1 ODD[1] of the TIMELY model

1.1 Purpose

The purpose of this model is to investigate the role of the delay time between herbivore attack and plant's defense reaction in induced defenses. The common understanding of delay time is "the shorter the better", therefore we want to check whether there exists an optimal delay time τ which is greater than zero and thus contradicts common belief. We focus on the variety of optimal values of τ for different scenarios of herbivore density.

1.2 Entities, state variables, and scales

The entities in the model are plants, larvae and patches. All state variables are given in table S1.

Agent	Variable	Description	Unit
Plant	x,y	Spatial coordinates	-
	$B_{\text{above}}(t)$	current biomass shoot	g
	$B_{\text{below}}(t)$	current biomass root system	g
	$d_a(t)$	above-ground defense level (percentage of defense compounds in relation to overall plant biomass)	%
	τ	delay time between the beginning of the larval attack and the start of the defense reaction of the plant and defense production	days
	D_c	fraction of produced biomass which is allocated to defense (for infested plants)	%
	$\text{MEMORY}_p[\text{t}]$	total biomass of larvae currently feeding on plant p	-
Larva	$\text{age}_l(t)$	Age of the larva (since hatching)	days
	$B_l(t)$	current biomass of larva	g
	$\text{mobile}_l(t)$	whether or not the larva can move between plants?	yes/no
	$\text{plant}_l(t)$	identity of the current host plant (set to "none" if the larva is moving)	-
	$\text{mortality}_l(t)$	Probability of larva to die in the current time-step	-
Patches	x_{patch}, y_{patch}	Spatial coordinates of the current patch	-

Table S1: Entities and state variables used in the individual-based model.

Plants

Rationale: The plants represent the fast-growing tobacco plant, *Nicotiana attenuata*. These plants are native in semi-arid regions of southwestern USA. They are growing under high competition pressure in monoculture-like natural populations and defend against herbivores/pathogens etc. by producing induced defenses.

[1] "ODD" (Overview, Design concepts, Details) is a generic format for describing agent-based models ([Grimm et al., 2010]).

Larvae

Rationale: The insect larvae are mobile, exponentially growing herbivores feeding on tobacco plants. During their growth they pass through five instars. At the beginning, larvae are bound to their host-plant, however, after reaching a certain weight and instar (third instar) they are able to move between plants, if necessary. Larvae chose to leave their host plant for two reasons: either the plant is nearly entirely consumed, or the defense-level (the percentage of defense compounds within the plant tissue) has reached a certain threshold. Switching plants comes to a cost, more energy is needed and the probability of being predated rises significantly when being on the ground.

Patches

A grid of patches is used to facilitate calculations (e.g. size of the ZOIs etc), however, the positions of plants and larvae were given continuous variables.

Scales

In order to make spatial calculations of resource competition easier, the Zone-of-Influences are projected onto a grid of patches. To avoid edge effects, we used a torus world with a size of 250 x 250 patches, which corresponds to a size of 15 x 15 m in reality. The state of each patch is characterized by its resource availability. We use a homogeneous environment, so all patches have the same, and constant degree of resource limitation for the above- and the below-ground part. One time step in the model represents $\frac{1}{6}$ day.
The simulation runs for 300 generations à 27 days (6 ticks a day). We chose 27 days as one generation, because this is the time the larvae need to complete their life circle on the plants.

Scale	**Value**	**Unit**
Number of patches	250 x 250	-
Patch size	16,7	cm
Time step	1/6	day

Table S2: Scales of the individual-based model.

Model parameters

All plants are characterized by their initial above- and belowground biomasses, $B0_{\text{above}}$ and $B0_{\text{below}}$; the plant's asymptotic biomass $B0_{\max}$ and the plant's intrinsic growth rate by mass, A_0.

Larvae are characterized by their initial biomass, $B0_l$ and a maximal biomass, $B_{l\ \max}$. When a larva reaches this mass, it goes to pupate and becomes thus inactive.

