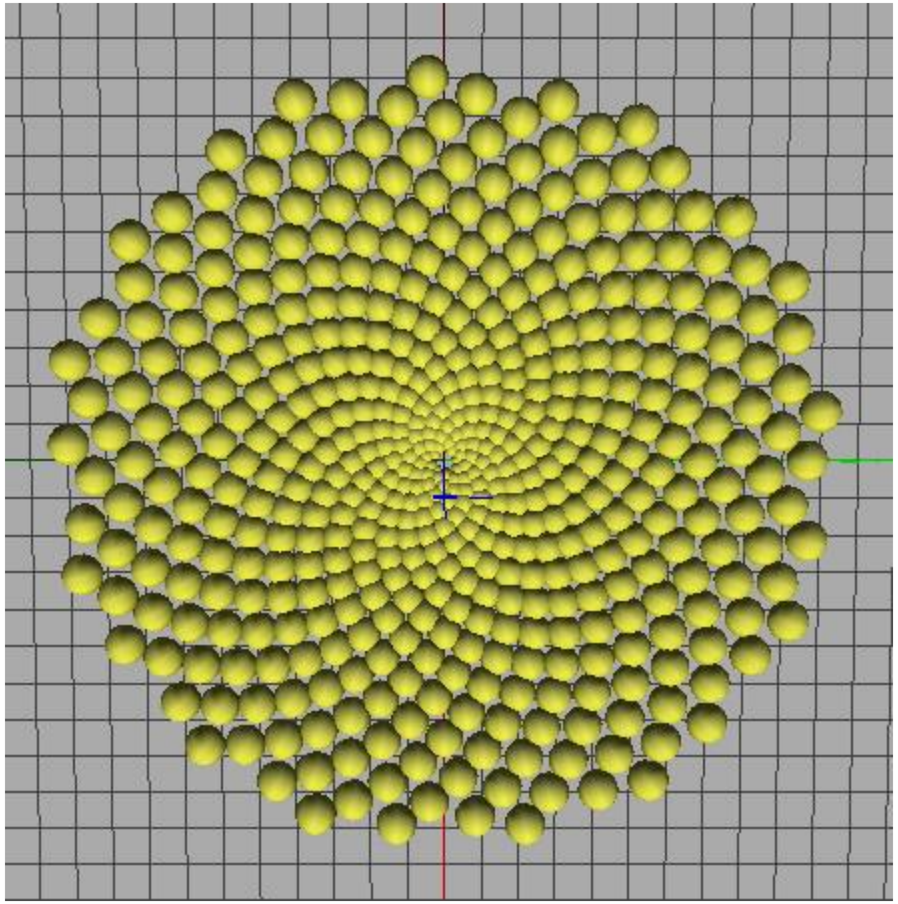
MWS 3+4

dr Wojciech Pałubicki

Modelowanie procesów biologicznych

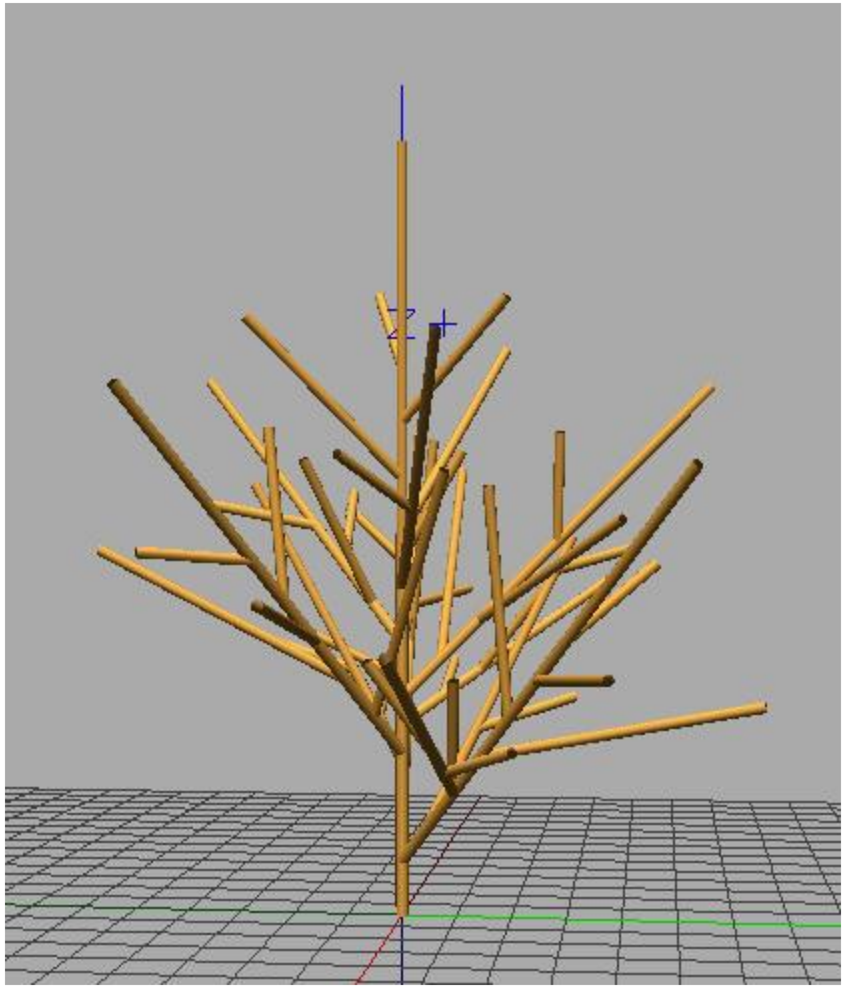
- **Model**: uproszczony opis świata
  - Za pomocy narzędzi analitycznych (matematyka, języki programistyczne)

Model Słonecznika

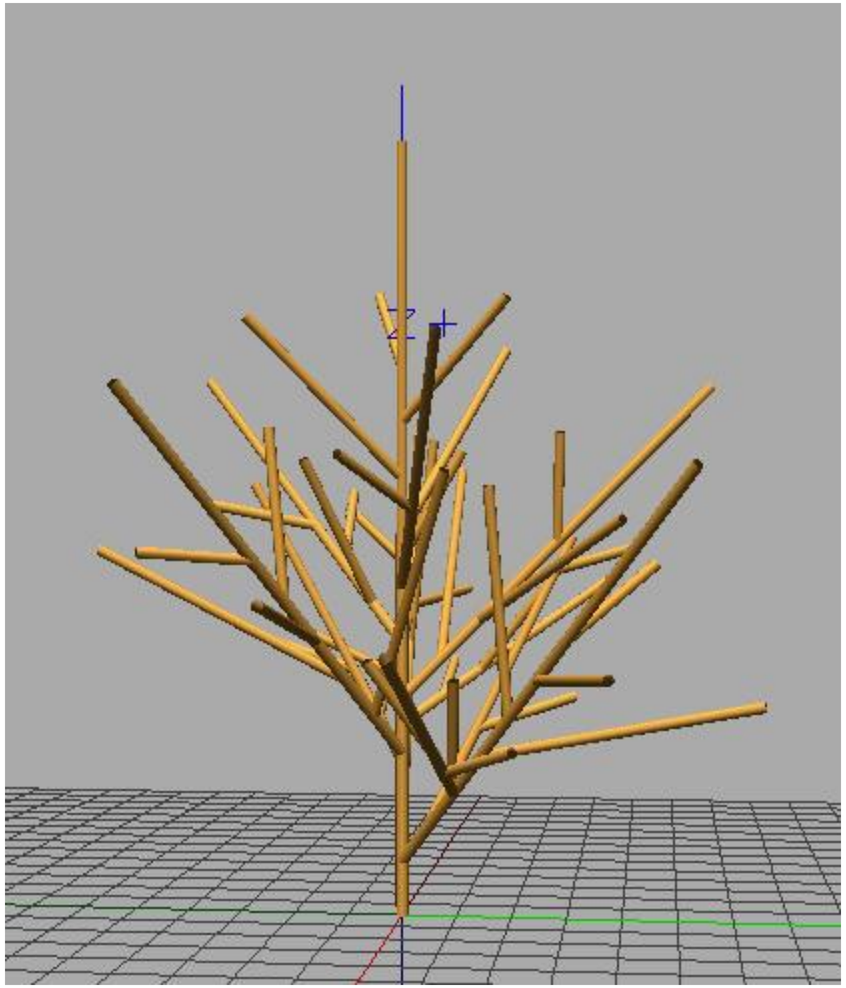


Fibonacci, 137.5

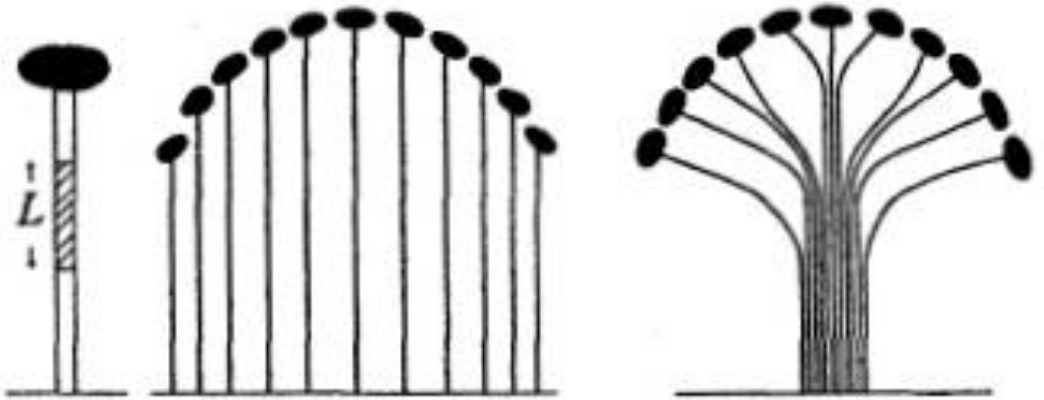
Tree Model (Fibonacci spiral)



