Supplementary Material

Delayed chemical defense: timely expulsion of herbivores reduces competition with neighboring plants (The American Naturalist)

Pia Backmann[1,2,3,*], Volker Grimm[1,2], Eckhard Finke[4], Gottfried Jetschke[5], Yue Lin[6], Matthijs Vos, Ian T. Baldwin[3] and Nicole M. van Dam[1,4]

June 28, 2018

[1]German Centre for Integrative Biodiversity Research (iDiv) Halle-Jena-Leipzig, 04103 Leipzig, Germany
[2]Helmholtz Centre for Environmental Research-UFZ, Department of Ecological Modelling, Permoserstr.15, 04318, Leipzig, Germany
[3]Max-Planck-Institute for Chemical Ecology (MPI-CE), Beutenberg Campus, 07743 Jena, Germany
[4]Friedrich-Schiller-University Jena, Institute of Ecology, 07743 Jena, Germany
[5]Münster University of Applied Science, Department of Mechanical Engineering, Stegerwaldstraße 39, 48565 Steinfurt, Germany
[6]Scion, Private Bag 3020, Rotorua, New Zealand
[7]Ruhr-Universität Bochum, Theoretical and Applied Biodiversity Research, Universitätsstraße 150, 44780 Bochum, Germany

[*]Correspondence author: Pia Backmann, Email: pia.backmann@tu-dresden.de

Contents

1 Figures and tables of the Supplementary Material

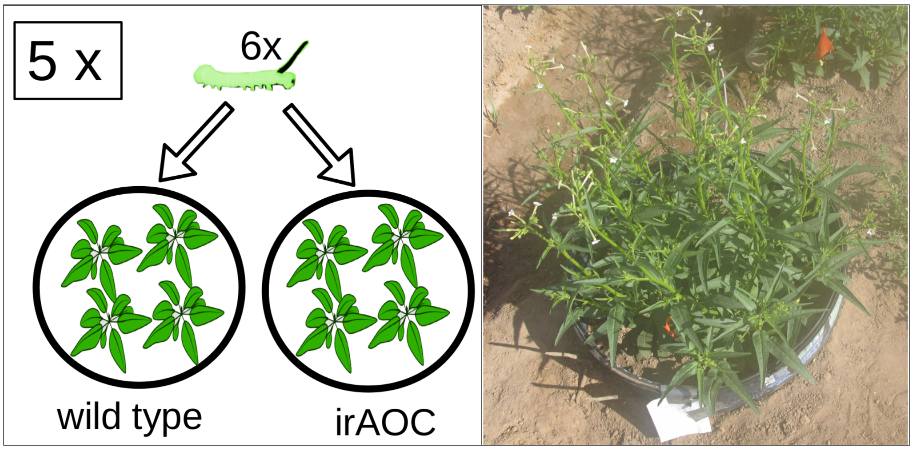


Figure S1: Left: Field experiment setup. The weight trajectories of *M. sexta* caterpillars on well defended (wild type) and low defended (irAOC) plants were measured. 30 freshly hatched 1st instar larvae were placed per plant line, six larvae per plant quadruplet. In one plant quadruplet, four plants of the same type (well defended or low defended) were planted. Each quadruplet was protected by a fluon-sprayed plastic ring of 40 cm height. The ring should prevent both, caterpillar escape and arthropod (lizard) feeding on caterpillars. Caterpillars were protected by a clip-cage for the first five days and could afterwards move freely between the plants of one quadruplet. The instar and weights of the caterpillars were recorded regularly. Right: a photo of one plant quadruplet with surrounding plastic ring.

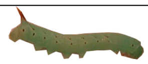
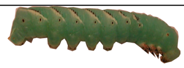
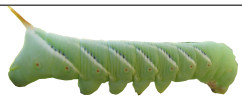
Instar	**Photo**	**Starting weight in mg**		**Age in days**	
		high defense	low defense	high defense	low defense
1.		1	1	1-6	1-5
2.		40±5	50±5	7-10	6-8
3.		130±10	150±10	11-15	9-11
4.		900±25	1100 ±30	16-20	12-16
5.		2000±40	2500 ±50	21-?	17-21

Table S1: Results of field experiment on growth (observed starting weight of different instars) and development (age of transition to next instar) of larvae growing on wild plants (high defense levels) and on plants which are unable to produce defense compounds (low defense).

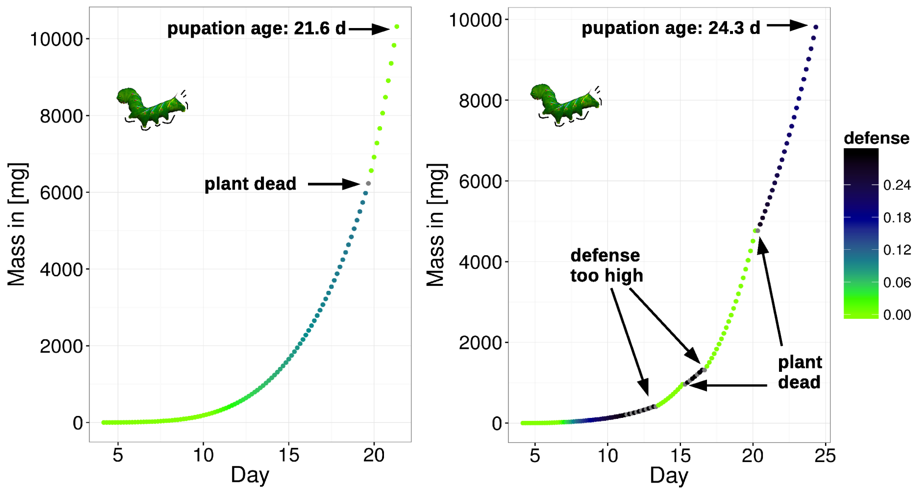


Figure S2: Simulation result: The weight of a single larva during one simulation plotted over time. The colors of the points show the defense-level of the larva's current host plant. Black/dark blue means, that the host plant has produced a large amount of defense compounds, green means that the plant is relatively defenseless. Arrows indicate death of the larva or moving of the larva to another plant. The reason for switching (either the host plant defense level has raised too high [defense-level > 0.24] or the host plant has been eaten) are indicated in the figure. Pupation age of the larva is noted as well. (a): a larva encountering host plants with low defense-levels; (b) a larva encountering both well and low defended host plants. Please note that in the simulations as in the field, about 2/3 of all larvae die before pupation.

