Towards a quantitative perspective in Networks of Bio-inspired Processors (NBP)

Sandra Gómez Canaval
Department Computer Science Systems
University College of Computer Science - UPM
Outline

Towards a quantitative perspective in NBPs. S. Gómez
Introduction

- Complex and hard problems in computation
  - NP complete

- Methods and paradigms to solve these problems in an efficient way
  - Bio-inspired models based on formal languages
  - Discrete approximations
Bio-inspired computational models

Inspired from the nature: How nature computes?
- Efficiently
- Distributed
- Massively parallelism
- In a real time

First step:
- Mathematical and computer science goals
- After biological goals.
NBP model

- Networks of bio-inspired processors
  - Maturity
  - Solves NP complete problems
    - Polynomial time with linear number of resources
  - Efficiency
  - Extensibility
  - Simplicity

Towards a quantitative perspective in NBPs. S. Gómez
Estado del arte: NBP

Características y poder computacional:

- Universales y computacionalmente completas
  - Resuelven problemas NP-completos

- Eficientes
  - Complejidad espacial: Número lineal de recursos
  - Complejidad temporal: polinomial

- Simples y Expresivas

- Extensibles / Escalables

- Distribuidas y paralelas

Towards a quantitative persoective in NBPs. S. Gómez
Networks of bio-inspired processors – NBP [Mitrana, 2001].

- Processors as generating languages devices
- Located in nodes of a network
- Data processing (as ADN strings) based on rewriting rules of a grammar
- Protocol Communication in the connections between nodes
- Parallelism in the processing and the communication phases
Alphabets: input and network
Underlying graph: network structure

Operations

X₁

Operations

X₂

Operations + protocol

X₃

Operations

Towards a quantitative perspective in NBPs. S. Gómez
Objetivos, justificación y motivación

- Acercamiento a la realidad biológica
- Orientación a un carácter cuantitativo
- Cambio en el enfoque del dominio de los problemas

Towards a quantitative perspective in NBPs. S. Gómez
Towards a quantitative perspective in NBP.

Input

$X_1$ $X_2$ $X_3$

Output

$w''_1$ $w''_2$ $w''_3$

NBP Metamodel Dynamic
Towards a quantitative perspective in NBPs. S. Gómez
$\Gamma$ configuration: $C: X_G \rightarrow 2^{V^*}$

Initial $\Gamma$ configuration in $w \in V^*$

$C_0^{(w)}(X_I) = \{w\}$ and $C_0^{(w)}(x) = \emptyset \ \forall \ x \in X_G - \{X_I\}$

Evolution step

$C \Rightarrow C'$ sii

$C'(x) = M^\alpha_x(C(x)) \ \forall x \in X_G$

Communication step

$C \Leftarrow C'$ sii

$C'(x) = (C(x) - \tau_x(C(x))) \cup \bigcup_{\{x,y\} \in E_G} (\tau_y(C(y)) \cap \rho_x(C(y)))$
A computation halts:

i. \( X_0 \) is non-empty: *acceptation computation.*

ii. There are two identical configurations obtained in consecutive steps

**Accepted language** by \( \Gamma \) is

\[
L(\Gamma) = \{ w \in V^* \mid \text{\( \Gamma \) computation in \( w \) accepting computation} \} \]
Towards a quantitative perspective in NBPs. S. Gómez
Networks of Evolutionary Processors: NEP
Networks of Evolutionary Processors: NEP

- **Evolutionary rule**: point mutations in a DNA sequence (insertion, deletion or substitution of a pair of nucleotides).