All patches have two floating point numbers between 0 and 1 which describe their resource limitations for the below- and aboveground compartments. The simulated environment is homogeneous and constant, this means that all patches have the same resource limitations and these values do not change over time.

Variable	Description	Unit
$B0_{\text{above}}$	initial biomass shoot (constant)	g
$B0_{\text{below}}$	initial biomass root (constant)	g
$B0a_{\max}$	ideal maximal above ground biomass of plant	g
$B0b_{\max}$	ideal maximal below ground biomass of plant	g
A_0	intrinsic mass growth factor of plant	
$B0_l$	initial biomass of larva	g
$B_{l\ \max}$	Maximal biomass of larva	g
tolerance$_l$	Maximal defense level of host plant, which larva tolerates, larva leaves plant above this threshold	%
F_l	Feeding rate: amount of biomass a larva consumes per g of larval body mass and day	-
U_l	Conversion factor of eaten biomass into larva mass	%
c_{death}	Death - mass relationship of larva	-
R_a	Resource limitation above ground	-
R_b	Resource limitation below ground	-

Table S3: Model parameter used in the individual-based model.

1.3 Process overview and scheduling

For each time step, the processes of above- and belowground resource competition, growth and mortality of each plant are performed. Individual plants first sense the above- and belowground resource qualities of the environment (levels of resource limitation of patches) within their shoot and root ZOIs, the areas (radius) of an individual plant's ZOIs are determined from its current shoot and root biomass correspondingly. When the above- or belowground ZOIs of neighboring plants are overlapping, plants compete only within the overlapping area. Thus, the overlapping area is divided according to the competition mode which reflecting the way of resource division. The growth rate of a plant is determined by the outcome of above- and belowground process, which is restricted by the compartment with minimum resource uptake rate according to growth function. The synthesized biomass is allocated to shoot and root optimally which follows the rule of functional balanced growth. If the biomass of a plant falls below 10 g it is considered dead and removed from the world. The defense production of the plant is calculated and the amount of biomass eaten by the larva infesting the plant (if one is present on the plant). Larvae feed on plant's above-ground biomass proportionally to their own weight.
The state variables of the plants are synchronously updated within the subroutines (i.e. changes to state variables are updated only after all individuals have been processed; [Grimm and Railsback, 2005]), which seems to be the more natural and realistic approach here because time steps are small and competition

is a continuous process.
Larval growth is calculated according to the amount of plant biomass consumed and the host plants' quality (good quality = low defense level of the plant). If a larva reaches its maximal bodymass $B_{l\,\max}$, it begins to pupate, meaning that it is removed from the simulation as it is no longer affecting the other entities. Small larvae are bound to stay on the initial host-plant, however, when a larva has reached a certain age and biomass, it becomes able to switch its host plant. This is done, when the current host plant's defense has reached the threshold value tolerance_l or when the shoot of the host plant has been totally consumed. Larvae can die with a certain probability, which depends on their size and the defense-level of their host plant. If the larva is currently moving in-between plants, it has a maximum chance of dying due to predation.

More complex processes are also explained further in the "sub-models" section. For a given sub-model, entities are processed in a randomized sequence, state variables are updated immediately (asynchronous updating).

The following pseudo-code describes the scheduling of the processes in each time-step:

Listing 1: Pseudo-Code of the main routine of the individual based simulation

```
 For each generation
[
    Set up new generation
    For each tick
    [
                For each plant
                [
                        Plant Mortality?
                        Calculate new biomass of plants:
                            calculate-sizes-of-ZOI
                            calculate-competition-indices
                            potential-plant-growth
                        plant-defense-production
                        smallest-compartment-defines-all
                        self-restriction-of-plant-growth
                        allometric-growth-adjustment
                ]

                For every larva
                [
                        Pupation?
                        larval-growth
                              subtract-larval-damage
                              from host plant above-ground biomass
                        if(defense-level > tolerance or host plant dead)
                        [
                          chose-host-plant
                        ]
                        Larval death?
                          calculate-current-larval-mortality
                ]
    ]
]
```

1.4 Design concepts

Basic principles

The ontogenetic plant growth model has been derived by Lin et al. (2013) from “Metabolic scaling theory” ([Lin et al., 2013]). This model has been combined with the ZOI approach, which means, that the physical space occupied by the plant, where resources necessary for growth can be obtained, is represented as two circles, one above-ground circle to allocate sunlight, one below-ground to allocate water and nutrients.