Trunk thickness

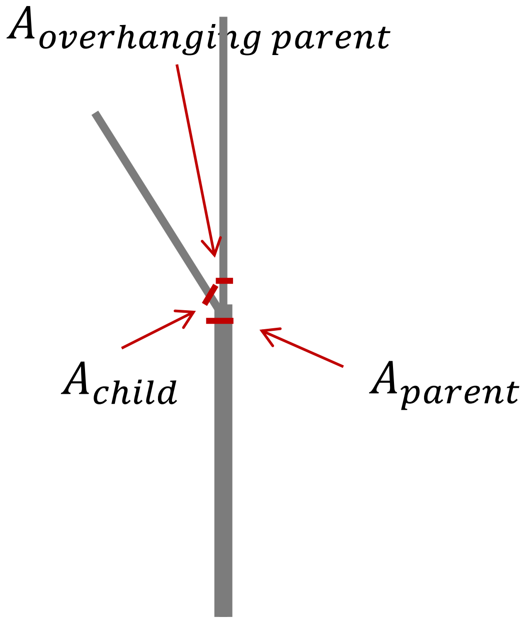


Pipe model

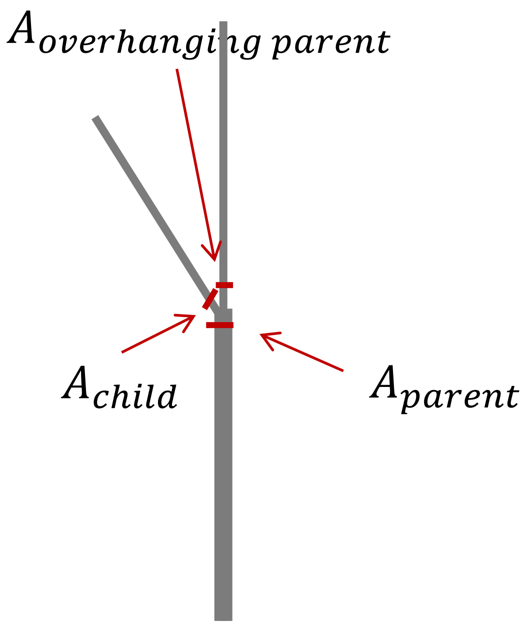


Shinozaki et al. 1964

Pipe model

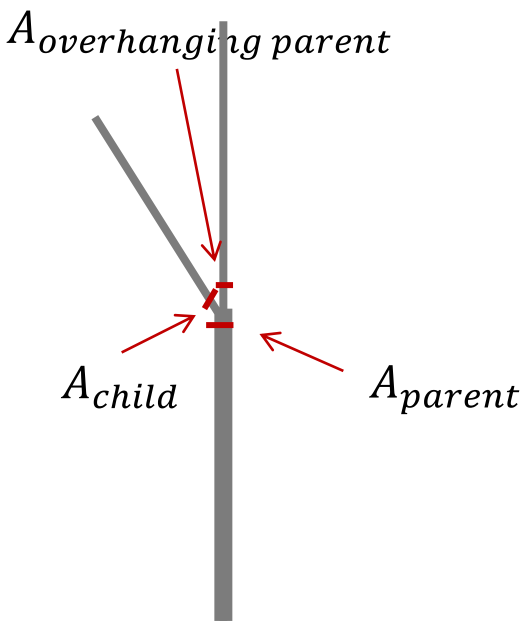


Pipe model



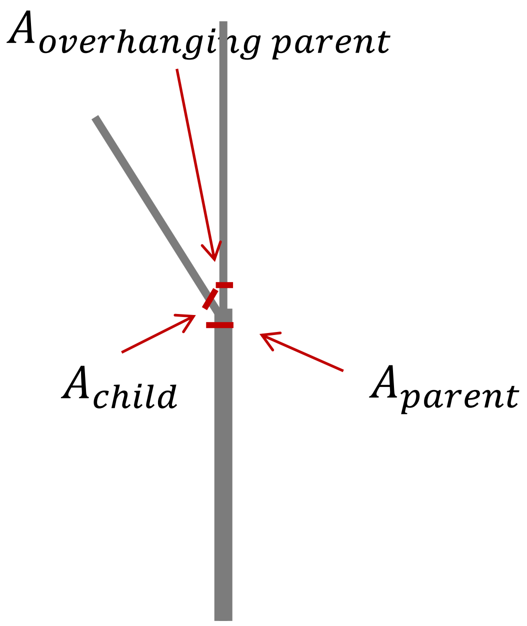
$$A_p = A_c + A_{op}$$

Pipe model



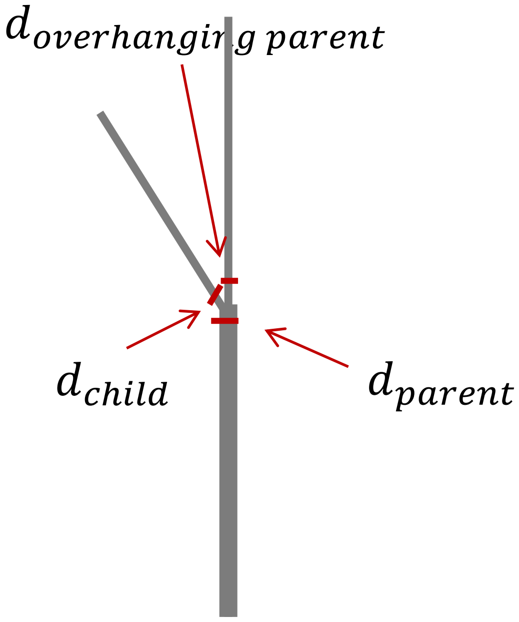
$$\pi r_p^2 = \pi r_c^2 + \pi r_{op}^2$$

Pipe model



$$r_p^2 = r_c^2 + r_{op}^2$$

Pipe model



$$d_p^n = d_c^n + d_{op}^n$$

$$n \in [1,3]$$

Context-sensitive L-Systems

$S < F \rightarrow E$ F stanie się E, jak stoi przed S

$F > S \rightarrow E$ F stanie się E, jak stoi za S

$T < F > S \rightarrow E$ F stanie się E, jak stoi przed T i za S

Context-sensitive L-Systems

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$$
\begin{array}{lll}
\omega & : & baaaaaaaa \\
p_1 & : & b < a \quad \rightarrow b \\
p_2 & : & \qquad\; b \quad \rightarrow a
\end{array}
$$

Context-sensitive L-Systems

S **<** F → E F stanie się E, jak stoi przed S

F **>** S → E F stanie się E, jak stoi za S

T **<** F **>** S → E F stanie się E, jak stoi przed T i za S

$baaaaaaaa$

$$\begin{aligned}
\omega &: \quad baaaaaaaa \\
p_1 &: \quad b < a \quad \rightarrow b \\
p_2 &: \quad \phantom{b <{}} b \quad \rightarrow a
\end{aligned}$$

Context-sensitive L-Systems

S < F → E F stanie się E, jak stoi przed S

F > S → E F stanie się E, jak stoi za S

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$$\begin{aligned} \omega &: \quad baaaaaaaa \\ p_1 &: \quad b < a \quad \rightarrow b \\ p_2 &: \quad \phantom{b<{}} b \quad \rightarrow a \end{aligned}$$

$baaaaaaaa$
$abaaaaaaa$

Context-sensitive L-Systems

S < F → E F stanie się E, jak stoi przed S

F > S → E F stanie się E, jak stoi za S

T < F > S → E F stanie się E, jak stoi przed T i za S

$$
\begin{aligned}
\omega &: \quad baaaaaaaa \\
p_1 &: \quad b < a \quad \rightarrow b \\
p_2 &: \quad\quad\;\; b \quad \rightarrow a
\end{aligned}
$$

$$
\begin{array}{l}
baaaaaaaa \\
abaaaaaaa \\
aabaaaaaa \\
aaabaaaaa \\
aaaabaaaa \\
\ldots
\end{array}
$$

Context-sensitive parametric L-Systems

$$A(x) < B(y) > C(z): \quad x + y + z > 10 \rightarrow E\left(\frac{x+y}{2}\right)F\left(\frac{y+z}{2}\right)$$

Context-sensitive parametric L-Systems

$$A(x) < B(y) > C(z): \quad x + y + z > 10 \rightarrow E\left(\frac{x+y}{2}\right)F\left(\frac{y+z}{2}\right)$$

$$\ldots A(4)B(5)C(6) \ldots$$

Context-sensitive parametric L-Systems

$$A(x) < B(y) > C(z): \quad x + y + z > 10 \rightarrow E\left(\frac{x+y}{2}\right) F\left(\frac{y+z}{2}\right)$$

$$\dots A(4)B(5)C(6) \dots$$

$$4 + 5 + 6 > 10$$

Context-sensitive parametric L-Systems

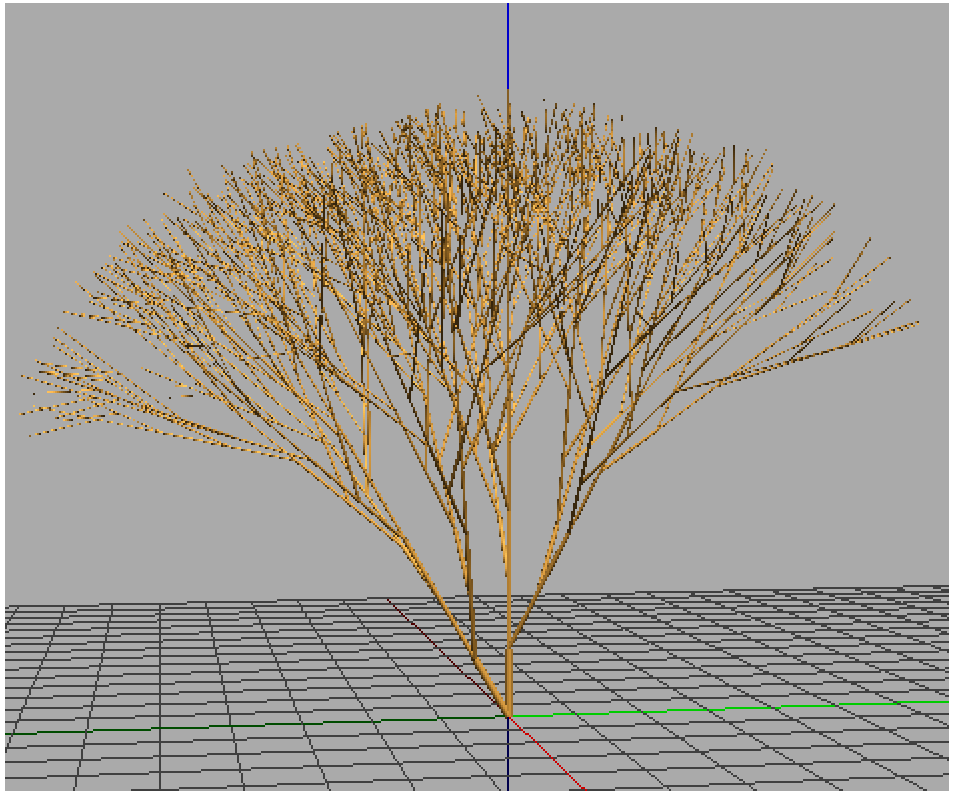
$$A(x) < B(y) > C(z): \quad x + y + z > 10 \rightarrow E\left(\frac{x+y}{2}\right)F\left(\frac{y+z}{2}\right)$$