- $\sigma: a \rightarrow b$ such that $a, b \in V \cup \varepsilon$

- Action rule: $\alpha = \{*, l, r\}$

<table>
<thead>
<tr>
<th>Evolutionary rule $\sigma$</th>
<th>Definition</th>
<th>Action rule $\sigma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substitution</td>
<td>$a, b \neq \varepsilon$</td>
<td>$\alpha = {\ast}$</td>
</tr>
<tr>
<td>Deletion</td>
<td>$a \neq \varepsilon \land b = \varepsilon$</td>
<td>$\alpha = {\ast, l, r}$</td>
</tr>
<tr>
<td>Insertion</td>
<td>$a = \varepsilon \land b \neq \varepsilon$</td>
<td></td>
</tr>
</tbody>
</table>

- $Sub_V, Del_V \in Ins_V$ set of all rules over $V$

Towards a quantitative perspective in NBPs. S. Gómez
## Networks of Evolutionary Processors: NEP

- Filtering strategy: $\beta \in \{s, w\}$
  - $s$: *strong*
  - $w$: *weak*

- Set of permitting/forbidding symbols

<table>
<thead>
<tr>
<th>Symbols</th>
<th>Input</th>
<th>Output</th>
<th>Strong</th>
<th>Weak</th>
</tr>
</thead>
<tbody>
<tr>
<td>Permitting</td>
<td>PI</td>
<td>PO</td>
<td>All</td>
<td>1 or more</td>
</tr>
<tr>
<td>Forbiddibg</td>
<td>FI</td>
<td>FO</td>
<td>None</td>
<td>None</td>
</tr>
</tbody>
</table>

Towards a quantitative perspective in NBPs. S. Gómez
Definition: Evolutionary processor associated to the node $x$ is a 5-tuple $(M_x, PI_x, FI_x, PO_x, FO_x)$ where:

- $M_x$ is a finite set of evolutionary rules such that $M_x \subseteq Sub_V$, $M_x \subseteq Del_V$ or $M_x \subseteq Ins_V$

- $PI_x, FI_x$ are the permitting/forbidding contexts/symbols respectively, such that $PI_x \cap FI_x = \emptyset$

- $PO_x, FO_x$ are the permitting/forbidding contexts/symbols respectively, such that $PO_x \cap FO_x = \emptyset$
Networks of Evolutionary Processors – NEP is a 8-tuple \((V, U, G, N, \alpha, \beta, X_I, X_O)\)

- \(V, U\) tal que \(V \subseteq U\)
- \(G = (X_G, E_G)\) underlying graph.
- \(N: X_G \rightarrow EP_U\) mapping \(x \in X_G\) with \(N(x) = (M_x, PI_x, FI_x, PO_x, FO_x)\)
- \(\alpha: X_G \rightarrow \{* , l, r\}; \quad \alpha(x)\)
- \(\beta: X_G \rightarrow \{s, w\}\) I/O filters
- \(X_I, X_O\) are input and output nodes

Towards a quantitative perspective in NBPs. S. Gómez
Polarized NEP

Towards a quantitative perspective in NBPs. S. Gómez
Networks of Polarized Evolutionary Processors – NPEP [Mitrana, 2012].

**Polarization**: filter strategy.

**Valuation mapping** for strings.

**Filtering protocol**: sign of the word **but does not** real numeric value.

Simulates cellular communication by ion channels
Polarized NEP

Valuation function: $\varphi$ de $U^*$ en $\mathbb{Z}$

$U=\{a,b,c\}$

<table>
<thead>
<tr>
<th>$\varphi(a)$</th>
<th>$\varphi(b)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-1</td>
</tr>
</tbody>
</table>

Polarity (sign) to each node

- $w=acd$ ?
- $a \rightarrow b$
- $w=bcd$ ?
- $w=bcd$ ?
- $w=bcd$ ?
- $d \rightarrow b$
Polarized Evolutionary Processor over $V$ is a pair $(M, \alpha)$:

- $M \subseteq \text{Sub}_V$, $M \subseteq \text{Del}_V$ or $M \subseteq \text{Ins}_V$
- $\alpha \in \{-, 0, +\}$ is the node polarity

NPEP is a 7-tuple $I' = (V, U, G, N, \varphi, X_I, X_O)$ where

- $V, U, V \subseteq U$
- $G = (X_G, E_G)$ underlying graph
- $N : X_G \to EP_U$ is a mapping from $x \in X_G$ to $N(x) = (M_x, \alpha_x)$
- $\varphi$ is a valuation from $U^*$ to $\mathbb{Z}$
- $X_I, X_O$ are the input and output nodes respectively
Polarized NEP Dynamics

\[ \Gamma \ \text{Configuration} = \text{NEP model} \]

\[ \Gamma \ \text{Initial configuration} = \text{NEP model} \]

