note that the arrows in the 'tower' (12) are functors, mapping *between* different hierarchical levels. Those pointing up put additional structures on the objects and those pointing down 'forget' some structures. The functors can be appropriately composed to map between categories from different levels. In particular, we have

$$\begin{array}{c}[a^i]\in\mathbf{R}\\ \Big\uparrow\Big\downarrow\\ S\in\mathbf{Ens}\end{array} \tag{13}$$

where the downward arrow is the forgetful functor for **R**. As the only categories we consider are 'concrete', i.e. there are forgetful functors from them to **Ens**, the category **Ens** underlies all categorical hierarchies, forming the *base category* of our study.

While adjoint functors provide connections between different hierarchical levels, objects on the same level are mapped to one another by morphisms. An **R**-morphism, for example, sends one natural system to a second, as in

$$[a^i] \xrightarrow{\phi} [b^j], \tag{14}$$

and together with its functorial image in **Ens** we have the commutative diagram

$$\begin{array}{ccc} [a^i] & \xrightarrow{\phi} & [b^j] \\ \downarrow & & \downarrow \\ S & \xrightarrow[\phi|_S]{} & S' \end{array} \tag{15}$$

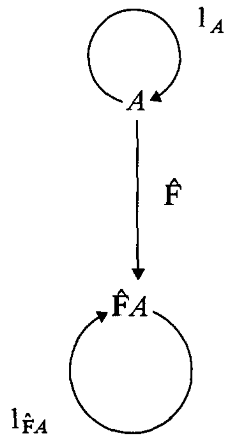
Morphisms can be used to compare objects on the same hierarchical level. Monomorphisms induce a partial ordering of objects, and this leads to the metaphor for growth and aging discussed in L–83.

6. Category of Diagrams. Let **A** and **B** be categories. The *functor category* $\mathbf{B}^{\mathbf{A}}$ has as objects all (covariant) functors from **A** to **B** and has as morphisms all natural transformations.

There are many situations in mathematics where a special part provides a universal description of the whole. For example (as we mentioned before), every Hilbert space is isomorphic to $L^2(\mu)$ for some measure μ, and thus the special Hilbert space $L^2(\mu)$ supplies a representation for all Hilbert spaces; in linear algebra $\mathbb{R}^n$ (respectively, $\mathbb{C}^n$) is canonical for all finite-dimensional real (respectively, complex) vector spaces; and so on. There are also many instances where a special part and its 'subparts' together describe the whole. The Stone Representation Theorem states that each Boolean algebra is isomorphic to a subalgebra of a power set algebra and hence the power set algebra is such a special part. Cayley's Theorem states that every group is isomorphic to a subgroup of the group of permutations over some appropriate set and hence permutation groups are prototypes in group theory.

It turns out that functor categories $\mathbf{B}^{\mathbf{A}}$ are similarly special in category theory. If **A** is the trivial category with a single object A and a single morphism $1_A \in \mathbf{A}(A, A)$, then a functor $\hat{\mathbf{F}}$ from **A** to **B** can be represented by the diagram (16); i.e. the functor category $\mathbf{B}^{\mathbf{A}}$ can be considered as consisting of the objects of **B** (and their identity morphisms).

If **A** is a category with two objects A_1 and A_2, morphisms 1_{A_1}, 1_{A_2} and a single $\phi \in \mathbf{A}(A_1, A_2)$, then **A** can be specified by diagram (17) (where the identity morphisms 1_{A_1} and 1_{A_2} are implied and hence omitted for simplicity). A functor $\hat{\mathbf{F}}$ from **A** to **B** can be represented by diagram (18).