The ZOIs are also used to calculate competition of neighbouring plants (in the area where the ZOIs of two or more plants overlap). Here the effects of different modes of competition for both above- and below-ground compartment and resource limitations are taken into account.

Adaptation

Some elements in the model implicitly represent adaptation: After being attacked by a larva, plants activate their defense production (after a certain time-delay τ). Therefore a fraction of biomass is allocated to defense and is no longer available for growing. If a larva leaves a plant, defense production ceases after τ time-steps. Mobile larvae can chose at each time-step whether they stay on a host plant or leave and go to another plant. This decision depends on the current defense-level $d_p(t)$ of the host plant. If the defense-level is high this means that larval growth is reduced and mortality increased. However, if a larva switches its host plants, it is more vulnerable (maximum mortality rate) during one time step.

Objectives

Larvae aim to gaining the biomass needed for pupation as fast as possible (pupation occurs when larvae have reached a critical biomass, $B_l(\max)$ which is equal for all larvae). They also need to minimize their risk of dying by choosing whether to stay on a plant or to switch host plants. Plants aim at surviving and maximizing biomass, which can be achieved by defending against larval feeding and by reducing competition by “sending” larvae to neighbor plants. This objectives are not considered explicitly by the plants, but implicitly via the given model rules and assumptions.

Sensing

Larvae can sense the following:

- when a plant is entirely eaten ($B_{\text{above}} \to 0$)
- the defense level $d_p(t)$ of their host plant
- their own biomass and age
- and whether they are developed enough to move between plants (mobile?)

Plants can sense:

- whether a larva is feeding on it
- the availability of resources in its ZOIs (above- and below-ground).

Interaction

Plant-Plant Interaction

Individual plants interact via the shoot and the root competition for resources which is represented by a “two-layer model”.

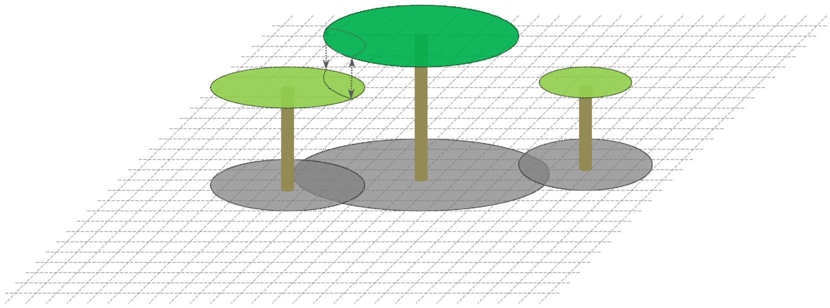


Figure S1: Two Layer Modell with two **Z**ones **O**f **I**nfluence. In green: the above-ground zone, in grey: the below-ground zone.

Plant-Herbivore Interaction

Herbivores feed on plants, this leads to reduced biomass or even plant death. Plants react to this by producing defense compounds and thus increasing their defense-level. The host plant's defense level reduces larval growth rate and increases larval mortality. At a certain threshold tolerance$_l$, the larva leaves the plant and searches a new one, because the advantage gained by leaving outmatches the increased death probability and energy costs during the commuting between plants.

Stochasticity

At the beginning, plants are given random coordinates and larvae are assigned to random plants. When a larvae commutes between plants, the plant where the larva goes is chosen among all plants within the dispersal kernel of the larva. The probability for a plant to be chosen as next host plant is anti-proportional to the plant's distance to the current position of the larva. Each larva dies at each time-step with a certain probability, mortality$_l(t)$ (depending on the quality of its food and its size). All these stochastic elements are introduced to represent variability without representing the underlying mechanisms.