**Evolutionary step**

\[ C \Rightarrow C' \text{ sii} \]

\[ C'(x) = M_x(C(x)) \ \forall x \in X_G \]

**Communication step**

\[ C \leftarrow C' \text{ sii} \]

\[ C(x) = (C(x) \setminus \{w \in C(x) | \varphi(w) \neq \alpha_x\}) \]

\[ \cup \bigcup_{\{x,y\} \in E_G} (w \in C(y) | \alpha_y \neq \varphi(w) = \alpha_x) \ \forall x \in X_G \]

Towards a quantitative perspective in NBPs. S. Gómez
Qualitative or Quantitative aspects?

- NPEP is motivated by mathematical and computer science goals, but not necessarily by biological goals.
- Application of NEP in other different domains
- It is necessary to consider not only their qualitative perspective but also the quantitative one.
- Quantitative aspects are a “sine qua non” condition within biological reality
- Although it's true that NPEP incorporates a numerical evaluation over the data that processes, this is not used from quantitative perspective.
Quantitative NEPs

Towards a quantitative perspective in NBPs. S. Gómez
In cellular and biological phenomena:

- Compare software simulation vs experiments
- Quantitative valuations
  - Concentrations, gradients, thresholds, etc...
- It is necessary a NEP model with quantitative elements: QNEPs
Parametric NEP: PNPEP

First model of the Quantitative NEP family.

Polarized NEP extension

Polarized NEP has a valuation mapping:
  But it is only qualitative valuation.

Now, we want to compute the exact weight of valuation of a word
Parametric NEP: PNPEP

In NPEP: $\varphi$ is a valuation from $U^*$ to $\mathbb{Z}$

If $U=\{n,N,k,K,p\}$

<table>
<thead>
<tr>
<th>Word</th>
<th>Mapping valuation</th>
<th>Polarity</th>
</tr>
</thead>
<tbody>
<tr>
<td>$nknkn$</td>
<td>+</td>
<td>+</td>
</tr>
<tr>
<td>$knnnkn$</td>
<td>+</td>
<td>+</td>
</tr>
<tr>
<td>$nn$</td>
<td>+</td>
<td>+</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Word</th>
<th>Mapping valuation</th>
<th>Polarity</th>
</tr>
</thead>
<tbody>
<tr>
<td>$nknkn$</td>
<td>+</td>
<td>1</td>
</tr>
<tr>
<td>$knnnkn$</td>
<td>+</td>
<td>5</td>
</tr>
<tr>
<td>$nn$</td>
<td>+</td>
<td>2</td>
</tr>
</tbody>
</table>
Must be filtering words having a concentration > 5 of symbols p

To aggregate symbols D,P,C,K,P in U alphabet

\[
\begin{align*}
\phi(C) &= -5 \\
\phi(B) &= 0 \\
\phi(K) &= 0 \\
\phi(K_1) &= 0 \\
\phi(P) &= 0 \\
\phi(K_2) &= -100
\end{align*}
\]
Parametric NEP: PNPEP

To fill this lack...

- A word can enter if overtakes a specific concentration threshold
- A word can enter if exist one and only one water molecule
- A word can enter if there are 1 Potassium and 2 Sodiums
Parametric NEP: PNPEP

New elements:

- **Projection function over words**

Si $U = \{n, N, k, K, p\}$

It is necessary a set of partitions over $U$

Towards a quantitative perspective in NBPs. S. Gómez
Evaluation of the projection over a specific interval

\[ w = \text{projection}(w, k) \]

\[ \text{Projection (w, k)} \]

\[ w = \text{projection}(w, n) \]

\[ \text{Projection (w, n)} \]

\[ 5 \leq \text{Potassium concentration} \leq 10 \]

\[ 100 \leq \text{Soddiun concentration} \leq 200 \]