(16)

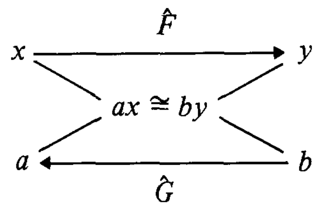
$$A_1 \xrightarrow{\ \phi\ } A_2 \tag{17}$$

$$\begin{array}{ccc} A_1 & \xrightarrow{\ \phi\ } & A_2 \\ {\scriptstyle \hat{F}}\downarrow & & \downarrow{\scriptstyle \hat{F}} \\ \hat{F}A_1 & \xrightarrow[\hat{F}\phi]{} & \hat{F}A_2 \end{array} \tag{18}$$

Hence $\mathbf{B}^{\mathbf{A}}$ can be considered as consisting of all copies in **B** of the 'pattern' (17), i.e. all morphisms $\psi \in \mathbf{B}(B_1, B_2)$. Note that diagram (15) is an example of the general diagram (18).

We thus see that when the domain category **A** is chosen suitably, objects and morphisms of any category **B** have representations in a functor category $\mathbf{B}^{\mathbf{A}}$; this gives a special role to functor categories. More generally, any category **A** can be specified by a diagram of arrows and the functor category $\mathbf{B}^{\mathbf{A}}$ can be regarded as the collection of all copies in **B** of this diagram (pattern). The functor category $\mathbf{B}^{\mathbf{A}}$ is therefore also called the *category of diagrams* in **B** (over **A**).

7. Adjoint-invariance Diagram. The adjoint-invariance diagram (AID) was introduced in L–R–83 as a mathematical morphology with which to analyse natural phenomena. The fundamental premises are that a representation of relevant features of the invariants of nature can be synthesized only when one has some measure of the appearances *and* their adjoints, namely the producers of these appearances (i.e. the projections and the projectors in R–L–83), and that invariants admit equivalent alternate descriptions. An AID has the form

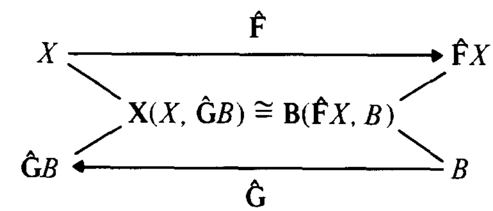


(19)

where $\hat{F}$: $x \to y$ and $\hat{G}: b \to a$ form a pair of adjoints and the middle line is an invariance of form, a natural isomorphism of structures.

The AID (19) is the diagram of the following category **A**. **A** has six objects: a, b, x, y, ax and by. The distinguished pair of morphisms $\hat{F} \in \mathbf{A}(x, y)$ and $\hat{G} \in \mathbf{A}(b,a)$ are adjoint to each other. This abstract adjointness, as we shall see shortly, has realizations in the various image categories. The objects ax and by are **A**-isomorphic. The 'inward' morphisms from a, x, b, y to ax and by are monomorphisms (generalized injections) and the 'outward' morphisms are epimorphisms (generalized projections). As before, all identity morphisms are implied. This six-object category **A** is given the name *AID-category*.

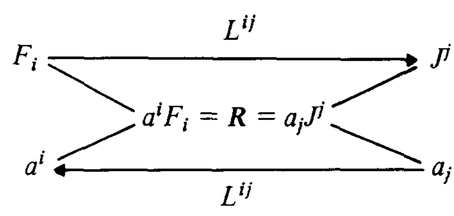
Let us consider several examples of functor categories over **A**. Since the form of an AID was suggested by that of a diagram depicting adjoint functors (L–R–83, Section 7), the latter should be an image of the former in an appropriate category. Indeed, a functor from **A** to the category **Cat** of (small) categories results in the diagram



(20)

which is diagram (24) of L–R–83. The AID (20) is, in other words, an element of $\mathbf{Cat}^{\mathbf{A}}$.