Observation

The following variables (population level) are stored at the end of each generation:

- Mean biomass (below, above and sum of both) of plants
- Number of larvae alive (still in simulation or having successfully pupated)
- Number of larvae which died
- Distribution of τ-values within the plant population (during the course of more generations)
- Number and size distribution of all plants
- Number of larval movements

- "Quality" of larval movements: Distribution of distances between plants, homogeneous or clustered distribution (as well: comparison of initial and end-state of the world)

1.5 Initialization

At initialization, all plants are given random coordinates. Either, the delay times, τ are drawn out of a uniform distribution $\in [0...10 days]$ (for the Genetic Algorithm simulations) or all plants can be given the same value of the delay time τ. The initial above- and below-ground biomasses are set to $30g \pm 3g$.
The herbivores are set randomly on the plants (as default setting only one larva per plant) and their initial body mass is set to $1mg$ which corresponds to the typical weight of a freshly hatched *Manduca sexta* larva (field data).

Agent	Variable	Range	Initial value
Plant	x,y	$\in$ [0, height/width]	random
	B_{above}	$\in [0, 500]$ g	$B0_{\text{above}} = 30$ g
	B_{below}	$\in [0, 500]$ g	$B0_{\text{below}} = 30$ g
	$d_a(t)$	$\in [0, 0.3]$	0
	τ	$\in [0, 10]$ days	uniform distribution $\in$ [0...10]
Larva	age	$\in [0, 35]$ days	0
	B_l	$\in [0, 10]$ g	$B0_l = 1$ mg
	mobile?	yes/no	no
	plant$_l(t)$	0 - max(plant)	random

Table S4: Initial values and typical ranges of the used variables

1.6 Input data

For this model no external input data is needed.

1.7 Submodels

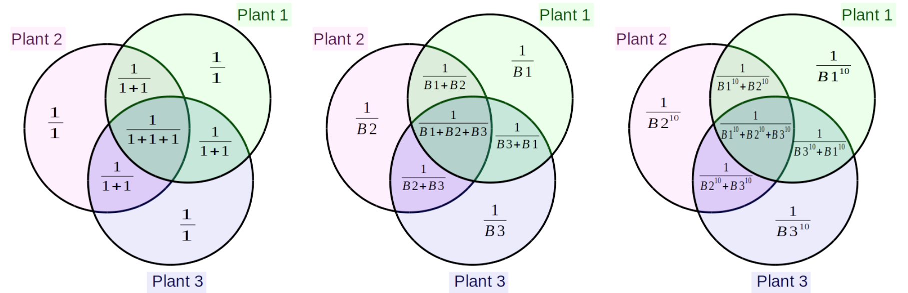
Plant competition

The plant's competition model, and partly also the code implementing them, have been adopted from Lin et al. ([Lin et al., 2013]).

Plant competition is represented using the two-layer ZOI model, which calculates the competition between plants in both layers, thus the root and the shoot, separately. As main idea, each plant is given a circular above- and below-ground zone-of-influence (ZOI) which equals the physical space occupied by this plant where it can obtain the resources necessary for growth. This space is allometrically related to the plant's body mass $B(t)$ (or, to be more precise, B_{above} and B_{below} for both, the root and the shoot compartment).
In the parts in which the ZOIs of two or several plants overlap, plants compete for resources. How much of the resources are taken from one plant depends on the number and sizes of all plants sharing resources of this certain ZOI and the

chosen competition modus. In the TIMELY model, one can chose between 4 competition modi:

- **off** = no competition, all plants get full resources
- **complete symmetry** = resources are divided equally among all plants
- **size symmetric** = resource intake is proportional to the plant's mass
- **allometric size asymmetry** = large plants obtain a disproportionately high share of the resources.