Polarity is divided between less generic intervals
Parametric NEP: PNPEP

- Valuation mapping NPEP is $\varphi: U^* \rightarrow \mathbb{Z}$
- Redefining $\varphi: U^* \rightarrow \mathbb{Z}^m$
- If $2^U = P = \{P_1, P_2, \ldots, P_m\}$ then

**Projection function:**

$$\pi_j(w, P_j) = a'_1, a'_2, \ldots a'_k$$

where $a'_i \begin{cases} a_i & \text{if } a_i \in P_j \\ \varepsilon & \text{otherwise} \end{cases}$

- If $\Pi = \{\pi_1, \pi_2, \ldots \pi_m\}$ then

$$\varphi(w) = \varphi_i(\pi_i(w, P_i)) \text{ for all } i \in \{1, 2, \ldots m\}$$

Towards a quantitative perspective in NBPs. S. Gómez
Parametric NEP: PNPEP

- Polarized NEP: polarity denoted by $\alpha \in \{-, 0, +\}$

- New polarization: **labels for $\alpha$**
  - Changing the notation: $\alpha \in \{(-\infty, 0), \{0\}, (0, +\infty)\}$

- Valuating the concentration of $p \geq 5$ then
  - $\alpha \in \{(-\infty, 0), \{0\}, (0, 5), [5, +\infty]\}$

### Classic notation vs Parametric Polarized NEP

<table>
<thead>
<tr>
<th>Classic notation</th>
<th>Parametric Polarized NEP</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha \in {(-\infty, 0), {0}, (0, +\infty)}$ = $\alpha \in {l_0, l_1, l_2}$</td>
<td>$\alpha \in {l_0, l_1, l_2 \ldots l_m}$</td>
</tr>
<tr>
<td>$\alpha \in {l_0, l_1, l_2}$</td>
<td>$\bigcup_{i=0}^{m} l_i = \mathbb{Z}$</td>
</tr>
</tbody>
</table>

Towards a quantitative perspexive in NBPs. S. Gómez
Parametric NEP: PNPEP

\[ \alpha \in \{(-\infty, 0), \{0\}, (0, 5), [5, +\infty)\} \]

\[ w_1 = knnnnknnnk \quad w_2 = nkknkn \quad w_3 = nn \]

Projection \((w_1, k)\): \[ kkkkkkkk \]

Projection \((w_2, k)\): \[ kk \]

Projection \((w_3, k)\): \[ \varepsilon \]

Towards a quantitative perspective in NBPs. S. Gómez
A parametric polarized evolutionary processor is a 3-tuple \((M, S, \alpha)\):

1. \(M \subseteq \text{Sub}_V\), \(M \subseteq \text{Del}_V\) or \(M \subseteq \text{Ins}_V\)
2. \(S \subseteq P\) is the set of partitions of \(U\) that this processor evaluates
3. \(\alpha \in \{l_x^0, l_x^1, l_x^2, \ldots l_x^m\}\), \(m=\text{card}(S)\)

Is the polarity partition
Parametric NEP: PNPEP

Networks of Parametric Polarized Evolutionary Processors –
PNPEP is a 8-tuple $\Gamma = (V, U, P, G, R, \varphi, X_I, X_O)$

$\Rightarrow V, U$ such that $V \subseteq U$

$\Rightarrow P$ is a partition over $U$

$\Rightarrow G = (X_G, E_G)$ is a underlying graph

$\Rightarrow N : X_G \rightarrow EP_U$ is the mapping form node to processors
$N(x) = (M_x, S_x, \alpha_x)$

