ANN for PESs: Methodology

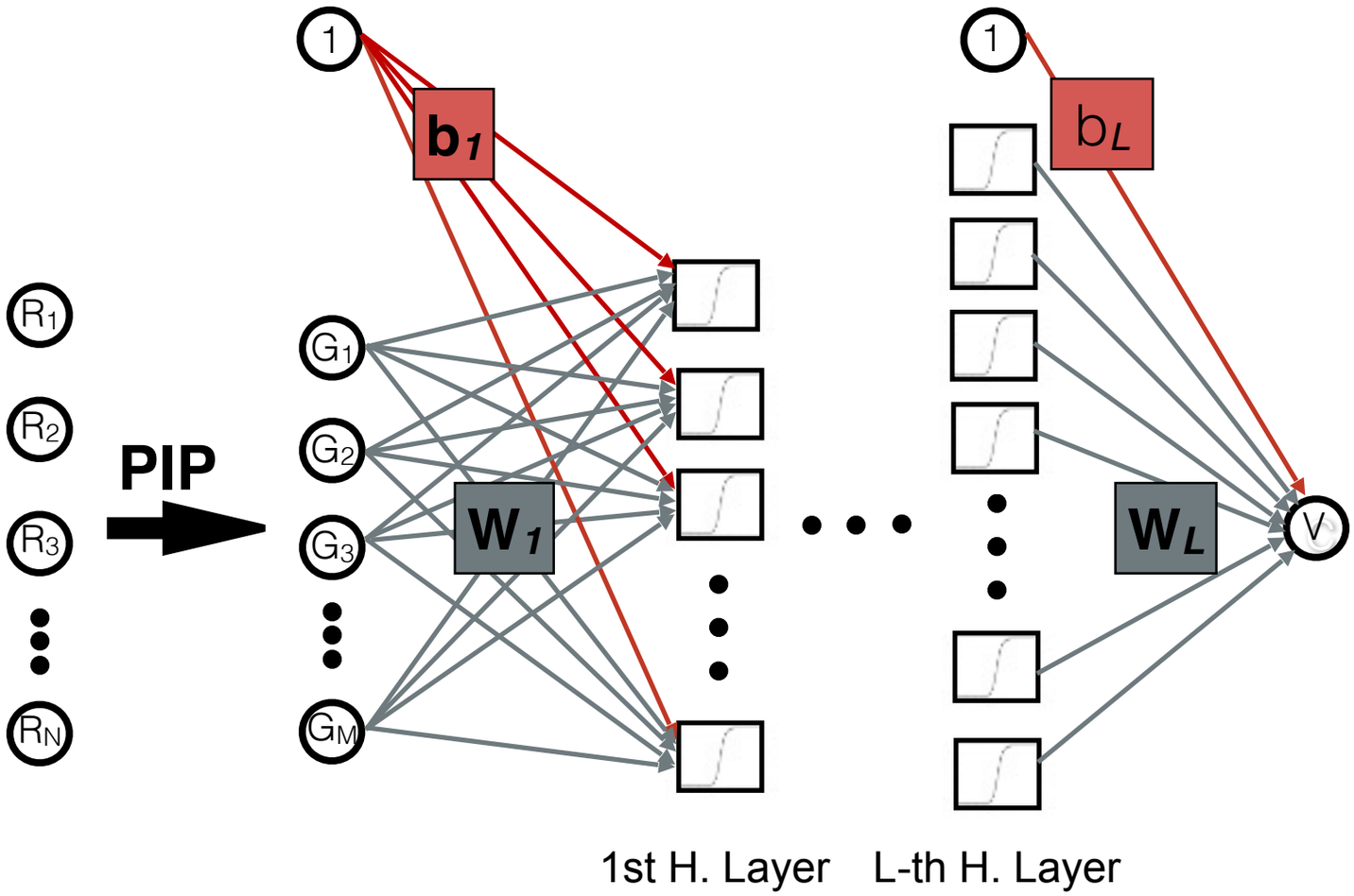
Multi-layer feed-forward Neural Networks (NN) have been adopted **as fitting functional:**

- ✦ Easy to implement;
- ✦ Easy to train;
- ✦ Easy to generalize to new systems;
- ✦ Easy to differentiate in **R**;
- ✦ Cost effective;
- ✦ Easy to be refined;
- ✦ Widely tested;
- ✦ Easy to be extended to the stochastic case.

Permutation Invariant Polynomials Neural Networks (PIP-NN):

theano

Lasagne



2. **G** is fed to a feed-forward neural network, and it **flows through its layers** as a series of weighted linear combinations alternated to non-linear functions

Output from the k-th Neuron of the i-th Layer

$$\begin{cases} z_i^k = \sum_{j=1}^{N_{i-1}} W_i^{jk} y_{i-1}^j + b_i^k \\ y_i^k = f_i\left(z_i^k\right) \end{cases}$$

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