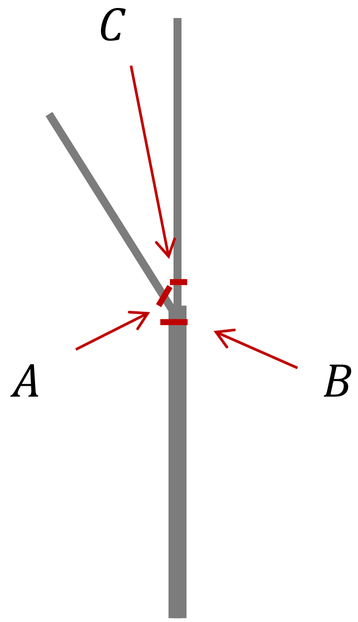
$$\dots A(4)B(5)C(6)\dots$$

$$4 + 5 + 6 > 10$$

$$B(5) \rightarrow E(4.5)F(5.5)$$

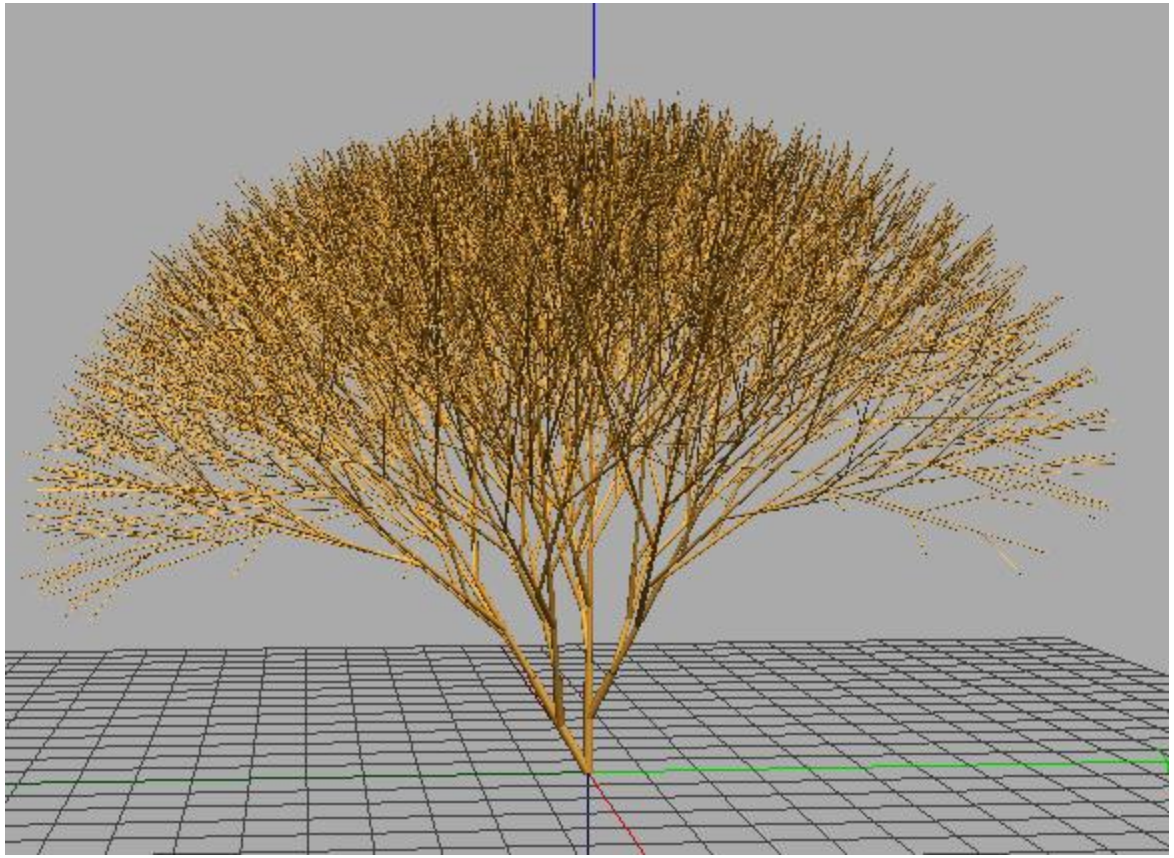
Context-sensitive pipe model



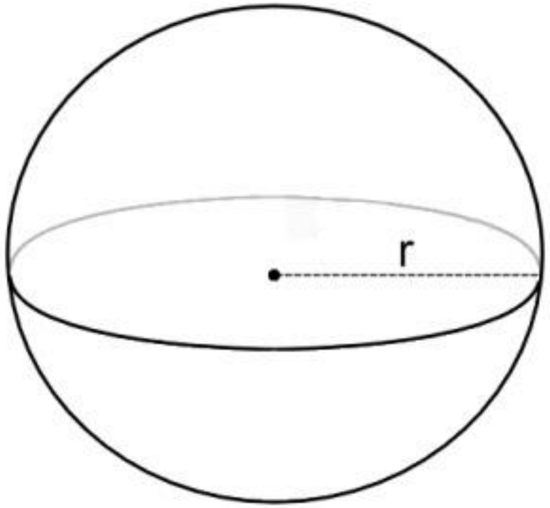


$$B(d_p) > [A(d_c)]C(d_{op}) \rightarrow d_p^n = d_c^n + d_{op}^n$$

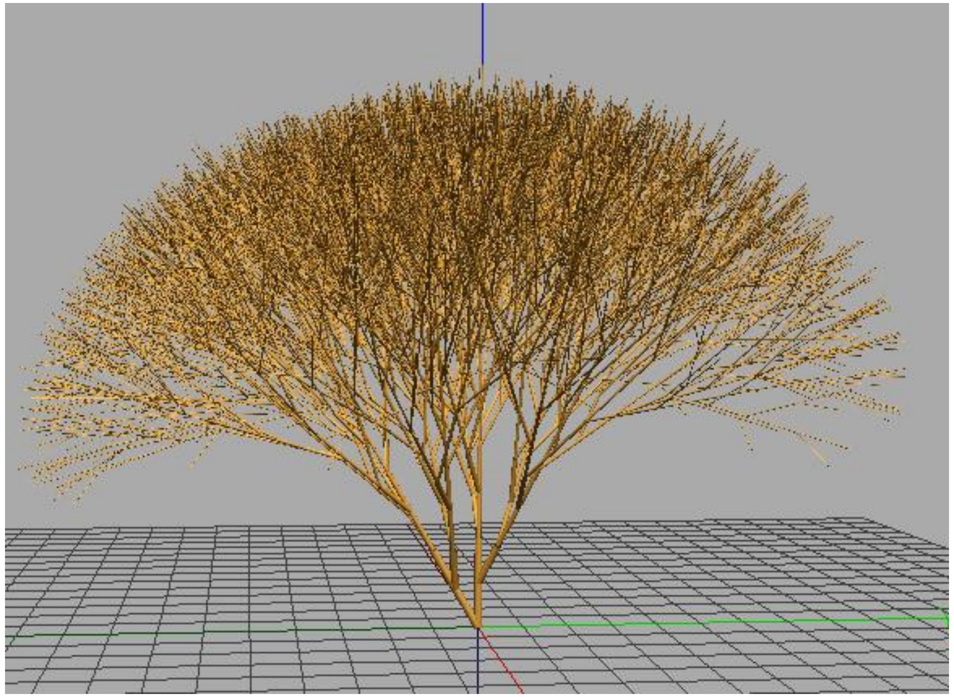
Za gęsta struktura drzewiasta



Przestrzeń i L-System



Objętość kuli ~ r^3

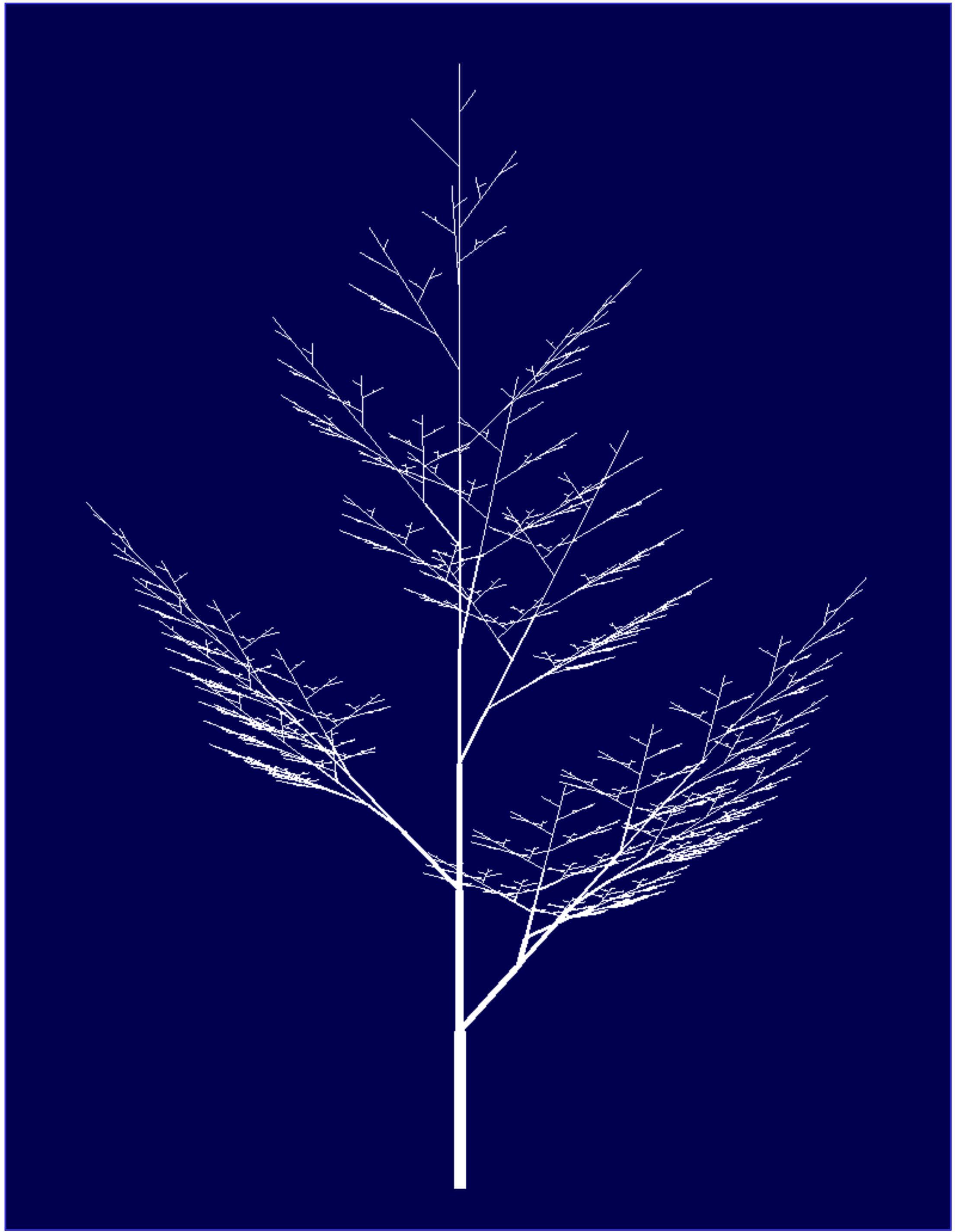


Liczba gałęzi ~ 2^r

Modelowanie drzew

First 3D tree model

Hisao Honda 1971



Recursive tree models

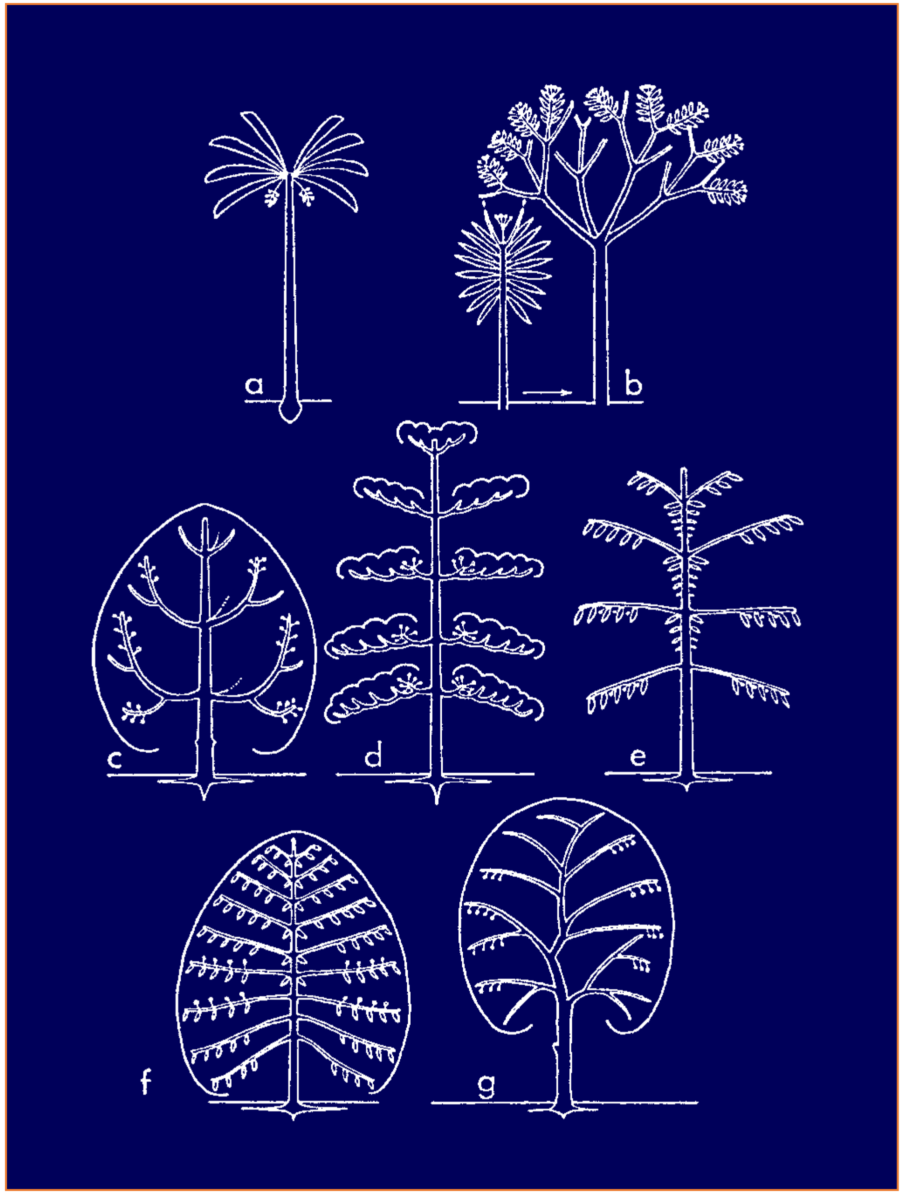
Aono and Kunii 1984
Reeves and Blau 1985
Bloomenthal 1985
Oppenheimer 1986
de Reffye et al. 1988
Weber and Penn 1995
Lintermann and Deussen 1999
Prusinkiewicz et al. 2001

Architectural models

Hallé, Oldeman, Tomlinson 1978

“Organization of trees reflects the precisely controlled genetic program which determines their development. [...]

This program is disrupted by environmental factors.”



F. Hallé, R.A.A Oldeman, P.B. Tomlinson:
Tropical trees and forests: An architectural analysis. Springer, Heidelberg 1978.