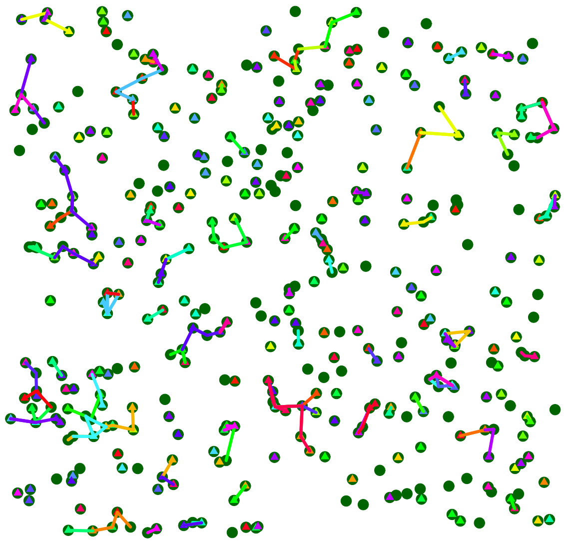


Figure S3: Movement trajectories of larvae during one simulation of 30 days, with 300 larvae and 400 plants. When a larva switches a plant, the probability to chose a plant decreases exponentially with distance. Plants are symbolized by dark green circles. Each line with a different color represents a different larva. At the beginning of the simulations, larvae were distributed randomly on the plants (the initial position of each larva is shown with a triangle), all further movement is shown by a line. When a line is present it means that at a larva moved at least once between both plants, repeated movement can be possible, too.

Test	Where to find	Options tested	Main findings
Larval mobility	Fig. ST24 (TRACE)	- immediately - at a certain age	**no significant effect**
Oviposition time	Fig. S7	- synchronously - in waves - continuously	**lower delay times if not in waves**
Larval movement pattern	Figs. ST8 – ST13 (TRACE) and ST23 (TRACE)	- $\frac{1}{\text{distance}}$ - $\frac{1}{\exp(\text{distance})}$	**effect on defense level and larval mortality**
Larval dispersal radius	Tabs. ST3, ST5 (TRACE) Figs. ST33 and ST35 (TRACE)	- 0.7 m - 4.7 m - 6.7 m	**shorter radius = higher larval mortality**
Plant density	Figs. S5 and S6	- 200 plants/225 m^2 - 300 plants/225 m^2 - 400 plants/225 m^2 - 500 plants/225 m^2	**lower density = higher delay times**
Plant growth rate	Tab. ST3 (TRACE) Figs. ST25 – ST32 (TRACE)	- 20% of energy - 80% of energy - 100% of energy	**no effect on mean(τ) higher growth rate = higher productivity**
Interplant competition	Fig. S4	- no competition - above & below	**mean(τ) $\to$ 0 when no competition**
Plant defense investment	Fig. S5	- no investment - 10% investment - 20% investment - 30% investment - 40% investment	**low investment = shorter delay times**

Table S2: Robustness analysis for testing the generality of the model. Data underlying this table are deposited in the Dryad Digital Repository, Data package title: Data from: Delayed chemical defense: timely expulsion of herbivores can reduce competition with neighboring plants, Journal: The American Naturalist, DOI: doi:10.5061/dryad.gh2m22t (Data from [Backmann et al., 2018])

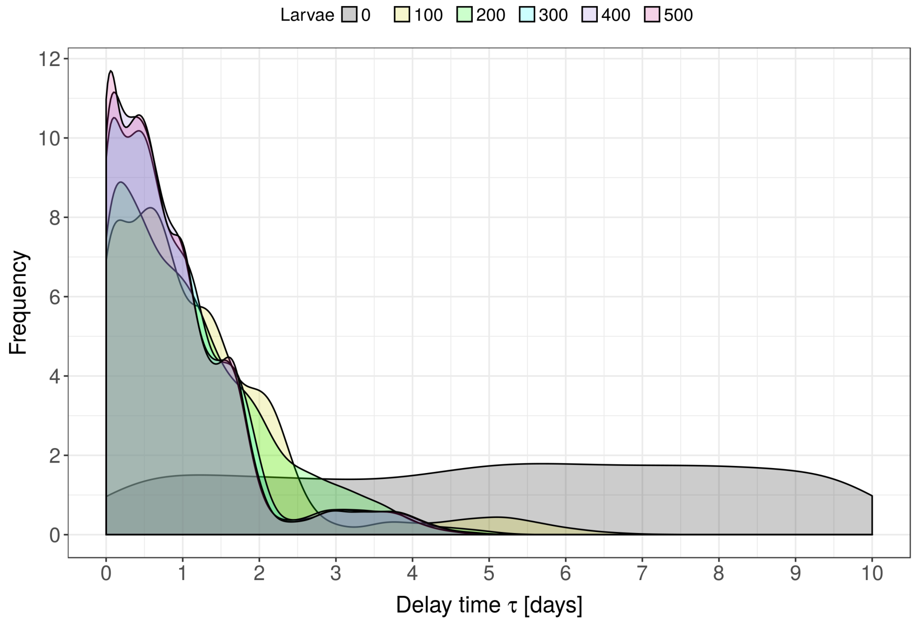


Figure S4: Simulations without inter-plant competition for resources: final frequencies of delay times τ for different initial numbers of larvae. The genetic algorithm started with randomly assigned delay times of the plants ($\tau \in [0, 10]$ days) in the first generation and ran for 300 generations.

Fig. S5 shows that if more energy of the plant is invested into defense allocation, optimal delay times are higher. This can be explained by the fact that the total delay between the insect's attack and plant's reaction (until an adequate defense level is produced) is the sum of both: the plant's delay time and the time needed for defense compound production. The latter takes longer if the plant can only allocate a small proportion of its energy into defense production. Therefore plants with weak defense production show shorter optimal delay times τ.

	mean(tau)	sd(tau)	mean(mass)	sd(mass)
default	4.7	2.4	57.0	3.6
alwaysmobile	5.2	2.7	48.1	5.1
fraction_0	3.7	2.6	53.1	1.8
fraction_10	0.9	0.8	59.6	1.6
fraction_20	1.8	1.6	61.0	2.8
fraction_40	6.1	2.0	54.7	3.5
200 plants	7.5	1.0	84.8	4.6
300 plants	7.0	1.0	66.4	2.4
400 plants	4.7	2.4	57.0	3.6
500 plants	3.5	2.2	48.1	3.0

Figure S5: We tested the influence of different parameter variations on the outcome of the genetic algorithm (the mean delay time τ after 300 generations). The first row of the table shows the default case of simulations with 400 plants and 300 larvae. In the second row we tested a simulation in which larvae were able to switch between plants all the time and not only when having reached the third instar. In rows 3 - 7 we tested different percentages of total allocation to defense production. In rows 8-11 we compared different plant densities.