A realization of the pattern (19) in the category **R** of description spaces (i.e. an element of $\mathbf{R}^{\mathbf{A}}$) is the duality-invariance diagram (DID) for the response tensor



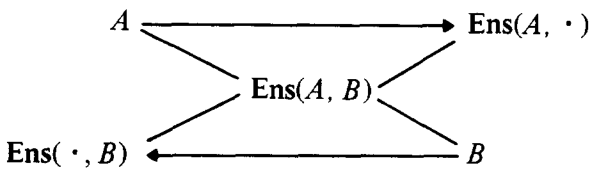
(21)

Recall (L–R–83) that *duality* is a function $\hat{\mathbf{D}}$ from a category **C** to **C** itself such that $\hat{\mathbf{D}}^2$ is the identity. Since

$$\mathbf{C}(X, \hat{\mathbf{D}}Y) \cong \mathbf{C}(\hat{\mathbf{D}}X, \hat{\mathbf{D}}^2 Y) \cong \mathbf{C}(\hat{\mathbf{D}}X, Y), \tag{22}$$

a duality is self-adjoint. Thus a DID (diagram 30) is a special type of AID.

An element of $\mathbf{Ens}^{\mathbf{A}}$ has the AID



(23)

which is the representation of the universal (M, R)-system

$$A \xrightarrow{\ f\ } B \xrightarrow{\ \Phi\ } \mathbf{Ens}(A, B) \tag{24}$$

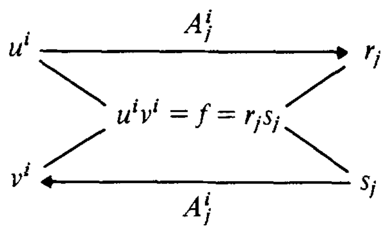
(L–R–83, Section 6). With appropriate choices of the category **B**, other AIDS and DIDS we considered (in L–R–83 and R–L–83) can similarly be described as elements of the functor category $\mathbf{B}^{\mathbf{A}}$.

8. Duality Vs Adjointness. In this section we compare and contrast an adjoint pair $(\hat{F}, \hat{G})$ with a self-adjoint pair $(\hat{D}, \hat{D})$, where $\hat{D}$ is a duality. Recall that a duality is self-adjoint.

Duality provides a canonical symmetric pair of alternate descriptions of phenomena. Its origin is the necessary intervention of sense perception in the knowledge of left and right, Yin and Yang, the two-ness of nature. The importance of duality appears in the enantiomorphic crystals discovered by Pasteur. Enantiomorphy arises as a consequence of the mixture of symmetry and dissymmetry. To Pasteur the dissymmetry of substances is even a prerequisite for life. This conception on the relationship between life and dissymmetry cannot be taken literally, but the union of symmetry and dissymmetry does lie in the very root of the generation of phenomena. A phenomenon can only exist in an environment possessing its characteristic symmetry or a lesser symmetry. It is the dissymmetry that creates the phenomenon. And it is this very nature of phenomena that necessitates the generalization from the symmetric pair $(\hat{D}, \hat{D})$ of alternate descriptions to the dissymmetric pair $(\hat{F}, \hat{G})$.

The difference between duality and adjointness is also a hierarchical one. Dualities often map between conjugate objects on the same level: force-and-flux, cause-and-effect, and enzyme-and-substrate are examples. Adjoints, on the other hand, often send objects between hierarchical levels: sets and vector spaces, natural systems and description spaces, and metabolism and repair are examples.

It is best to illustrate the above with the AID of a bilinear form representing the structure of a chemical reaction



(25)

(which is Figure 5 of R–L–83) and the DID of a response tensor (diagram 21).

In both diagrams (25) and (21) the top arrows represent operators 'summing over i', while the bottom arrows act with 'summing over j'. In terms of bra- and ket-vectors (R–L–83), we have

$$|r_j\rangle = \langle u^i | A^i_j$$
$$\langle v^i | = A^i_j | s_j\rangle \tag{26}$$

for diagram (25) and

$$|J^i\rangle = \langle F_i | L^{ij}$$
$$\langle a^i | = L^{ij} | a_j\rangle \tag{27}$$

for diagram (21). Since $L^{ij} = \langle a^i, a^j\rangle^*$ is *real symmetric*,

$$(L^{ij}\text{: sum over } i) = (L^{ji}\text{: sum over i}), \tag{28}$$

whence equations (27) can be replaced by

$$\langle J^i | = L^{ji} | F_i\rangle$$
$$\langle a^i | = L^{ij} | a_j\rangle. \tag{29}$$

Note that $\hat{D} = (L^{ij})$ is a duality at the level of tensor spaces (L–R–83), Section 4), and hence self-adjoint—which is, incidentally, also a property of real symmetric matrices. Thus, the top and bottom arrows of diagram (21) become 'the same' and diagram (21) takes the form of a DID (diagram 30).