Architectural models do not suffice

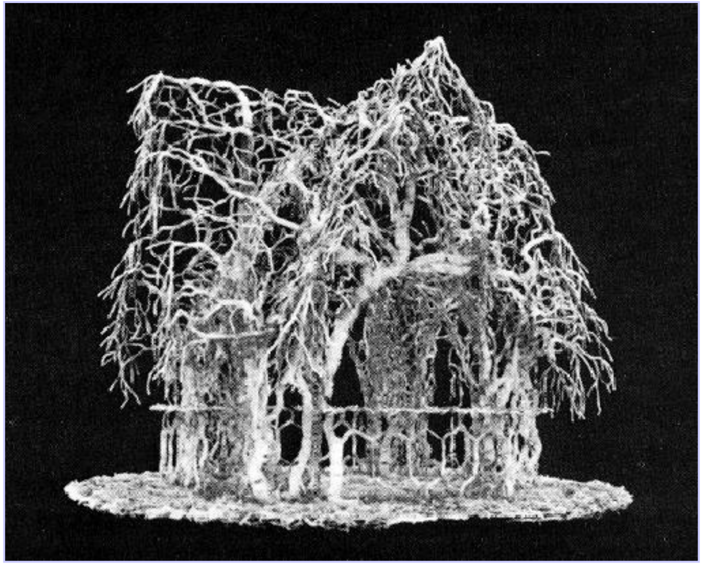
Sachs & Novoplansky 1995,
Sachs 2004

“The form of a tree is generated by self-organization in which alternative branches compete with one another, following no strict plan or pre-pattern.”

T. Sachs and A. Novoplansky. Tree form: Architectural models do not suffice. *Israel Journal of Plant Sciences*, 43:203-212, 1995.

Space-based models

Ulam 1962
Cohen 1967
Arvo and Kirk 1988
Greene 1989
Chiba et al. 1994
Prusinkiewicz et al. 1994
Mech and Prusinkiewicz 1996
Benes 2002
Rodkaew et al. 2003
Runions et al. 2007

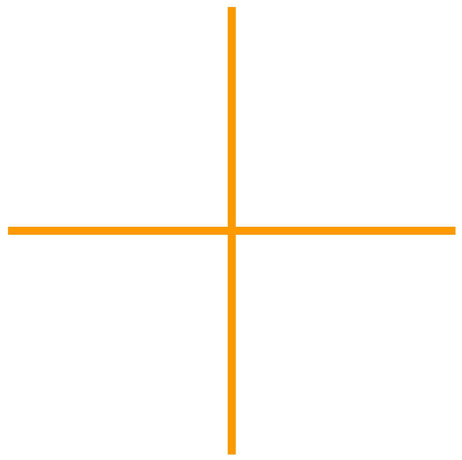


Self-organization of branches in space

- Self-organization
    - Process in which global pattern and structure emerge from interactions among the lower-level components of the system.
- Database amplification
    - Simple mechanism (economically encoded in the genome) can generate complex patterns and structures
- Reason for modelling
    - The emergence of form through self-organization is difficult to comprehend without models

