Efficient Behavior of Photosynthetic Organelles via Pareto Optimality, Identifiability and Sensitivity Analysis

Appendix Supplementary Information

PoSA pseudo-code

Giovanni Carapezza, Renato Umeton, Jole Costanza, Claudio Angione, Giovanni Stracquadanio, Alessio Papini, Pietro Lió, Giuseppe Nicosia

Algorithm 1 PoSA Algorithm

Require: $[f, y, Q, N, K, \alpha, \beta]$
/* f output of the model */
/* y knockout vector */
/* $[Q, N, K, \alpha, \beta]$ parameters of PoSA*/

Given $Y = \{b_1, b_2, \ldots, b_s, \ldots, b_p\}$
for $s \leftarrow 1$ to p **do**
  Select the pathway b_s

  for $q \leftarrow 1$ to Q **do**

    for $\alpha \leftarrow 1$ to K **do**
    /* perform Mutation Operator on y */
      $\tilde{y}(q, \alpha) \leftarrow \text{Mutation}(y, \beta)$

      for $h \leftarrow 1$ to N **do**
      /* perform Mutation Operator on b_s */
        $\tilde{b}_s(\alpha, q, h) \leftarrow \text{Mutation}\Big(b_s, \dfrac{\alpha}{K}\Big)$

      /* evaluate scale factor Δ */
        $\Delta_s(h, \alpha, q) = \dfrac{\sum \tilde{b}_s(\alpha, q, h)}{W_s}$

      /* evaluate an Elementary Effect on pathway b_s */
        $EE_s(h, \alpha, q) = \dfrac{f(\tilde{y}(i, \alpha)) - f(b_1, b_2, \ldots, \tilde{b}_s, \ldots, b_p)}{\Delta_s(h, \alpha, i)}$
      end for
    end for
  end for
  $\mu_s{}^* \leftarrow \text{mean}(EE_s)$ /* evaluate the $\mu_s{}^*$ sensitivity index */
  $\sigma_s{}^* \leftarrow \text{var}(EE_s)$ /* evaluate the $\sigma_s{}^*$ sensitivity index */
end for
return $[\mu*, \sigma*]$

Algorithm 2 Mutation Operator

Require: $[x, a]$

/* $a \in \{0, 1\}$ is a real constant and defines the maximum number of mutations in the Boolean vector x of W_x elements*/

/* Select randomly an integer value A in $[1, a \cdot M_x]$ */

$A \leftarrow$ random $(1, aW_x)$

/* Select randomly A bits on x vector */

$ind \leftarrow$ random $(1, W_x, A)$

$\tilde{x} \leftarrow \text{not}(x\,[ind]\ )$

return $\tilde{x}$