Contrariwise, $A^i_j = \Pi_j \Pi^i$ (notation of R–L–83, Section 5) is not symmetric with respect to the indices, so $F = (A^i_j$: sum over $i)$ and $G = (A^i_j$: sum over $j)$ are not equal. They are, however, an adjoint pair: an adjoint of a matrix is the conjugate transpose (transpose for a real matrix). Thus diagram (25) does indeed have the form of an AID (19).

$$\begin{array}{ccc} x & \xrightarrow{\hat{D}} & y \\ & \searrow \quad ax = by \quad \swarrow & \\ & \swarrow \qquad\qquad \searrow & \\ a & \xleftarrow[\hat{D}]{} & b \end{array} \tag{30}$$

The duality $\hat{D} = (L^{ij})$ sends causes to effects, mapping on the same level. Recalling the concepts of categorical hierarchies of Section 5, this self-adjoint operator can therefore be likened to a morphism. The adjoint pair $(\hat{F}, \hat{G})$, as in the chemical example of Section 5 in R–L–83, functions between atomic and molecular descriptions, i.e different levels. So adjoint operators which are not self-adjoint are comparable to functors. In conclusion, 'self-adjointness' of maps can be established as a test for whether objects are on the same hierarchical level.

9. Transformation of Diagrams. We now return to morphisms in functor categories, i.e. natural transformations of functors. First let **A** be the two-object category from Section 6. If $\hat{\mathbf{U}}$ and $\hat{\mathbf{V}}$ are two functors from **A** to **B**, then a natural transformation $\Phi \in \mathbf{B}^{\mathbf{A}}(\hat{\mathbf{U}}, \hat{\mathbf{V}})$ has the diagram

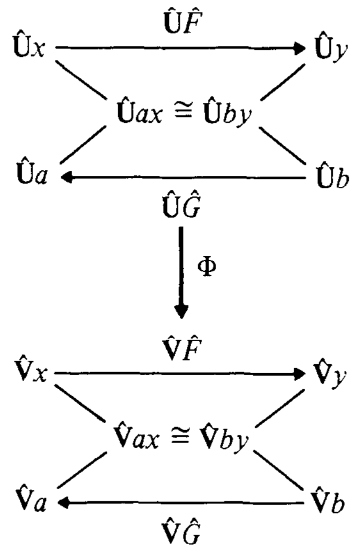
$$\begin{array}{ccc} \hat{\mathbf{U}}A_1 & \xrightarrow{\hat{\mathbf{U}}\phi} & \hat{\mathbf{U}}A_2 \\ \Phi \downarrow & & \downarrow \Phi \\ \hat{\mathbf{V}}A_1 & \xrightarrow[\hat{\mathbf{V}}\phi]{} & \hat{\mathbf{V}}A_2 \end{array} \tag{31}$$

which generalizes diagram (18). The top and bottom arrows can be considered as *analogues* of each other. Diagrams of the form (31) have interesting interpretations in the concept of *similarity* in physics and biology, and these implications are discussed in detail in Rosen (1978, Chapter 7).