S. Camazine et al. (2001): Self-organization in biological systems, Princeton University Press.

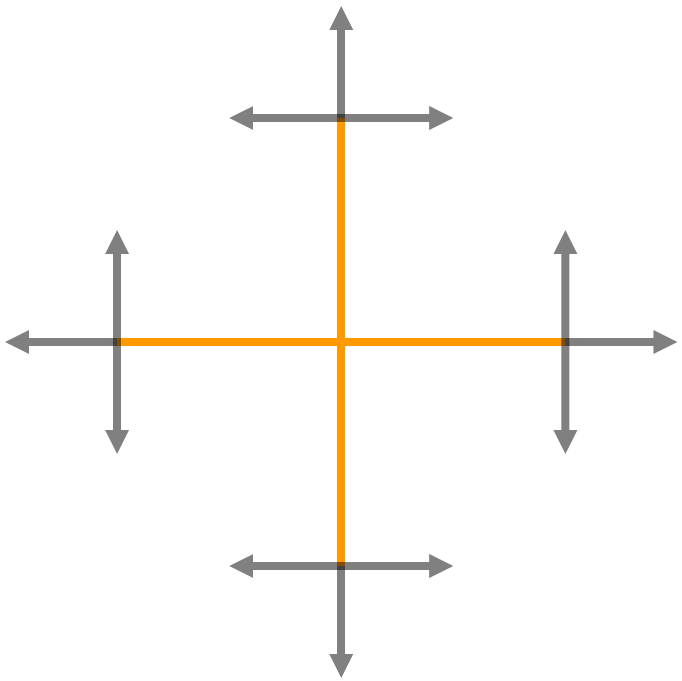
Example – Cellular Automaton



Consider a branching structure…

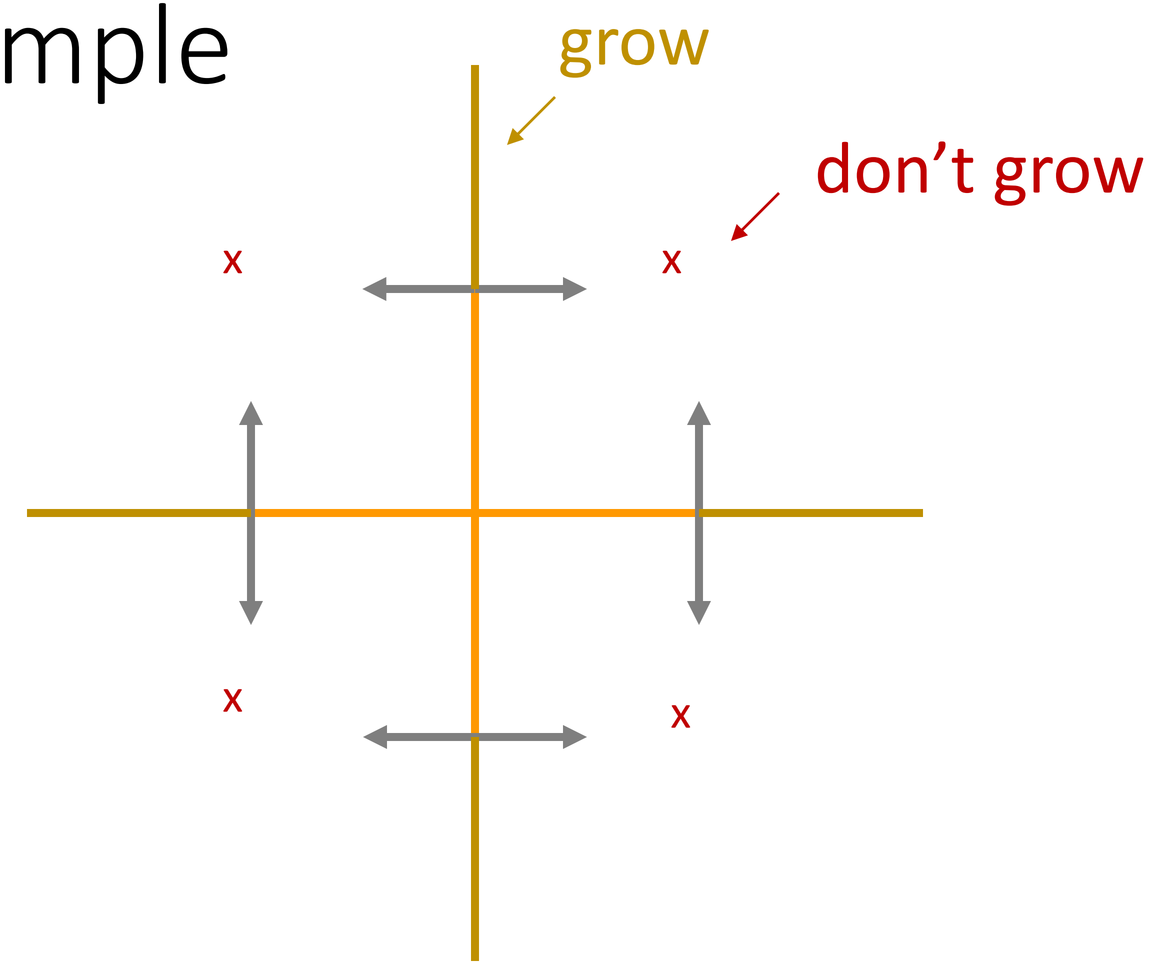
S. Ulam (1962): Patterns of growth of figures.
Proceedings of Symposia on Applied Mathematics 14, 215-224.

Example



At the end of each branch there are 3 buds.

Example



Rule 1: If there is enough space, grow.
Rule 2: If there isn’t enough space, don’t grow.

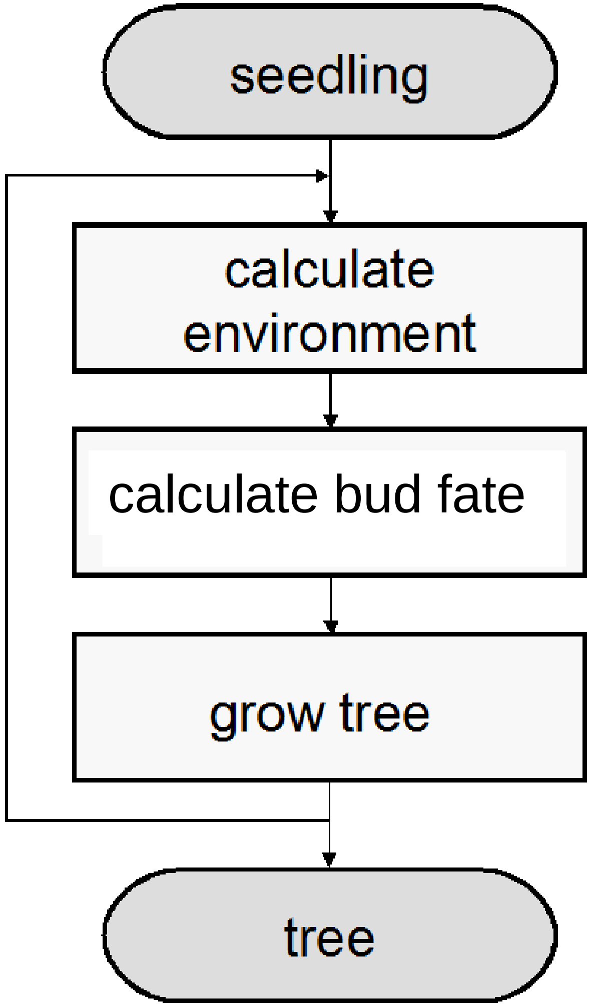
What structures will emerge?

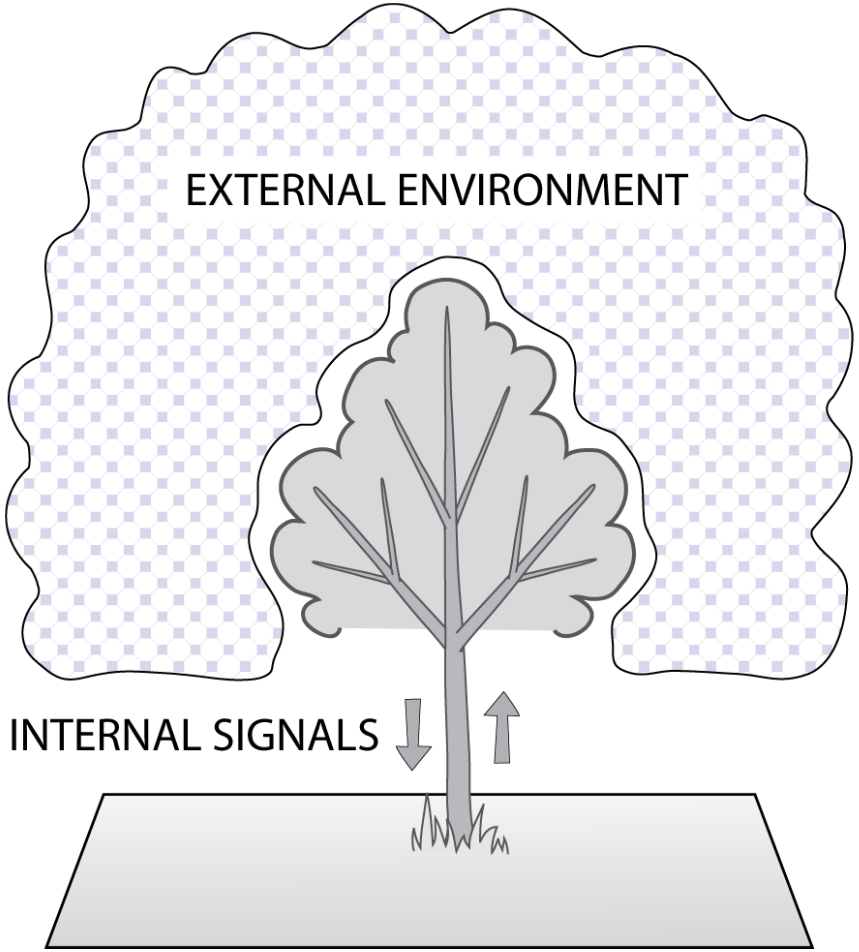
Synchronous growth

Asynchronous growth

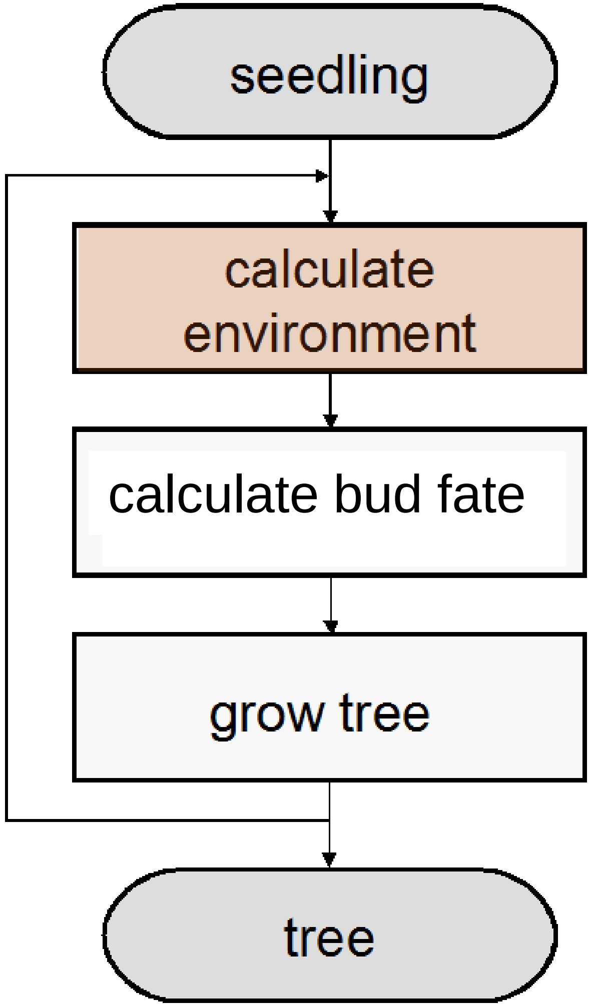
Combining Architectural and Self-organizing Models