We tested which optimal delay times would evolve for different plant densities. Here it shows that lower plant densities lead to higher delay times with smaller variance (Fig. S4). The explanation for this is that lower plant densities result in both: A) reduced inter-plant competition and B) higher herbivore loads (as we simulated with the fixed number of 300 larvae per simulation). The lower the herbivore load, the lower the pressure to optimize the defense reaction - therefore higher plant numbers have a greater variance of possible delay times (Fig. S6). For higher plant numbers, the herbivore load of the single plant becomes smaller which results in a less specialized defense reaction of the plants. This shows that for our model results the herbivore load is more important than the severity of competition. However, competition still is an important co-factor. We tested in Fig. S4 which mean delay times would evolve (by using the GA) without inter-plant competition. It shows that in that case the shortest possible delay time would be favored by evolution. Therefore, plants only have to delay their response when being challenged by both, herbivore attacks and strong inter-plant competition.

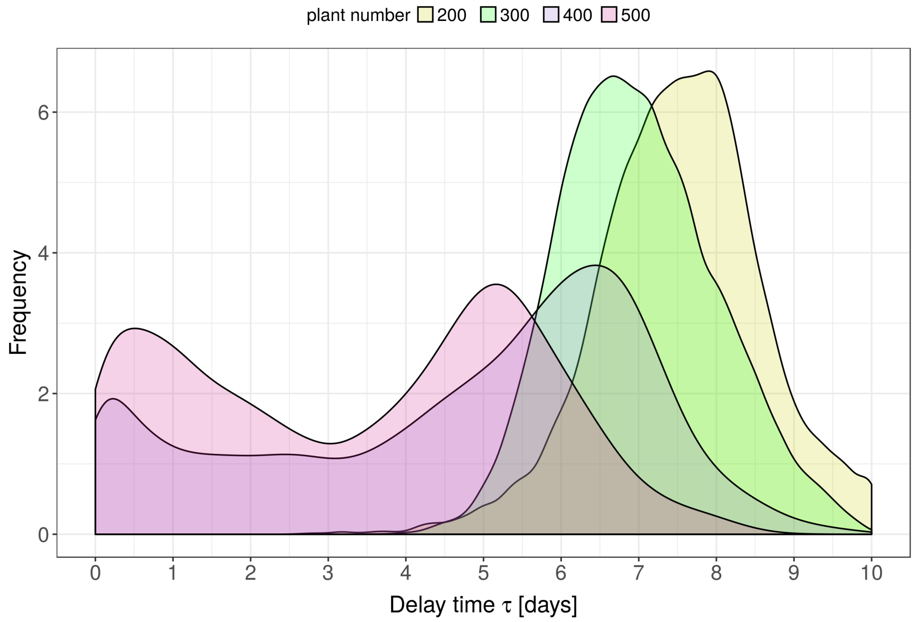
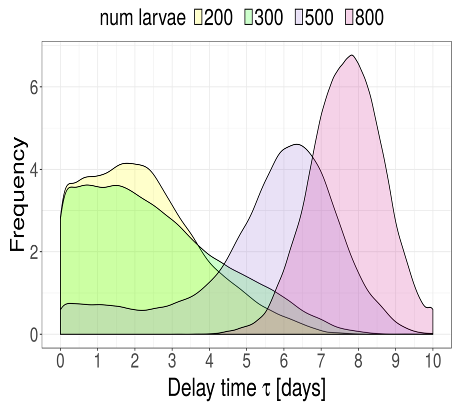
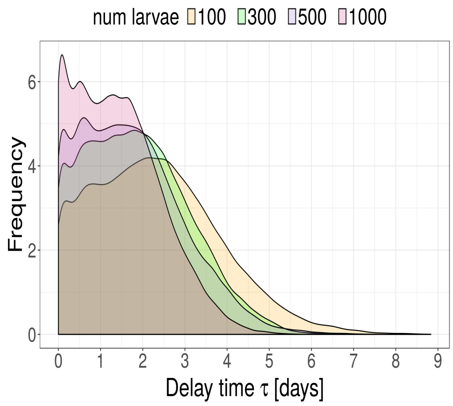


Figure S6: Result of the genetic algorithm (distribution of delay times among the plants of the 300th generation) for simulations with different plant densities (from 200 – 500 plants). Lower densities lead to higher delay times. Hereby, lower plant densities mean A) less inter-plant competition and B) more larvae per single plant (as the number of larvae was set constant for all densities). It seems as if B) has the largest effect on the optimal defense time, as the resulting curves of low plant densities have sharper peaks (less variance).

For the *Manduca*-*Nicotiana* system all plants germinate synchronized after a fire and *Manduca* moths reach the plants in larger groups at a certain time. However, in order to generalize the model we also included (and tested) the case for unsynchronized germination and larvae which are put on the plants at different times (Fig, S7). The results show that longer delay times are beneficial for plants as long as herbivores attack the plants in waves (we tested one or two waves). If herbivores arrive continuously on the plant, no beneficial effect of longer delay times could be measured. However, insect outbreaks (or waves) are a common phenomenon and not exclusively restricted to the *N. attenuata* – *M. sexta* system ([Myers, 1988], [Crawley et al., 1983], [Berryman et al., 1987], [Poorter et al., 1989], [Berryman, 1996], [Bjørnstad et al., 2002]).



(a) oviposition in waves



(b) continuous oviposition

Figure S7: Result of the genetic algorithm (distribution of delay times among the plants of the 300th generation) for different oviposition modes. Left figure: simultaneous oviposition in two waves. Here, for each wave half of the total number of larvae was put simultaneously on randomly chosen plants. Two consecutive waves happened with 14 days delay. Right figure: continuous oviposition.