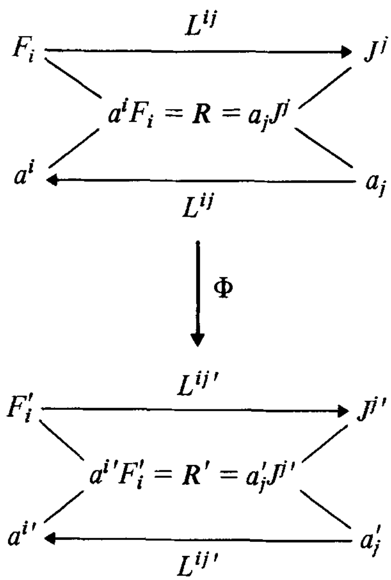
When **A** is the six-object AID category, a natural transformation Φ of two functors $\hat{\mathbf{U}}$ and $\hat{\mathbf{V}}$, realized in a category **B** as two AIDs, takes the form as in diagram (32).

For example, in the category **R** two functors can be realized as DID representations of two response tensors $\boldsymbol{R}$ and $\boldsymbol{R}'$, which are alternate descriptions (projections, R–L–83) of the inaccessible underlying invariant I. Then a natural transformation Φ of one to the other acts as a means for comparing the two descriptions of phenomena under different sets of projectors and has the morphology as in diagram (33).

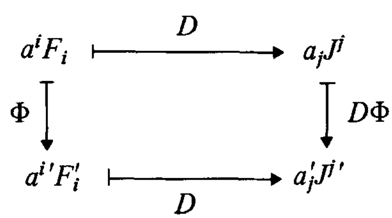
Diagram 33 can be simplified to the bilinear coordinate-transformation diagram (34) (L–R–83, Section 5).


$\hat{U}\hat{F}$
$\hat{U}x$
$\hat{U}y$
$\hat{U}ax \cong \hat{U}by$
$\hat{U}a$
$\hat{U}b$
$\hat{U}\hat{G}$
Φ
$\hat{V}\hat{F}$
$\hat{V}x$
$\hat{V}y$
$\hat{V}ax \cong \hat{V}by$
$\hat{V}a$
$\hat{V}b$
$\hat{V}\hat{G}$

(32)


L^{ij}
F_i
J^j
$a^iF_i = R = a_jJ^j$
a^i
a_j
L^{ij}
Φ
$L^{ij\prime}$
F_i'
$J^{j\prime}$
$a^{i\prime}F_i' = R' = a_j'J^{j\prime}$
$a^{i\prime}$
a_j'
$L^{ij\prime}$

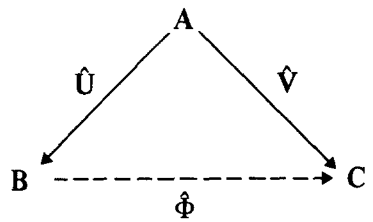
(33)


D
a^iF_i
a_jJ^j
Φ
$D\Phi$
$a^{i\prime}F_i'$
$a_j'J^{j\prime}$
D

(34)

Noting the resemblance of diagram (34) to diagram (31), we see that an alternate description is a kind of similarity.

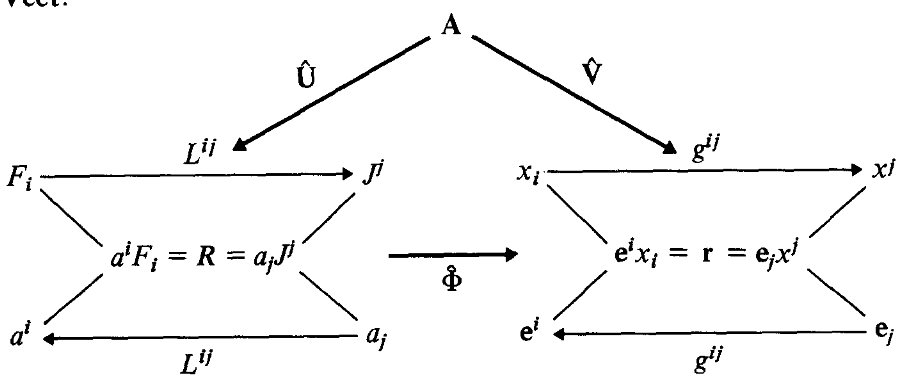
The above discussion on functorial images of diagrams over **A** in one category **B** may be extended as follows. Let **A**, **B**, and **C** be three categories with functors $\hat{\mathrm{U}}$: **A** → **B** and $\hat{\mathrm{V}}$: **A** → **C** and let a functor $\hat{\Phi}$: **B** → **C** exist such that the diagram



(35)

commutes. Then the functor $\hat{\Phi}$ serves as a comparison for diagrams over **A** realized in the *different* categories **B** and **C**. (When **B** = **C** the situation is reducible to that before.)