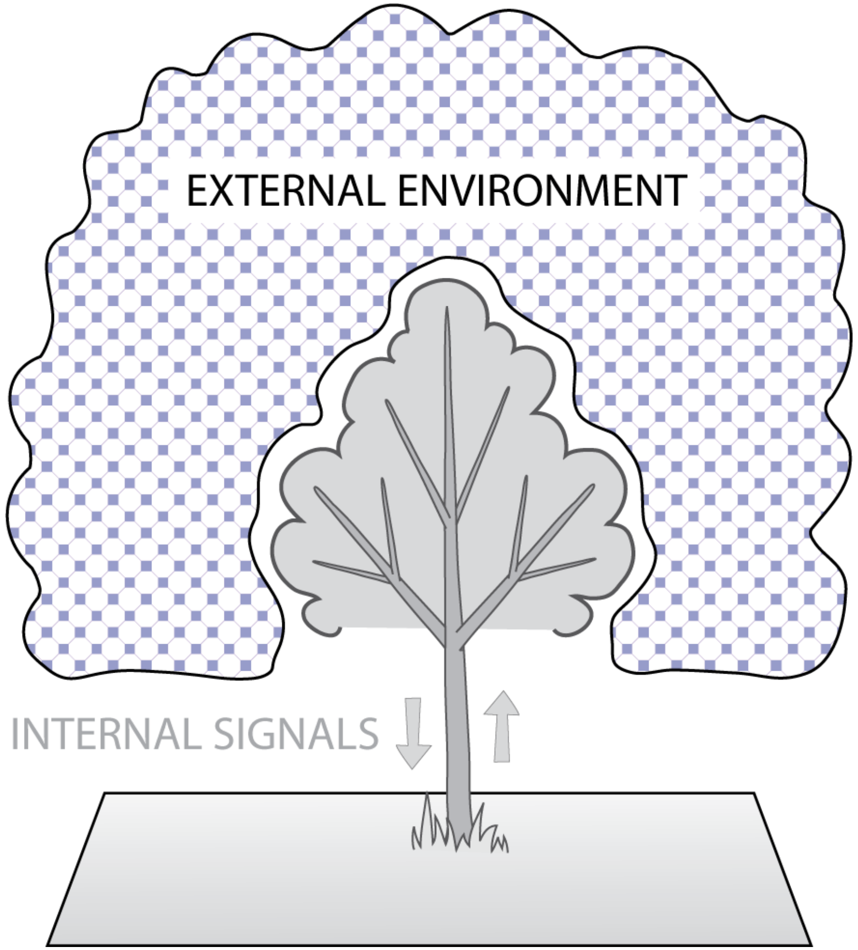
Simulation Overview



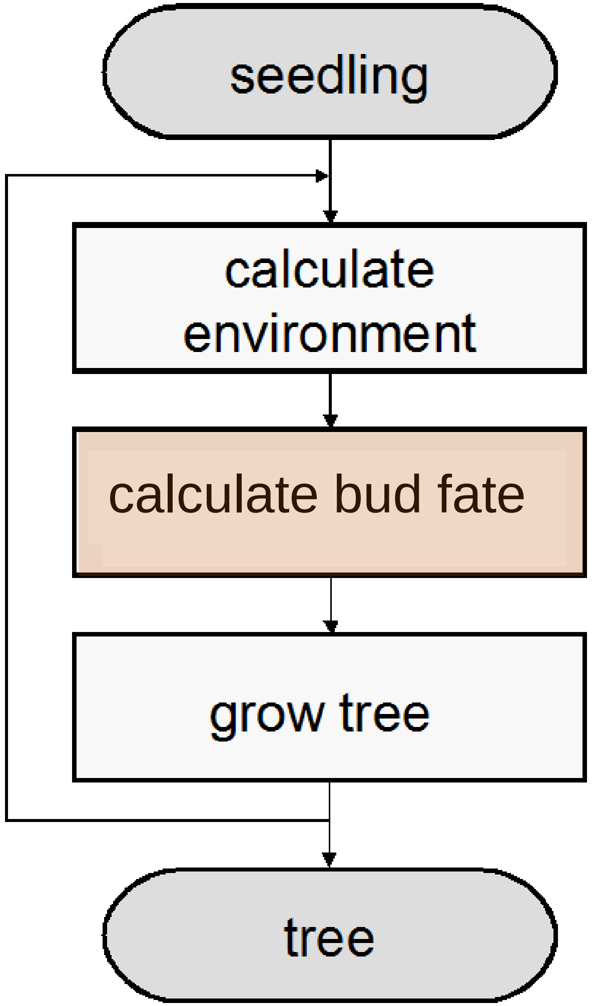


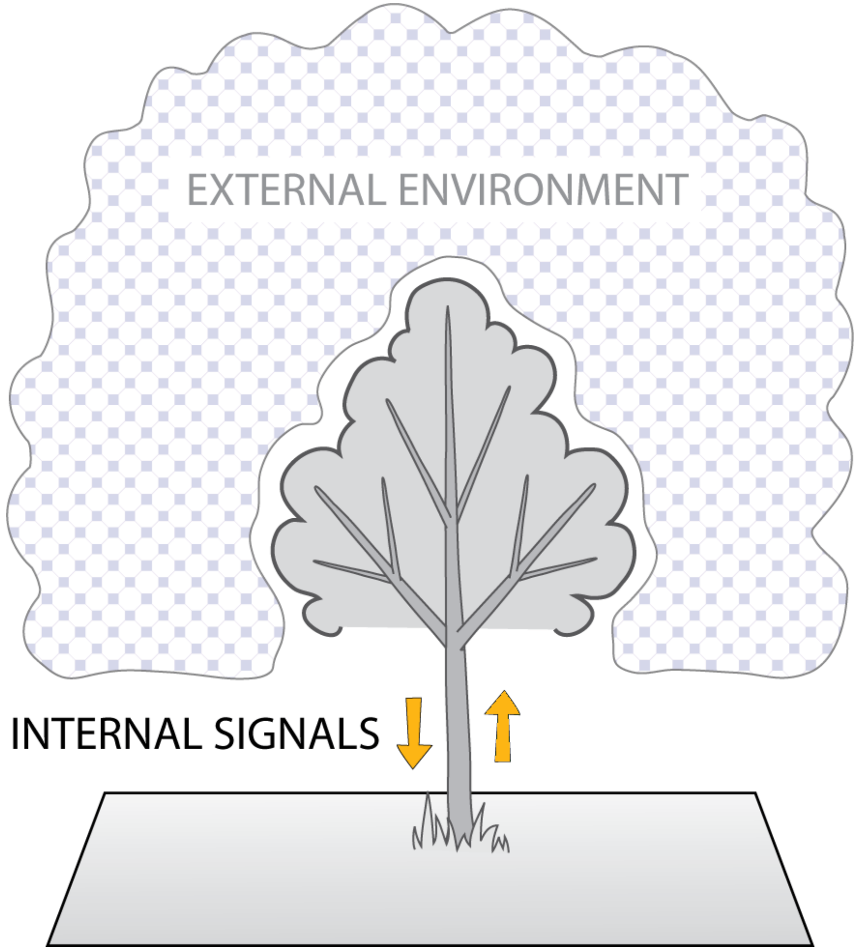
Simulation Overview



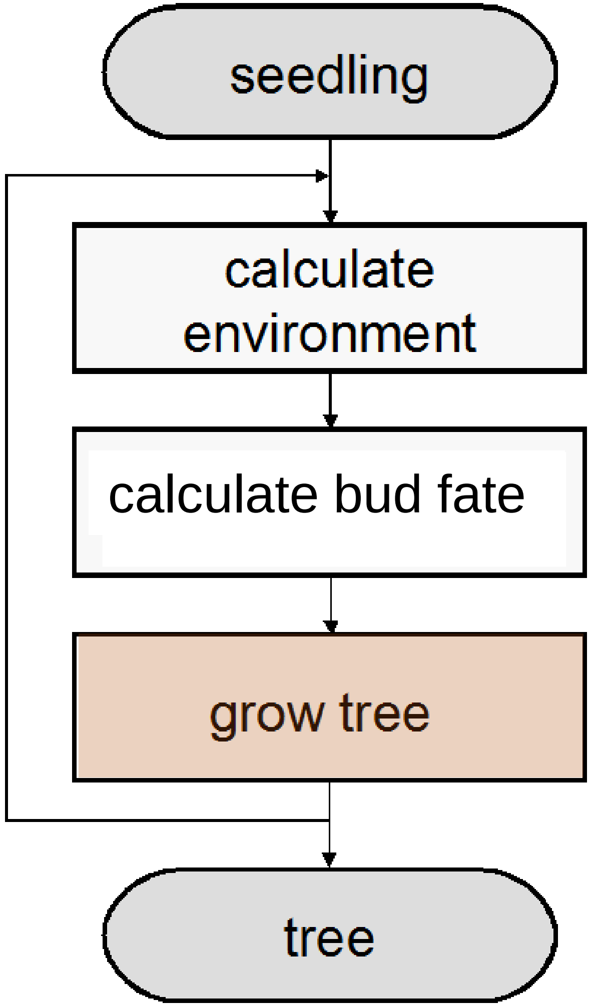