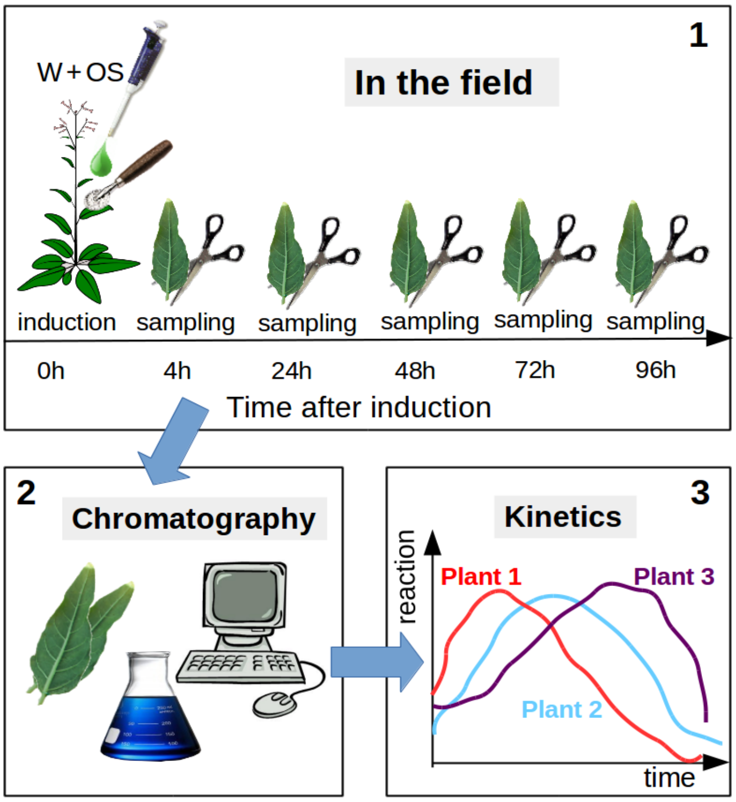


Figure S8: Measurement of the kinetics of plant reaction after induction with W+OS (wound + oral secretion): divide the plants into unelicited (control) plants and plants, where one leaf is elicited with W+OS (use a pattern wheel to produce three rows of holes on each side of the mid vein of the leaf, then apply 20 mL of larval oral secretion (OS) to the wounds) to simulate herbivory. Leaves of control and elicited plants are harvested at 0, 4, 24, and 48, 72 and 96 h after elicitation, and control samples were taken simultaneously from untreated plants. Leaf samples are analyzed by chromatography for defense compound concentrations. As a result, we can determine for every plant the temporal development of certain defense compound accumulations (e.g. DGTs, phenolics, terpenes). Hence, we can calculate the variation of delay times within a natural plant population. The corresponding analyses are in progress [05/2018].

2 ODD* of the TIMELY model

2.1 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.

2.2 Entities, state variables, and scales

The entities in the model are plants, larvae and patches. All state variables are given in table SO1.

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 SO1: 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.Plants are also characterized by there circular "zone-of-influence" (ZOI),

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

which are derived separatelely from the above- and below-ground biomass (see below).

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. The latter is due to the fact, that 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. However, switching plants as well comes to a cost, more energy is needed and the probability of being predated rises significantly when being on the ground. Normally, larvae tend to chose plants in the neighbourhood as new host plants. We represented this behaviour by a dispersal kernel decreasing inversely proportional with the distance to the former host plant.

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 SO2: 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 SO3: Model parameter used in the individual-based model.

2.3 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.