As an example, again let **A** be the AID category. In the beginning of our sequence of papers on the phenomenological calculus the morphology $R = a^i F_i$ and the DID of the response tensor were suggested by those of a radius vector $\mathbf{r} = \mathbf{e}^i x_i$. Thus R and $\mathbf{r}$ are *models* of each other. This *modelling relation* is represented by the functor $\hat{\Phi}$ between **B** = **R** and **C** = **Vect**:



(36)

We shall return to other realizations of the modelling relation shortly.

10. Pattern Generation. Rosen's (1981) note on a unified approach to pattern generation points out the close relationship between the concepts of abstract patterns and fibre bundles. A *fibre bundle* (E, B, X, p) consists of a *total space* E, a *base space* B, a *fibre* X and a *bundle projection* p: $E \to B$ such that there exists an open covering $\{U\}$ of B and, for each $U \in \{U\}$, a homeomorphism $\phi_U : U \times X \to p^{-1}(U)$ such that the composite

$$P \circ \phi_U : U \times X \to p^{-1}(U) \to U \tag{37}$$

is the projection on the first factor. In other words, the bundle projection and the projection $B \times X \to B$ are locally equivalent. The *fibre over* $b \in B$ is $X_b = p^{-1}(b)$, and each X_b is homeomorphic to X. Intuitively, one can think of a fibre bundle as a union of fibres X_b for $b \in B$, hence parametrized by B and 'glued together' by the topology of the total space E.

A *cross-section* of a fibre bundle (E, B, X, p) is a map $f: B \to E$ such that $p \circ f = 1_B$. Thus a cross-section selects for every $b \in B$ a point $f(b)$ in the fibre X_b. Rosen's basic suggestion is that if the base space B is identified as the domain (of constitutive parameters) over which patterns are to be formed and the fibre X as the set of states which may be assigned to each point of that domain, then a pattern is obtained by selecting for each $b \in B$ one allowable state from $X \cong X_b$. This simply says that 'pattern' and 'cross-section' are the same concepts. Denoting the space of all cross-sections (patterns) by P, we see that the problem of pattern generation is most appropriately formulated in the space P: a pattern-generating mechanism is a dynamics in P.

The category **R** of description spaces can be considered as the fibre bundle $(E, (H^*)^m, H^m, p)$, where E consists of all dyadic response tensors of the form $R = a^i F_i$ with $a^i \in H^*$ and $F_i \in H$, and $p(R) = \{a^i: i = 1, \ldots, m\}$. For each m-tuple of constitutive parameters $\{a^i\} \in (H^*)^m$ the fibre $X_{\{a^i\}}$ is the description space $[a^i]$. It is clear that each $X_{\{a^i\}}$ is isomorphic to the fibre H^m. When the isomorphism identification $H \cong H^*$ is made, we have the dual representation of this fibre bundle

$$(E, (H^*)^m, H^m, p) \cong (E, H^m, (H^*)^m, q), \tag{38}$$

with $q(R = a_j J^j) = \{a_j\} \in H^m$. Note that p and q constitute the dual collection of projectors $\{\hat{\mathbf{P}}_i\}$ and $\{\hat{\mathbf{Q}}^i\}$ in R–L–83.