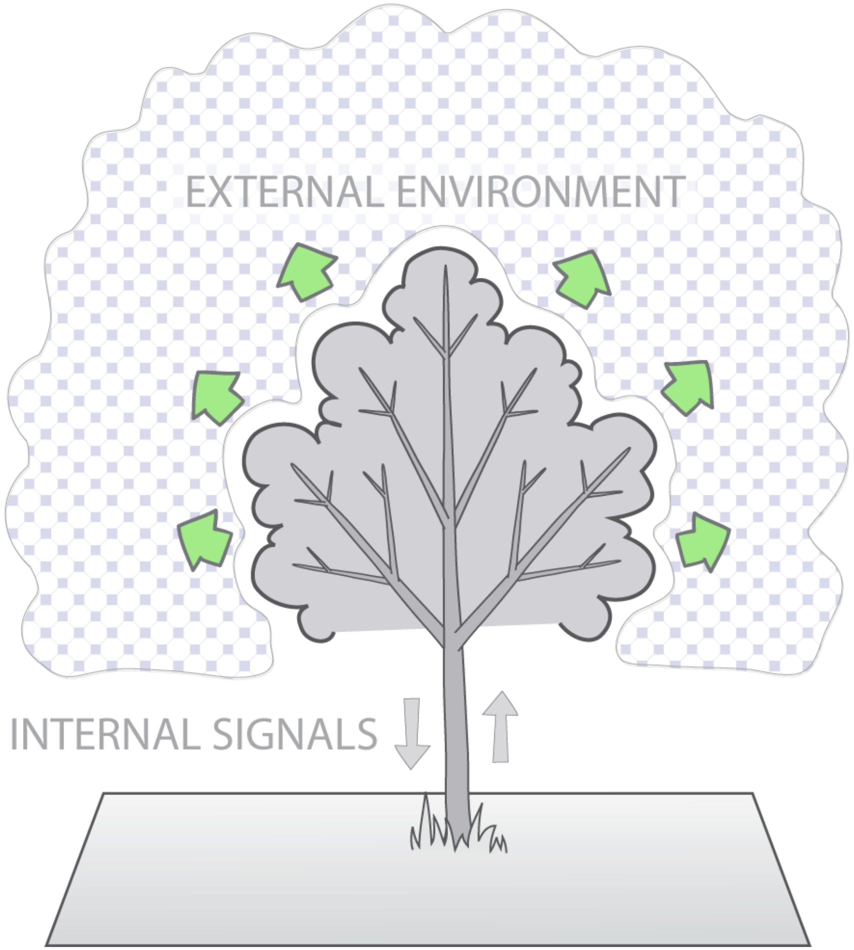
Simulation Overview



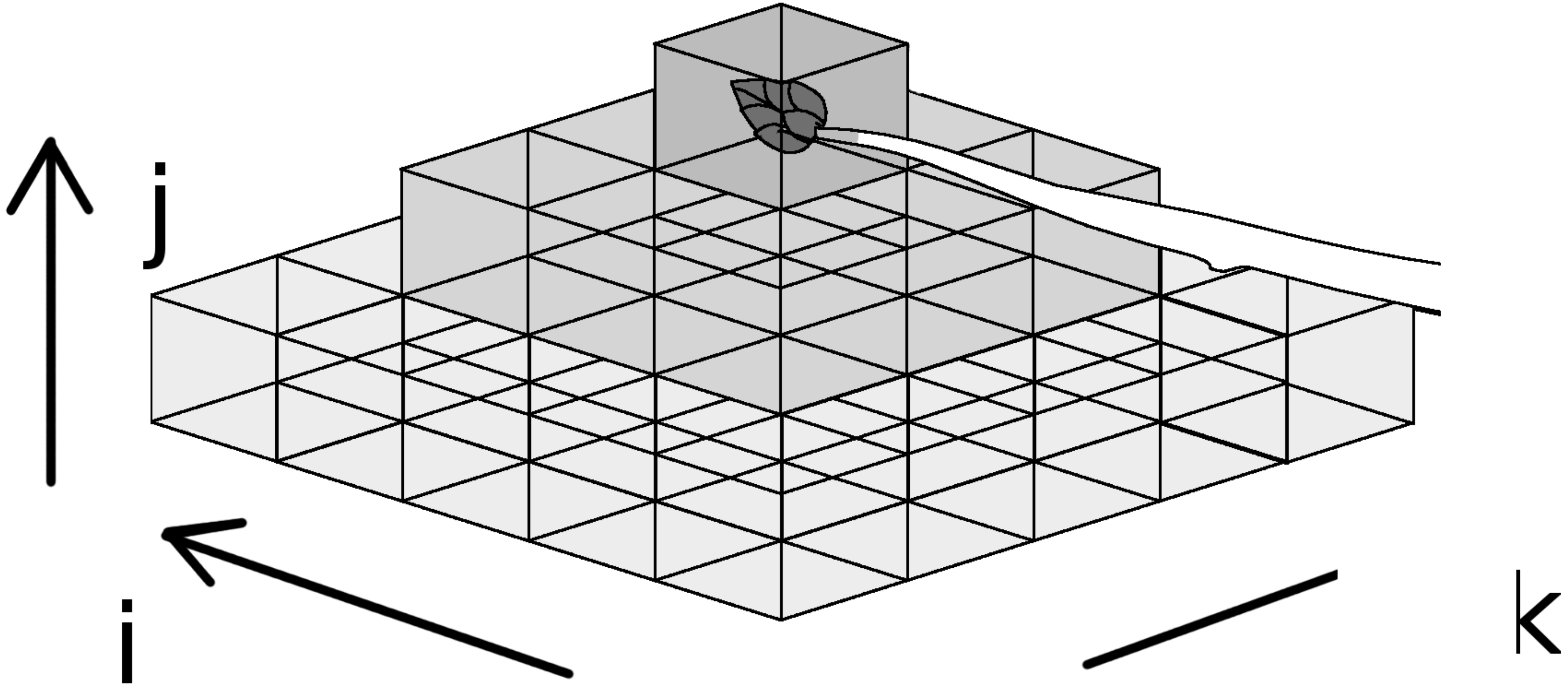


Simulation Overview

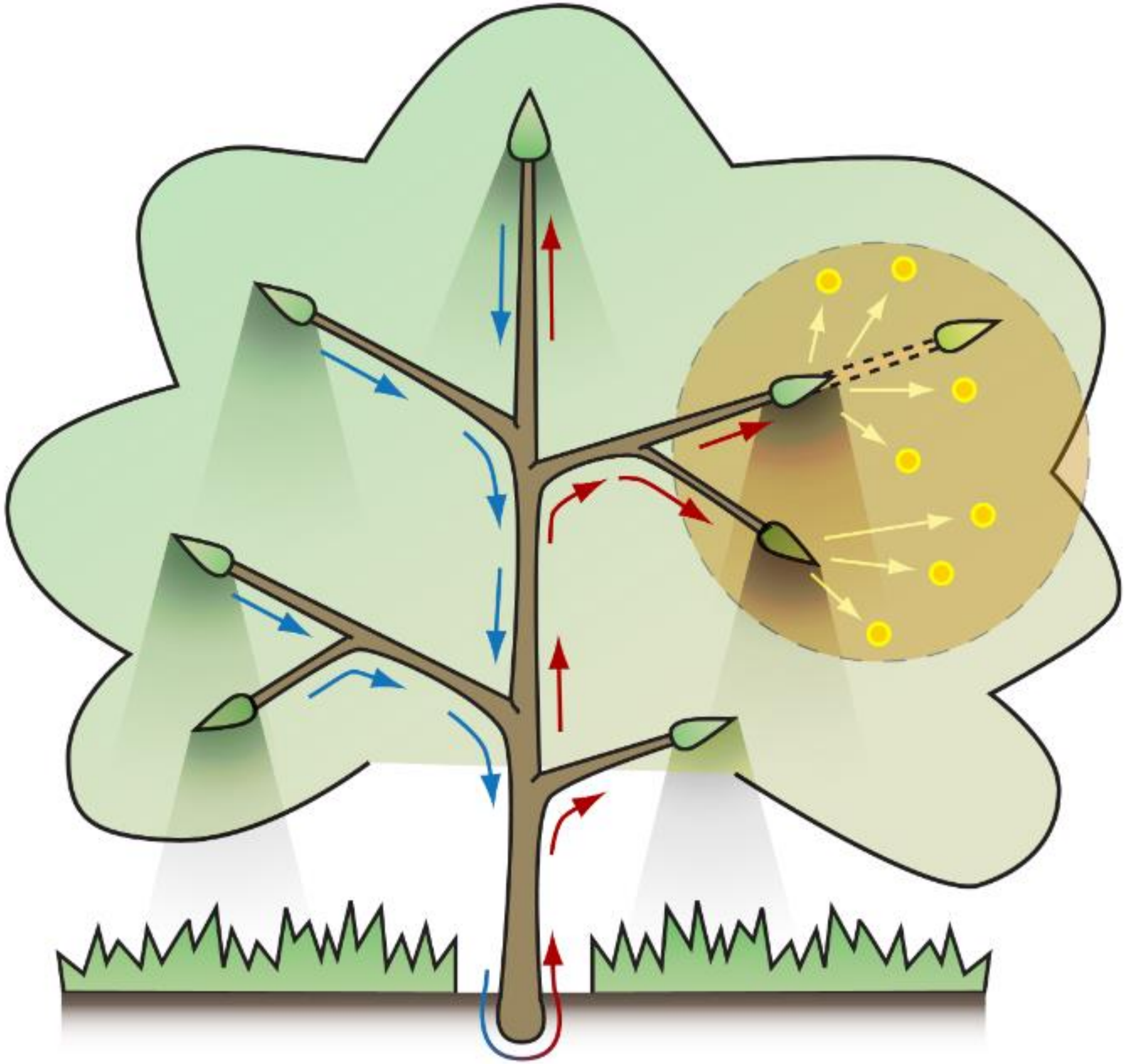




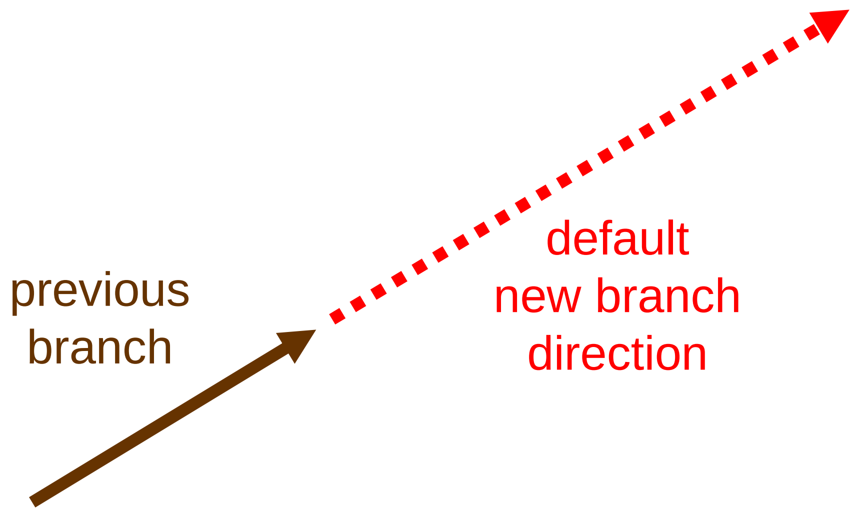
Calculating Environment