All the processes mentioned above will be 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
                ]
    ]
]
```

2.4 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".

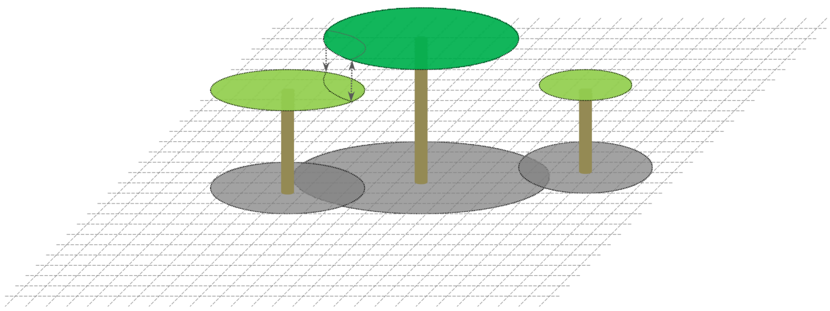


Figure SO1: Two Layer Modell with two **Z**ones **O**f **I**nfluence. In green: the above-ground zone, in grey: the below-ground zone.

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, $\text{mortality}_l(t)$ (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)

2.5 Initialization

When being initialized, 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 SO4: Initial values and typical ranges of the used variables

2.6 Input data

For this model no external input data is needed.

2.7 Submodels

All subsections here represent sub-models which are implemented in the code of the model as functions.

Create plants [number_plants]

Set up a new generation
The simulation runs for 300 generations of plants. For each generation, 400 plants are created and given random x and y coordinates. It is supposed that the plants with the largest biomass have the largest fitness values, therefore the genotypes of plants are chosen proportionally to their total biomass at the end of the preceding generation. For the first run, the τ-value of each plant is drawn from a uniform distribution $\in$ [0...10 days]. The larvae are distributed randomly on the plants (when possible maximal one larva per plant).

Plant Mortality?

A plant with a shoot biomass of $B_{\text{above}}(t) <= 10$ is considered as dead and are removed immediately and the larva feeding on this plant switches to another plant if it is mobile, if not it dies.

Calculate plant biomass

Plant growth is calculated 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 an 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. In the parts in which the ZOIs of two or several plants overlap, plants compete for resources.
Additionally, if a plant is currently in the "defense" modus (triggered by a feeding herbivore on the plant), a certain fraction of the plant's available energy is put into defense compound production, which reduces the plant's growth rate.

The above-ground biomass of the plant is also reduced by larval feeding if the plant is currently infested by an herbivore.

In the following subsections, the different modules (functions) of the simulation program are explained in the order in which they are executed. The name of the subsection-captions correspond to the function names in the code. The plant's growth and competition model, and partly also the code implementing them, have been adopted from Lin et al. ([Lin et al., 2013]).

calculate-sizes-of-ZOI (above and below-ground)
The plant's ZOIs (for both, root and shoot) are represented by circles within which resources necessary for growth can be accessed by the plant. 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). "Allometric" means that the relationship between plant density N (of a population) and mean biomass of the surviving plants, M, can be described by a power law: $M = c_0 \cdot \gamma$. With: c_0 = growth constant. We use the exponent $\gamma = -4/3$.
This relationship leads to the area $A_{\text{ZOI}(p)}(t)$ obtained by a single plant, p:

$$A_{\text{ZOI}(p)}(t) = c_0 \cdot B_p(t)^{3/4} \tag{1}$$

calculate-competition-indices (above and below-ground)
Each ZOI of a plant is given a competition index ($C_a(t)$ for above-ground and $C_b(t)$ for below-ground) showing the proportion of the plant's resource intake of all the resources available of this ZOI. It can take values between 1 (the plant gets all resources within this patch) and 0 (plant receives no resources).
It depends on the number and sizes of all plants sharing resources of this certain ZOI and the chosen competition modus.

The equations shown below are valid for above- and below-ground compartment ($C_a(t)$ and $C_b(t)$), however, to keep the ODD simple, we here demonstrated the calculation for the competition index $C(t)$ of one unspecified ZOI:

- **Competition modus: "off"**
  Each plant p receives all resources available within its ZOI:

$$C(t)(\text{ZOI of plant p}) = 1 \ \ \forall p$$

- **Competition modus: "complete symmetry"**
  Ressources of patches shared by several plants are divided equally among all plants:

$$C(t)(\text{ZOI of plant p}) = \sum_{i=1}^{N} \frac{1}{N} \cdot \left(1/\sum_{j=1}^{M} (1) \right)$$

  with N = number of patches in ZOI, M = number of plants sharing the current patch.

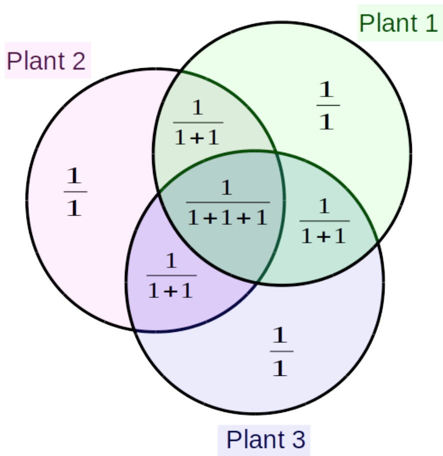


Figure SO2: **Complete size symmetric competition**. Each plants gets in the areas where its ZOI is overlapped by the ZOI(s) of other competing plants an equal share of the resources available.

- **Competition modus: "size symmetric"**
  Each plant's share of resource intake is directly proportional to the plant's mass:

$$C(t)(\text{ZOI of plant p}) = \sum_{i=1}^{N} \frac{1}{N} \cdot \left(B_p/\sum_{j=1}^{M} B_j \right)$$

  with N = number of patches in ZOI, M = number of plants sharing the current patch and B_j = biomass of competing plant j (including biomass of plant p in the center).

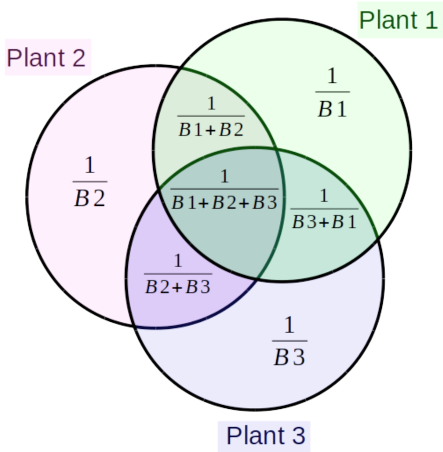


Figure SO3: **Size symmetric competition**. Here, each plants obtains, in the areas where its ZOI is overlapped by the ZOI(s) of other competing plants, a share of resources which is proportional to its size.

- **Competition modus: "Allometric size asymmetry"**
  Bigger plants obtain a disproportionately high share of the resources within the overlapping area of the ZOIs:

$$C(t)(\text{ZOI of plant p}) = \sum_{i=1}^{N} \frac{1}{N} \cdot \left(B_p^{10} / \sum_{j=1}^{M} B_j^{10} \right)$$