(a) complete symmetry (b) size symmetry (c) allometric size asymmetry

Figure S2: Different modi of plant competition. In all examples, three plants compete for resources in the overlapping areas of their ZOIs.

For our simulations, we used the modus "allometric size-asymmetry" to calculate the competition index for the above-ground ZOI of a plant and the modus "size-symmetric" for the below-ground ZOI of a plant. This reflects that competition for above-ground resources can be pre-emptive (e.g., via shading), which this is not so for below-ground resources.

Plant growth

To calculate the new biomass of the plant (performed at each time step): First, it is calculated how much resources each plant gets (under consideration of inter-plant competition and resource restrictions).Then, if the plant is currently induced, the plant's defense production is subtracted. To ensure that plant growth is restricted to a realistic size, a self-limiting growth term is multiplied which compares the maximal biomass with the current biomass:

$$\Delta GR = \Delta gr \cdot \left[1 - \left(\frac{B(t)}{B_{\max}(t)}\right)^{\frac{1}{4}}\right] \tag{1}$$

The gain of biomass is restricted to the minimal gain of one of both compartments of the plant. To prevent a strongly reduced growth rate because of a very small compartment, the size-differences between above- and below-ground compartment are reduced by adjusting the plant's growth according to the proportions of above- and below-ground ZOIs.

Plant defense production

If plant p is infested by (an) herbivore(s), it allocates, after a certain delay time, τ, a fraction of its biomass production to defense. We call this "the plant is induced". The current amount of defense compounds produced by plant p is calculated with regard to its current gain in biomass and the fraction of newly produced biomass which can be allocated to defense, D_c:

$$\Delta\text{defense}(t) = \Delta gr(t) \cdot D_c \tag{2}$$

For each time-step in which the plant is induced, the costs for producing plant defenses are subtracted from the biomass the plant has produced during that time step. The defense is allocated above- and below-ground, thus both, above- and belowground growth rates are reduced equally. However, as larvae are feeding above-ground they are only affected by defense compounds found in the shoot tissue. A higher defense level leads to increased larval mortality and decreased larval growth rate. The new defense level is calculated as follows: The newly produced defense $\Delta\text{defense}(t)$ is added to the defense compounds which have been already present in time step $t-1$.

$$d_a(t) = \frac{1}{B_{\text{above}}(t)} \Big(\overbrace{d_a(t-1) \cdot B_{\text{above}}(t-1)}^{\text{defense last time step}} + \Delta\text{defense}_a(t) \; - \; \overbrace{F_l \cdot B_l(t) \cdot d_a(t-1)}^{\text{defense eaten by larva}} \Big) \tag{3}$$

With:
F_l = feeding rate (per g) of the larva and $B_l(t)$ = (sum of) mass(es) of larva(e) currently feeding on the plant.

The plant stops being induced after all larvae have left the plant and the additional delay time has passed. This means that the delay time τ delays both, the onset and the offset of defense production.

Priming

In plant defense, priming is a physiological process by which a plant prepares to respond more quickly or aggressively to future biotic or abiotic stress ([Frost et al., 2008]). Priming has not been observed for *Nicotiana attenuata* plants (so, if one plant is induced and produces defense compounds this does not affect its neighbouring plants). Therefore, we did not perform simulations with priming. However, to keep our model general and allow also for simulations of other plant species where priming occurs, we included a priming option which can be switched on or off into our model. If "priming" is activated, each induced plant primes its surrounding plants within a certain radius (for the time of the induction). The delay time of primed plants is halved so that they react faster to herbivore attack.

larval-growth

Larval growth depends on two factors:

1. the amount of consumed biomass during the last time-step
2. the quality (thus defense-level) of their food

When a larva reaches the maximal weight, it leaves the plant to pupate. This means it is set inactive and does not interact with other agents (plants, larvae) any more for the rest of the simulation.