A pattern in the fibre bundle **R** is then a map Φ which picks for each $\{a^i\}$ a response tensor $a^i F_i$ (hence an m-tuple $\{F_i\}$ in the fibre H^m). It then becomes a similarity transformation

$$\Phi: a^i F_i \mapsto a^{i'} F_i' \tag{39}$$

for different constitutive parameters $\{a^i\}$ and $\{a^{i'}\}$. Further, taking the duality (38) into account one immediately recovers the commutative diagram (34) above. A pattern-generating mechanism, formulated as a dynamics $\Phi = \{\Phi_t\}$ in the space of cross-sections P, takes the form as in diagram (40) which completes the cycle and brings us back to diagram (1) of an **N**-dynamics.

11. Differential Geometry of Proteins. A structural and dynamical representation of protein patterns is given in Louie and Somorjai (1982). The

$$\begin{array}{ccc} a^iF_i(t_1) & \stackrel{\Phi}{\longmapsto} & a^{i'}F'_i(t_1) \\ T_{t_2-t_1} \downarrow & & \downarrow (\Phi T)_{t_2-t_1} \\ a^iF_i(t_2) & \underset{\Phi}{\longmapsto} & a^{i'}F'_i(t_2) \\ \Cap & & \Cap \\ X_{\{a^i\}} & & X_{\{a^{i'}\}} \end{array} \tag{40}$$

primary structure of a protein molecule, its sequence of amino acids, can be described as a finite word over an alphabet of 20 letters. The higher-order (secondary, tertiary and quaternary) structures, on the other hand, are most appropriately described by the shape of a space curve (representing the protein backbone) lying on certain surfaces embedded in $\mathbb{R}^3$.

The map which sends the primary sequences of proteins to their three-dimensional spatial structures can then be formulated as a cross-section of a fibre bundle. The base space is the *genotype* of proteins while the fibre is the *phenotype*. The molecular dynamics of proteins are best described as dynamics in the space of cross-sections (patterns) of this fibre bundle.

Let $\{a^i\}$ be a finite word over the set of 20 amino acids, representing the genotype of a protein, and let $\{F_i\}$ be its phenotype, describing the shape of the backbone space curve of the protein. Then a similarly transformation between proteins is given by the map (39) and a pattern-generating protein dynamics is given by diagram (40).

Since a space curve is uniquely determined by a pair of continuous functions (κ, τ), the curvature and torsion, the response tensor a^iF_i admits the alternate description (κ, τ). This yields the modelling relation (35) for the differential geometry of proteins:

$$\begin{array}{ccc} & \text{protein} & \\ \swarrow & & \searrow \\ R = a^iF_i & \longrightarrow & R = (\kappa, \tau) \end{array} \tag{41}$$

Protein dynamics can also be studied in the framework of this alternate description, namely as a dynamics in the space of pairs of continuous functions (κ, τ). This is discussed in Louie and Somorjai (1983).

Finally, this alternate description of proteins as pairs of continuous functions has useful implications in the study of enzyme–substrate recognition. Recall (L–R–S–82) that an enzyme can be described by a function of bounded variation which acts as the integrator in a Stieltjes integral, in which a continuous function describing the substrate is the integrand. The pair (κ, τ) can be considered as a function of bounded variation when κ and τ represent the curvature and torsion of an enzyme backbone curve. Then the mechanism of enzyme–substrate recognition is given by the operator

$$\int_K \cdot \, \mathrm{d}(\kappa, \tau) \tag{42}$$

and represented by the diagram

$$\begin{array}{ccccc} S \in \text{substrates} & \rightarrowtail & F \in C(K) & \searrow & \\ & & \downarrow & & \\ & & \langle F, a\rangle = \int F \mathrm{d}a & & aF \in T_1^1(C(K)) \\ & & \uparrow & & \\ e \in \text{enzymes} & \rightarrowtail & a = (\kappa, \tau) \in NBV(K) & \nearrow & \end{array} \tag{43}$$

(cf. Figure 4 of L–R–S–82). We shall discuss the above ideas and the differential geometry of enzymes in a forthcoming paper.

This paper is dedicated to Dr. I. W. Richardson.

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