  with N = number of patches in ZOI, M = number of plants sharing the current patch and B_j = biomass of plant j (including biomass of plant p).

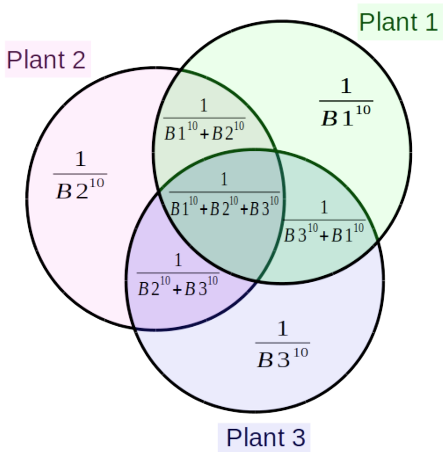


Figure SO4: **Allometric size asymmetric competition**. Bigger plants obtain a disproportionately high share of the resources within the overlapping area of the ZOIs.

We distinguished between several different competition modi, all modi were

tested for calibration purposes.
For the final 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.The same settings were used by Lin et al. (2013); they reflect the general notion that competition for above-ground resources can be pre-emptive (e.g., via shading), which this is not so for below-ground resources.

potential-plant-growth
Restrictions in resource availabilities, R_a and R_b, within the plant's above- and below-ground ZOIs reduce the potential growth rate of the current plant and are taken into account.
Both, R_a and R_b are $\in$ [0...1] (with 0 = no resources available and 1 = all resources available) and are kept as constant values for the whole simulation.

Above-ground growth rate of a plant:

$$\Delta gr_{\text{above}}(t) = A_{\text{ZOI}_a}(t) \cdot R_a \cdot C_a(t) \cdot c0_a \tag{2}$$

Below-ground growth rate of a plant:

$$\Delta gr_{\text{below}}(t) = A_{\text{ZOI}_b}(t) \cdot R_b \cdot C_b(t) \cdot c0_b \tag{3}$$

with $c0_a$ = growth constant for above-ground growth and $c0_b$ = growth constant for below-ground growth and $C_a(t)$ and $C_b(t)$ as competition indices for both above- and belowground compartment.

Especially in the later stages of plant growth, the wild tobacco is challenged by more and more severe water shortages in the below-ground compartment. Therefore the resource limitation R_b is set to a higher value (more limitation) for the below-ground compartment than in the aboveground compartment.

plant-defense-production
If plant p is infested by herbivores, it allocates a certain fraction of its biomass production to defense, therefore its growth rate is reduced. The current amount of defense compounds produced by plant p is calculated with regard to its current gain in biomass, $\Delta gr_{\text{above}}(t)$ and $\Delta gr_{\text{below}}(t)$, its individual time-delay τ_p and the fraction of newly produced biomass which can be allocated to defense, D_c.
For above-ground:

$$\Delta\text{defense}_a(t) = \Delta gr_{\text{above}}(t) \cdot D_c \cdot \text{sign}\left(\text{MEMORY}_p\left[t - \tau_p\right]\right) \tag{4}$$

And below-ground:

$$\Delta\text{defense}_b(t) = \Delta gr_{\text{below}}(t) \cdot D_c \cdot \text{sign}\left(\text{MEMORY}_p\left[t - \tau_p\right]\right) \tag{5}$$

With:

$$\text{sign}(x) = \left\{ \begin{array}{ll} 1 & \text{if } x > 0 \\ 0 & \text{otherwise} \end{array} \right\} \tag{6}$$

The ”memory“ array, MEMORY_p [ ] of plant p stores in each element $\in [1...\text{tickmax}+\tau_p]$ the sum of all masses of larvae which have been present on the plant at the corresponding time-step t of the simulation:

$$\text{MEMORY}_p\,[t] = \sum_{i=0}^{L(t)} B_l(i,t) \tag{7}$$

with $L(t)$ = number of larvae present on plant p at time step t, $B_l(i,t)$ = current body mass of larva i . The array has the length of all ticks + the delay-time τ_p of plant p (see Fig. SO5).

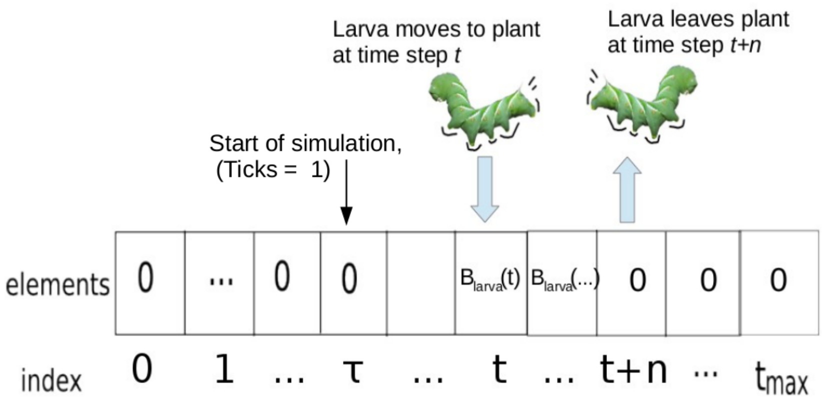


Figure SO5: "Memory" of the plant: The presence of larvae on the plant is recorded at every time-step in an array containing in each of its element the sum of the current biomass of all larvae present (at a certain time-step).

This means that the defense is induced when at time-step $t - \tau_p$ there has been at least one larva feeding on the plant.
We chose this quite complex representation of the plant's memory to be able to modify the representation of the plant defense production for test purposes and in later publications. It is very likely that a plant reacts not only, when a larva is feeding, but also to the quantity of the feeding load.

The costs for producing plant defenses (which are zero, if the plant is currently not induced and 0.3 of the plant's growth if the plant is induced) are subtracted from the biomass produced in this time step:

$$\Delta gr_{\text{above}} = A_{\text{ZOI}_a}(t) \cdot R_a \cdot C_a(t) \cdot c0_a \cdot (1 - \Delta\text{defense}_a) \tag{8}$$

$$\Delta gr_{\text{below}} = A_{\text{ZOI}_b}(t) \cdot R_b \cdot C_b(t) \cdot c0_b \cdot (1 - \Delta\text{defense}_b) \tag{9}$$

The defense is allocated above- and below-ground, thus both, above- and belowground growth rates are reduced equally.

smallest-compartment-defines-all
The growth rate of the limitating compartment (with minimal resource uptake)

is used as growth rate of the whole plant:

$$\Delta gr(t) = \begin{cases} 2 \cdot \Delta AGR & \text{if } \Delta AGR < \Delta BGR \\ 2 \cdot \Delta BGR & \text{if } \Delta AGR > \Delta BGR \end{cases} \tag{10}$$

self-restriction-of-plant-growth
As the plants have to provide higher maintenance costs when the plant's biomass is bigger, there is a maximal biomass for plants, $B0_{\max}$. This value is the maximal biomass a plant can attain under "perfect" conditions, meaning that there is no resource shortage ($R = 1$ and no plant-plant competition, thus $C(t) = 1$). To deduce from the artificial value $B0_{\max}$ the maximal biomass the plant can maintain under realistic conditions (at the specific time-point) ,$B_{\max}(t)$, resource shortages and competition are added:

$$B_{\max}(t) = B0a_{\max} \cdot (C_a(t) \cdot R_a)^4 + B0b_{\max} \cdot (C_b(t) \cdot R_b)^4 \tag{11}$$

Thus, to ensure that plant growth is restricted to this realistic size, a self-limiting growth term is multiplied which compares the maximal biomass with the current biomass, $B(t) = B(t-1) + 2 \cdot \min(\Delta gr_{\text{above}}, \Delta gr_{\text{below}})$:

Self-restricted above-ground growth, ΔAGR:

$$\Delta AGR = \Delta gr_{\text{above}} \cdot \left[1 - \left(\frac{B(t)}{B_{\max}(t)}\right)^{\frac{1}{4}}\right] \tag{12}$$

Self-restricted below-ground growth, ΔBGR:

$$\Delta BGR = \Delta gr_{\text{below}} \cdot \left[1 - \left(\frac{B(t)}{B_{\max}(t)}\right)^{\frac{1}{4}}\right] \tag{13}$$

allometric-growth-adjustment
Above-ground and below-ground growth is determined by the proportion of the sizes above- and belowground ZOIs. To prevent a strongly reduced growth rate because of a very small compartment the plant aims to reduce the size-differences between root and shoot by allometric growth plasticity:

$$\Delta B_{\text{above}}(t) = \frac{\Delta gr(t) \cdot \Delta BGR^{\frac{3}{4}}}{\Delta AGR^{\frac{3}{4}} + \Delta BGR^{\frac{3}{4}}} \tag{14}$$

$$\Delta B_{\text{below}}(t) = \frac{\Delta gr(t) \cdot \Delta AGR^{\frac{3}{4}}}{\Delta AGR^{\frac{3}{4}} + \Delta BGR^{\frac{3}{4}}} \tag{15}$$

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

Amount of consumed food
The amount of biomass consumed is proportional to the larva's current body mass. The bigger the larvae is the more it can consume (if plant material is still

available).

Food quality
If a larva feeds on a plant with a high defense-level, the elevated concentration of toxins is negatively correlated to larval growth. The less defended a plant, the better the larval performance.

Field experiment data
To have a realistic estimate of larval growth curves (depending on the quality, thus the defense level of its host plant) we conducted field experiments were 30 individuals of *Manduca sexta* were placed on plants being unable to defend and 30 individuals were placed on maximally defended plants as neonates. 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.
Implementation in the model - calculate-larval-growth
We used this data to calibrate larval growth.
We found the following mass - age relationships for larvae raised on defenseless plants vs larvae raised on maximally defended plants respectively:

$$\text{Defenseless\_Formula} : B_l(t) = \exp(-8.355) \cdot \text{age}_{\text{nodef}}(t)^{5.856} \tag{16}$$

$$\text{MaxDefense\_Formula} : B_l(t) = \exp(-6.329) \cdot \text{age}_{\text{def}}(t)^{4.661} \tag{17}$$

For calculating the new larval mass at each time-step , we used the fit of the measured growth-curves (see Fig. 2 of main document) given in equations 16 and 17 as "extreme values".
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. According to the current larval mass, $B_l(t)$, we used two different x-values, so-called "ages" of larvae in both equations, they are calculated as following:

$$\text{age}_{\text{nodef}}(t-1) = \big(B_l(t-1) \cdot \exp(8.355)\big)^{1/5.856} \tag{18}$$

$$\text{age}_{\text{def}}(t-1) = \big(B_l(t-1) \cdot \exp(6.329)\big)^{1/4.661} \tag{19}$$

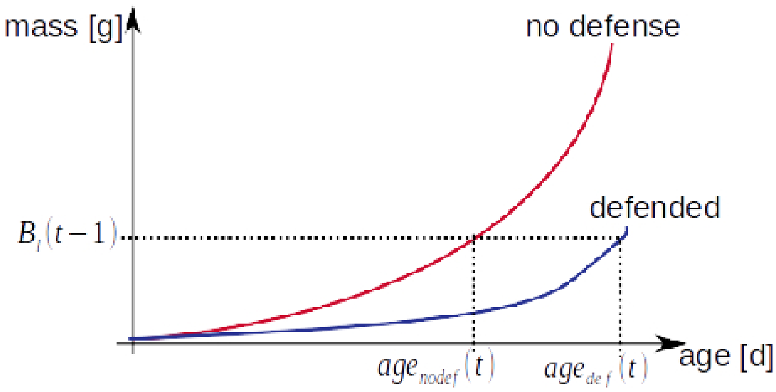


Figure SO6: The calculation of both larval ages.

Then, for both ages, the time passed the last tick is added:

$$\text{age}(t) = \text{age}(t-1) + 1\text{ tick} = \text{age}(t-1) + 1/6\text{ day} \tag{20}$$

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 17. In comparison to that, a larvae feeding on a completely undefended plant (defense-level = 0) would show a performance as described in equation 16.

To calculate the potential growth of a larva feeding on a plant with an intermediate defense-level, the following formula has to be applied:

$$B_l(t, d_a(t)) = \frac{(\text{tolerance}_l - d_a(t))}{\text{tolerance}_l} \cdot \text{Defenseless\_Formula} + \frac{d_a(t)}{\text{tolerance}_l} \cdot \text{MaxDefense\_Formula} \tag{21}$$

with: $d_a(t)$ = current above-ground defense-level of the host plant and tolerance_l, the maximum defense level tolerated by the larva.

One can e.g. see that if the plant has a current defense level of $d_a(t) = 0$, the Defenseless_Formula is applied to 100 % – if on the other hand the plant defense is maximal, the MaxDefense_Formula is used to 100%.

calculate-larval-damage
Larval damage is calculated according to the current mass of the larva and the biomass of the current host plant.

Potential damage caused by the larva:

$$\Delta\text{damage}(t) = \frac{B_l(t) - B_l(t-1)}{U_l} \tag{22}$$

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

$$\text{damage}(t) = \begin{cases} \min\left[\Delta\text{damage}(t), B_{\text{above}}(t)\right] & \text{if larva on host plant} \\ 0 & \text{if larva not on host plant} \end{cases} \tag{23}$$

The calculated, potential larval damage is taken from the plant's above-ground biomass $B_{\text{above}}(t)$. If $B_{\text{above}}(t) < \text{damage}(t)$, the damage is set to B_{above} and the plant is considered as dead with zero above-ground biomass. Larval damage is subtracted from above-ground plant biomass only, as larvae are feeding only on above-ground parts of the plant. If the larva is moving to another plant in the current time step, no damage is calculated.

Complete growth equation
To summarize, to calculate the new biomass of the plant, first the restrictions in resource availability are considered, then the plant-plant competition is included and plant's defense production subtracted. As last step, the self-restriction in plant growth is considered and the gain of biomass is restricted to the minimal gain of one of both compartments of the plant and 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.

Additionally, if a larva currently is feeding on the plant, the produced damage by the larva is subtracted from the gain in biomass of the above-ground compartment:

$$B_{\text{above}}(t) = B_{\text{above}}(t-1) + \Delta B_{\text{above}}(t) - \text{damage}(t) \tag{24}$$