The amount of biomass consumed is proportional to the larva's current body mass:

$$\Delta\text{damage}(t) = \frac{B_l(t) - B_l(t-1)}{U_l} \tag{4}$$

with U_l = conversion factor (how much of the plant's material eaten by a larva is converted into larval mass).

As larvae are feeding on the leaves and stem of the plant, larval damage is subtracted from above-ground plant biomass only. If the plant's above-ground biomass is smaller than the larval damage, the damage is set to the plant's above-ground biomass and the plant is considered as dead.

Larvae are affected by the defense-concentration in the plant tissue; the higher the concentration, the lower their performance, meaning that they show a decreased growth rate and an increased mortality rate. To have a realistic estimate of the influence on plant defense on larval growth curves, we conducted field experiments. Here we placed 30 neonate larvae of *Manduca sexta* on plants which are unable to defend and 30 individuals on maximally defended plants. The masses (in g) were measured every second day and the mean of the masses of all larvae raised on defenseless plants and the mean of all larvae raised on maximally defended plants were plotted against their age in days. We found the following mass - age relationships for larvae raised on defenseless plants vs larvae raised on maximally defended plants respectively:

$$\text{Defenseless\_Formula} : B_l(t) = \exp(-8.355) \cdot \text{age}_{\text{nodef}}(t)^{5.856} \tag{5}$$

$$\text{MaxDefense\_Formula} : B_l(t) = \exp(-6.329) \cdot \text{age}_{\text{def}}(t)^{4.661} \tag{6}$$

In the model, the maximum defense level tolerated by the larva is $\text{tolerance}_l = 0.24$, a larva feeding on a plant with this defense-level would show a typical growth curve as shown in equation 6. In comparison to that, a larvae feeding on a completely undefended plant (defense-level = 0) would show a performance as described in equation 5. As the model plants are in most cases neither fully induced nor totally undefended, we mixed both fit functions to obtain a realistic estimation of larval growth, according to the host plant's current defense-level.

Larva-choose-new-host-plant

Larvae are considered mobile when they reach a certain body mass and age. This corresponds to the field observations that only larvae of an instar >=3rd instar are capable to cover larger distances. At each time-step, all mobile larvae have the possibility to change their host plants. Moving comes at the costs of higher death probability of the larva (for one time-step). The larvae switch their host plant for two reasons:

- the host plant's defense level $d_a(t)$ excesses the value tolerance_l
- the host plant has been totally consumed

For moving, the next host plant is chosen randomly from all plants within the dispersal kernel of the larva. Here the probability of a plant to be chosen scales negatively with the exponential of the distance to the larva's current position. The commuting time is set (independently of the next plant's position) to one tick, which means that the larvae cannot, for the length of one tick, consume plant biomass and thus do not gain weight. To keep the model simple, moving does not cost energy.

Larval-death

Each larva has a state variable "mortality$_l(t)$" $(0 \ldots 1)$ which indicates the probability of dying during the next tick and which is updated at the end of each time-step. For every larva a random number $z \in [0 \ldots 1]$ is drawn and compared to the variable "mortality$_l(t)$". If it is smaller, the larva dies and is removed immediately from the world. A larva which is on plant (P_i) with defense-level $Def(P_i)$ has the following mortality "mortality$_l(t)$ for the next time step (1/6 day):

$$\text{mortality}_l(t) = \frac{(\text{death coefficient} + 1.5 \cdot \text{Def}(P_i) - 0.1)/6}{1 + log(\text{biomass}_{\text{larva}}) \cdot exp(1)} \tag{7}$$

The default death coefficient is set to 0.25. When a larva switches plants it is more exposed to predators (spiders, ants, lizards) which are present on the soil surrounding the plants. Therefore it is given a mortality penalty which depends on the distance the larva travels. The further the larva moves, the higher the mortality:

$$\text{mortality}_l(t) = \frac{\text{death coefficient} + (\text{distance} * 1.5/\text{movement}_{\text{radius}})/6}{1 + log(\text{biomass}_{\text{larva}}) \cdot exp(1)} \tag{8}$$