$\Rightarrow \varphi$ is a valuation from $U^*$ to $\mathbb{Z}^m$

$\Rightarrow X_I, X_O$ are the input and output node respectively

Towards a quantitative perspective in NBPs. S. Gómez
Parametric NEP: PNPEP

\[ V = \{ s, S, p, P, v, V, A \} \quad \text{y} \quad U = \{ n, N, k, K, b, B, a, t, q, f, ñ \} \]

\[ P = \{ P_0 = \{ n \}, P_1 = \{ k \}, P_2 = \{ K, N, K, g, B, a, q, f, ñ, t \} \} \]

\[ \varphi(p) = 1 \quad \varphi(k) = -1 \]

\[ \alpha \quad \text{Intervalo polarización} \quad \alpha_{x_i} \quad S \]

\[ [0, 5), [5, +\infty) \quad l_{xi}^{1} \quad P_1 \]

\[ w_1 = k n n n k n n n k \]

\[ w_2 = n k n k n \]

\[ w_3 = n n \]
Parametric NEP: Dynamic

\[ \Gamma \text{ Configuration} = C : X_G \rightarrow 2^{U^*} \]
\[ \Gamma \text{ Initial configuration} = \text{NPEP model} \]

**Evolutionary step**

\[ C \Rightarrow C' \text{ sii} \]
\[ C'(x) = M_x(C(x)) \quad \forall x \in X_G \]

**Communication step**

\[ C \leftarrow C' \text{ sii} \]
\[ C'(x) = (C(x) \{ w \in C(x) \mid \varphi_i(w) = \varphi(\pi_i(w)) \notin \alpha_{x,i} \forall \pi_i \in \Pi \}) \cup \bigcup_{x,y \in E_G} \{ w \in C(y) \mid \varphi_i(w) = \varphi(\pi_i(w)) \in \alpha_{x,i} \exists \pi_i \in \Pi \} \]

Towards a quantitative perspective in NBPs. S. Gómez

Computation = NPEP
Na – K Pump simulation using Parametric NEP
Conceptos básicos

Sustancia química: $a \in V$

Solución o entorno químico: $w \in V^*$

Concentración de una sustancia: $|w|_{a}, a \in V, w \in V^*$

Reacción química: $R = \{\sigma_1, \sigma_2, \ldots, \sigma_n\}, n \in \mathbb{N}, \sigma_i \in (Sub_V \cup Ins_V \cup Del_V)$

Estado del sistema en un tiempo $i > 0$: $C_i(x)$ para todo $x \in X_G - \{X_I\}$

Towards a quantitative perspective in NBPs. S. Gómez
Simulating cellular transport with PNPEP

八十

Bomba Sodio-Potasio: transporte activo

<table>
<thead>
<tr>
<th></th>
<th>Concentración extracelular</th>
<th>Concentración intracelular</th>
<th>Potencial reposo</th>
<th>Potencial reposo Células excitable</th>
</tr>
</thead>
<tbody>
<tr>
<td>Na</td>
<td>145 mEq/L</td>
<td>[5; 15] mEq/L</td>
<td>-20mV -120mV</td>
<td>-70mV</td>
</tr>
<tr>
<td>K</td>
<td>5mEq/L</td>
<td>140 mEq/L</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Towards a quantitative perspective in NBPs. S. Gómez
Towards a quantitative perspective in NBPs.

Simulating cellular transport with PNPEP

Graphical representation of cellular transport pathways with nodes and connections.
Towards a quantitative perspective in NBPs.

NPEP Paramétricas: Bomba Na-K

Diagram showing various parameters labeled as $X_0$, $X_1$, $X_2$, $X_{2.0}$, $X_{2.1}$, $X_{2.2}$, $X_{2.3}$, $X_{2.4}$, $X_{2.5}$, $X_{2.6}$, $X_{1.1}$, $X_{1.2}$, $X_{1.3}$, $X_{1.4}$, and $X_{2.0}$.

Graphs showing time versus mS/cm² and mV, with labels for aperture, cierre, and inactivo.
Open problems and future work

- PNPEP as a first model in a family of QNEPs - Quantitative NEPs,
  - Will may address probabilistic, estocastic, and more additional quantitative elements.
  - To study the dynamic of evolutionary trajectory NEPs.
  - To calculate evolutionary distances
  - To classify and to distribute based on quantitative criterions
  - Behavior based on learning
  - To optimize based on multiobjectives
Thanks for your attention