$$B_{\text{below}}(t) = B_{\text{below}}(t-1) + \Delta B_{\text{below}}(t) \tag{25}$$

Calculate-plant-defense-level

The current above-ground defense-level in a plant ($d_a(t) \in [0...0.3]$) is calculated at each time step when the new biomass of the plant has been calculated. Only the defense concentration of the shoot is calculated, because the larvae are feeding above-ground only and thus are affected only by defense compounds found in the shoot tissue. The fraction of the above-ground biomass which has been newly allocated to defense in time step t (see page 22, equation 4), $\Delta\text{defense}_a(t)$, is added to the defense compounds which have been already present in time step $t-1$. The amount of defense compounds being eaten by the larva is subtracted:

$$d_a(t) = \frac{1}{B_{\text{above}}(t)} \Big(\overbrace{d_a(t-1) \cdot B_{\text{above}}(t-1)}^{\text{defense last time step}} + \Delta\text{defense}_a(t) - \overbrace{F_l \cdot B_l(t) \cdot d_a(t-1)}^{\text{defense eaten by larva}} \Big) \tag{26}$$

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.

A higher defense level leads to increased larval mortality and decreased larval growth rate.

Pupation?

When a larva reaches the maximal weight, $B_l(\text{max})$ 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.

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

Apart from that the larvae stay put.

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):

$$\text{mortality}_l(t) = \frac{(\text{death coefficient} + 1.5 \cdot \text{Def}(P_i) - 0.1)/6}{1 + log(\text{biomass}_{\text{larva}}) \cdot exp(1)} \tag{27}$$

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:

$$\text{mortality}_l(t) = \frac{\text{death coefficient} + (\text{distance} * 1.5/\text{movement}_{\text{radius}})/6}{1 + log(\text{biomass}_{\text{larva}}) \cdot exp(1)} \tag{28}$$

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.

3 Genetic algorithm

Genetic algorithms (GAs) are a biologically-inspired computer science technique that combine notions from Mendelian genetics and Darwinian evolution to search for good solutions to problems. The GA works 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 plants. For the first generation a population of plants with random τ values is created. For each following generation, 400 plants are created and 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. As result, the distribution of genotypes for every generation is recorded and the biomasses of all plants, the number of dead plants and larvae at the end of the simulation.

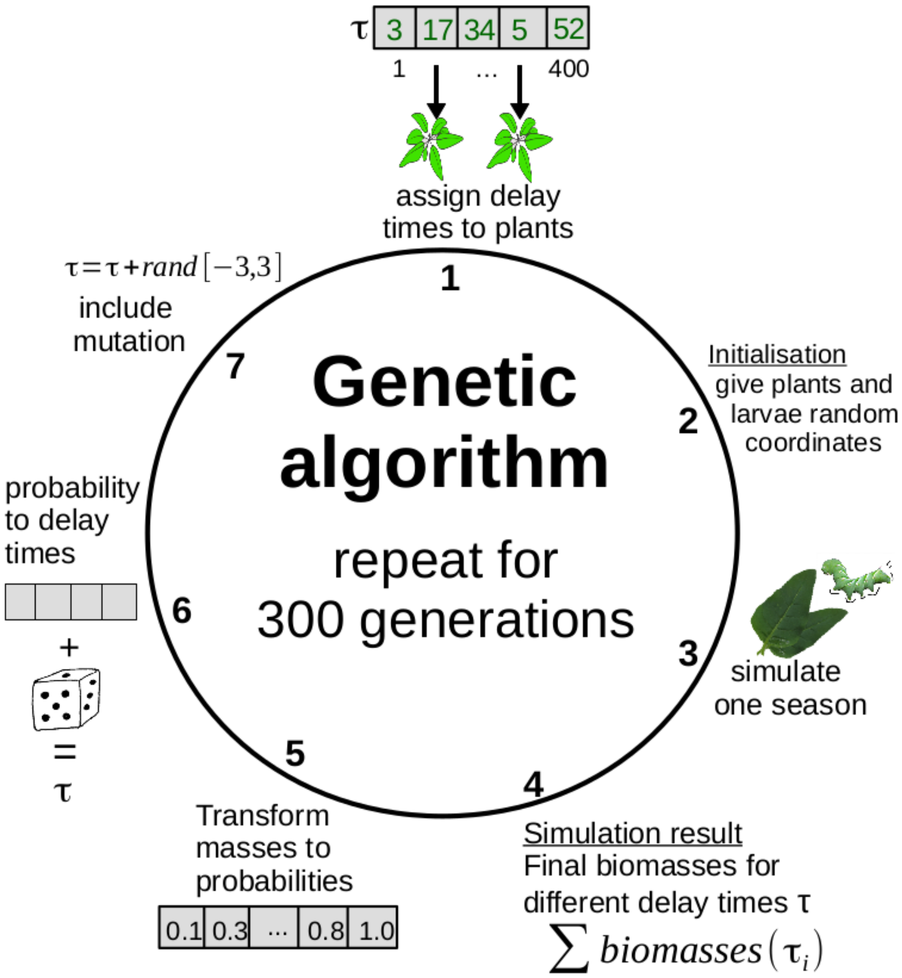


Figure SO7: Flow chart of the genetic algorithm used to detect optimal values of delay times $\tau \in [0, 10]$.

We tested the development of the τ- distribution within the plant population for different plant and herbivore densities.

Test for frequency of τ values
In our simulations, we found that for each herbivore density, a different delay time τ was optimal. The distribution of τ values within one population sharpened over the number of generations. For higher herbivore pressure, the distribution of τ values was sharper than for low herbivore pressures. We assumed that the distribution itself (and not only the mean value of τ) was an important feature. To test whether this was a stable outcome we repeated the GA with all plants given the same value of τ for the first generation. The chosen τ was the resulting optimum after 300 generations of GA. We then compared the curve and sharpness of the resulting distribution with the curve of the 300th generation after a random initialization.

References

[Backmann et al., 2018] Backmann, P., Grimm, V., Finke, E., Jetschke, G., Lin, Y., Vos, M., Baldwin, I. T., and van Dam, N. (2018). Data from: Delayed chemical defense: timely expulsion of herbivores can reduce competition with neighboring plants. *The American Naturalist*.

[Berryman, 1996] Berryman, A. A. (1996). What causes population cycles of forest lepidoptera? *Trends in Ecology & Evolution*, 11(1):28–32.

[Berryman et al., 1987] Berryman, A. A. et al. (1987). The theory and classification of outbreaks. *Insect outbreaks.*, pages 3–30.

[Bjørnstad et al., 2002] Bjørnstad, O. N., Peltonen, M., Liebhold, A. M., and Baltensweiler, W. (2002). Waves of larch budmoth outbreaks in the european alps. *Science*, 298(5595):1020–1023.

[Crawley et al., 1983] Crawley, M. J. et al. (1983). *Herbivory. The dynamics of animal–plant interactions.* Blackwell Scientific Publications.

[Frost et al., 2008] Frost, C. J., Mescher, M. C., Carlson, J. E., and De Moraes, C. M. (2008). Plant defense priming against herbivores: getting ready for a different battle. *Plant physiology*, 146(3):818–824.

[Grimm et al., 2010] Grimm, V., Berger, U., DeAngelis, D. L., Polhill, J. G., Giske, J., and Railsback, S. F. (2010). The odd protocol: a review and first update. *Ecological modelling*, 221(23):2760–2768.

[Grimm and Railsback, 2005] Grimm, V. and Railsback, S. F. (2005). Individual-based modeling and ecology:(princeton series in theoretical and computational biology).

[Lin et al., 2013] Lin, Y., Berger, U., Grimm, V., Huth, F., and Weiner, J. (2013). Plant interactions alter the predictions of metabolic scaling theory. *PloS one*, 8(2):e57612.

[Myers, 1988] Myers, J. H. (1988). Can a general hypothesis explain population cycles of forest lepidoptera? *Advances in Ecological Research*, 18:179–242.

[Poorter et al., 1989] Poorter, H. et al. (1989). Interspecific variation in relative growth rate: on ecological causes and physiological consequences. *Causes and consequences of variation in growth rate and productivity of higher plants*, 24:45–68.