Genetic algorithm

Genetic algorithms (GAs) work by generating a random population of solutions to a problem, evaluating those solutions and then using cloning, recombination and mutation to create new solutions to the problem. For this model, we have written a simple genetic algorithm by ourselves. The simulation runs for 300 generations of 400 plants. For the first generation, the τ-value of each plant is drawn from a uniform distribution $\in$ [0...10 days]. We supposed that the plants with the largest biomass have the largest fitness values. Therefore, for each following generation, the heritable trait, thus the delay times, τ of plants are chosen proportionally to the total biomass of plants that had this value of τ at the end of the preceding generation. Additionally, a mutation is included (every resulting genotype is randomly added a number $\in [-3, 3]$.) This has been done to avoid being trapped in local minima.

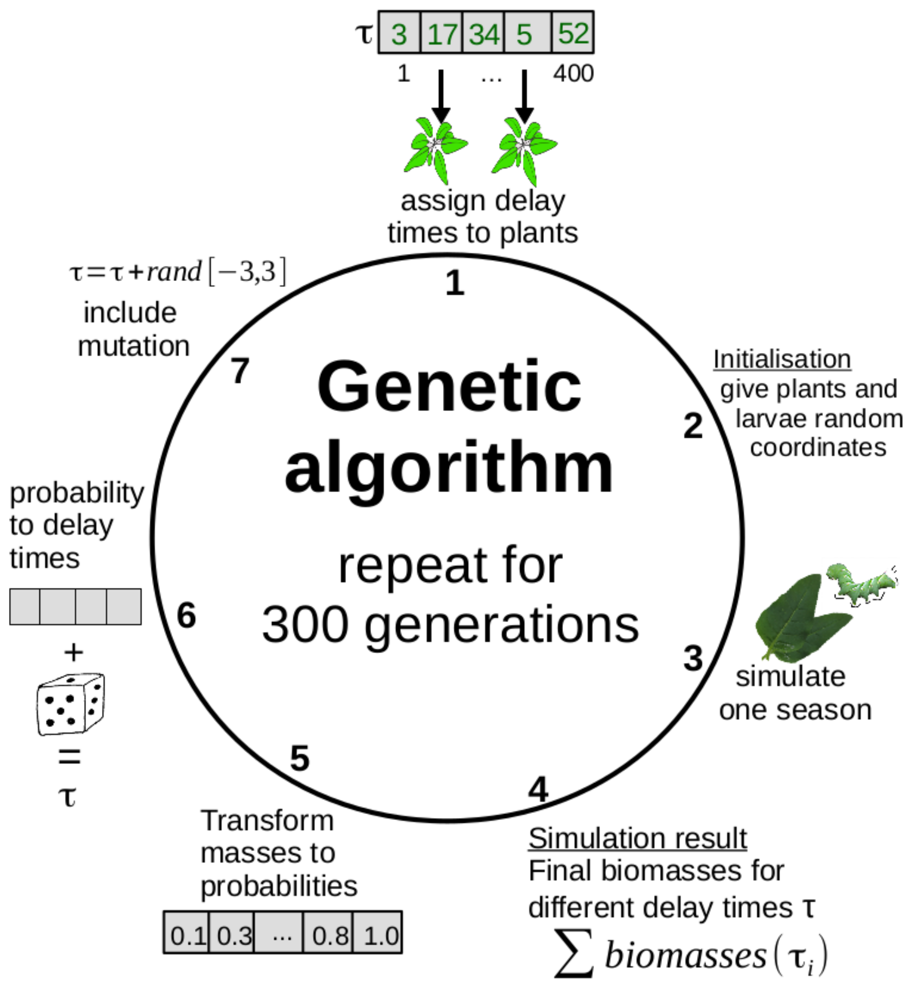


Figure S3: Flow chart of the genetic algorithm used to detect optimal values of delay times $\tau \in [0, 10]$.

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