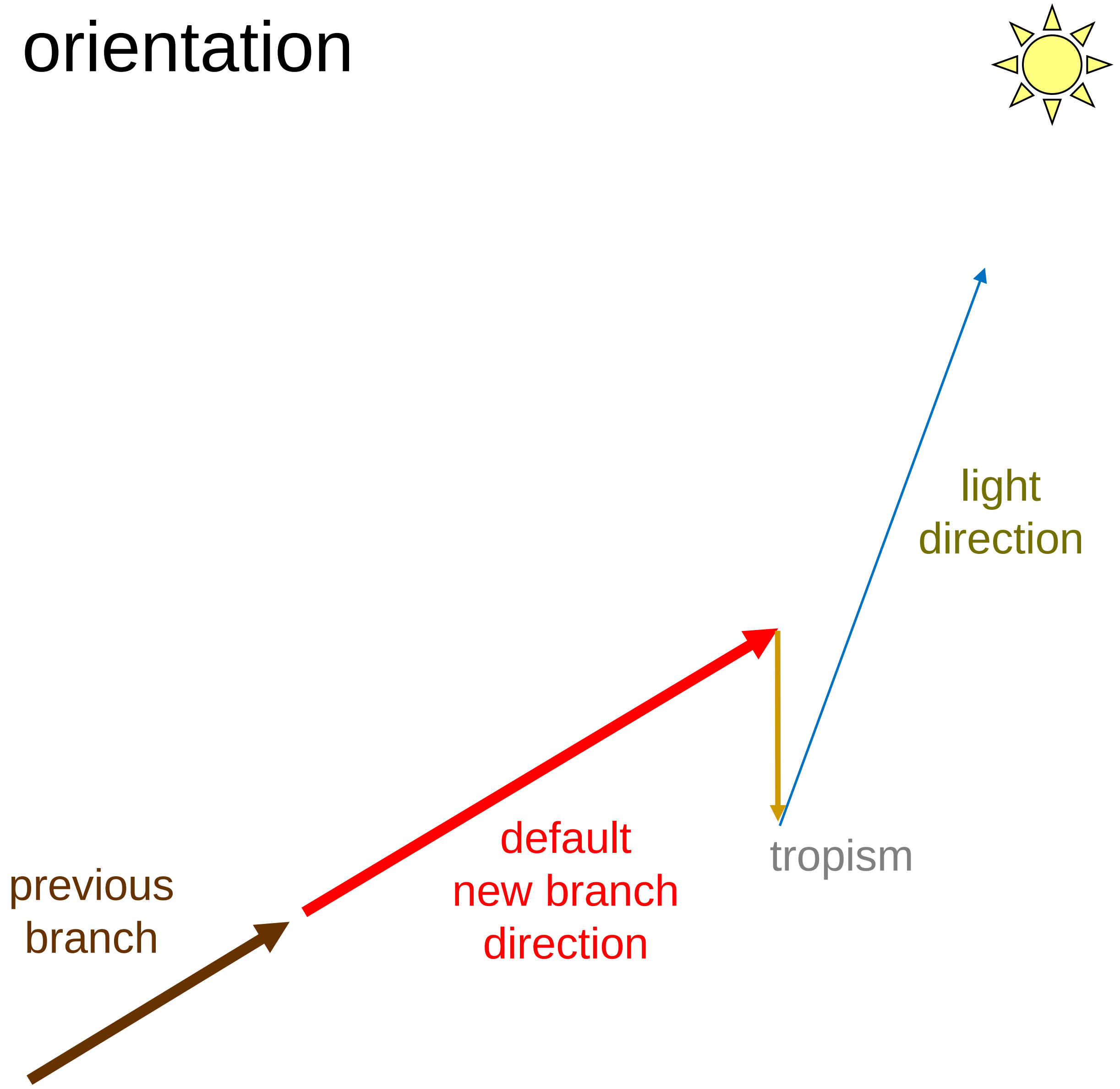
Shadow propagation



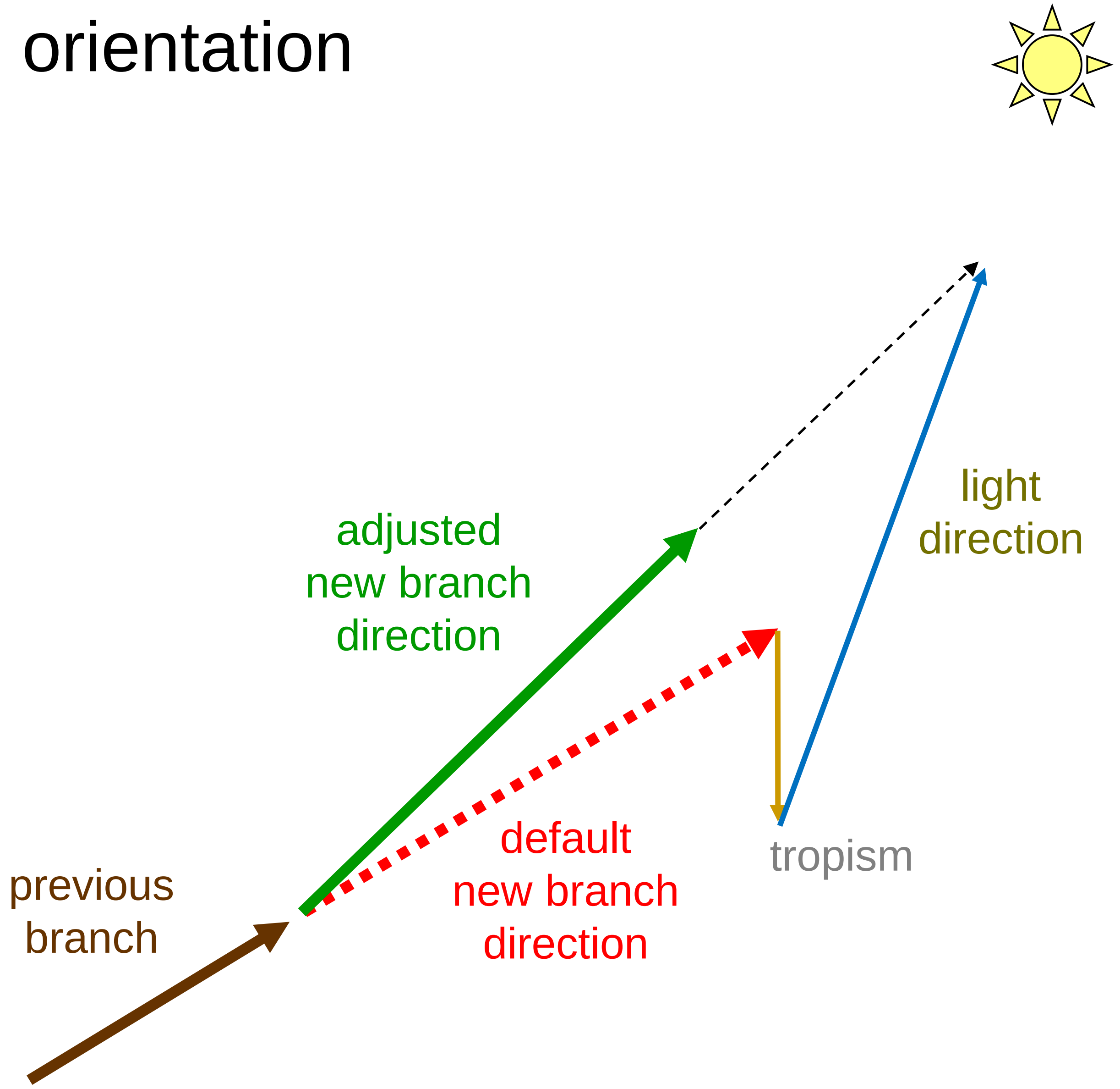
Branch orientation



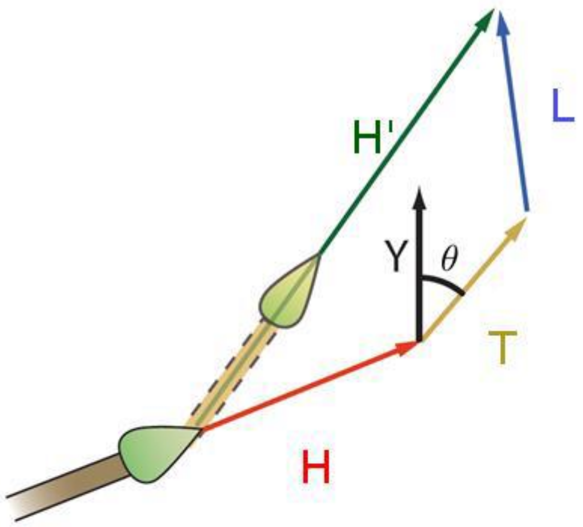
Branch orientation

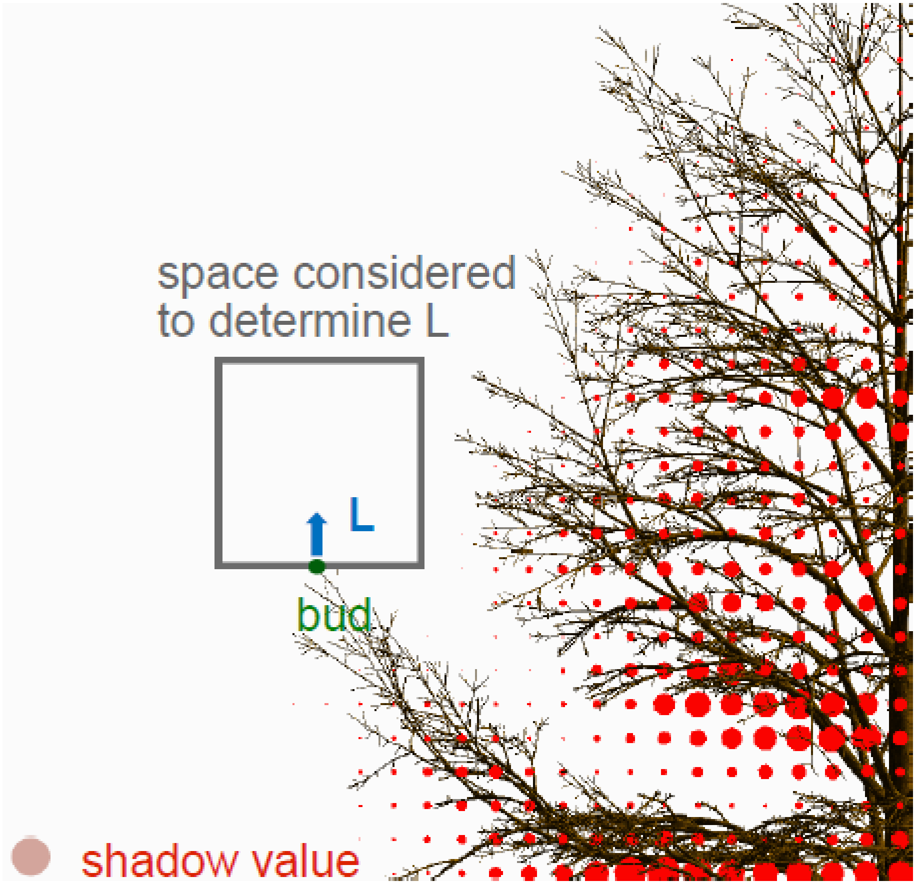


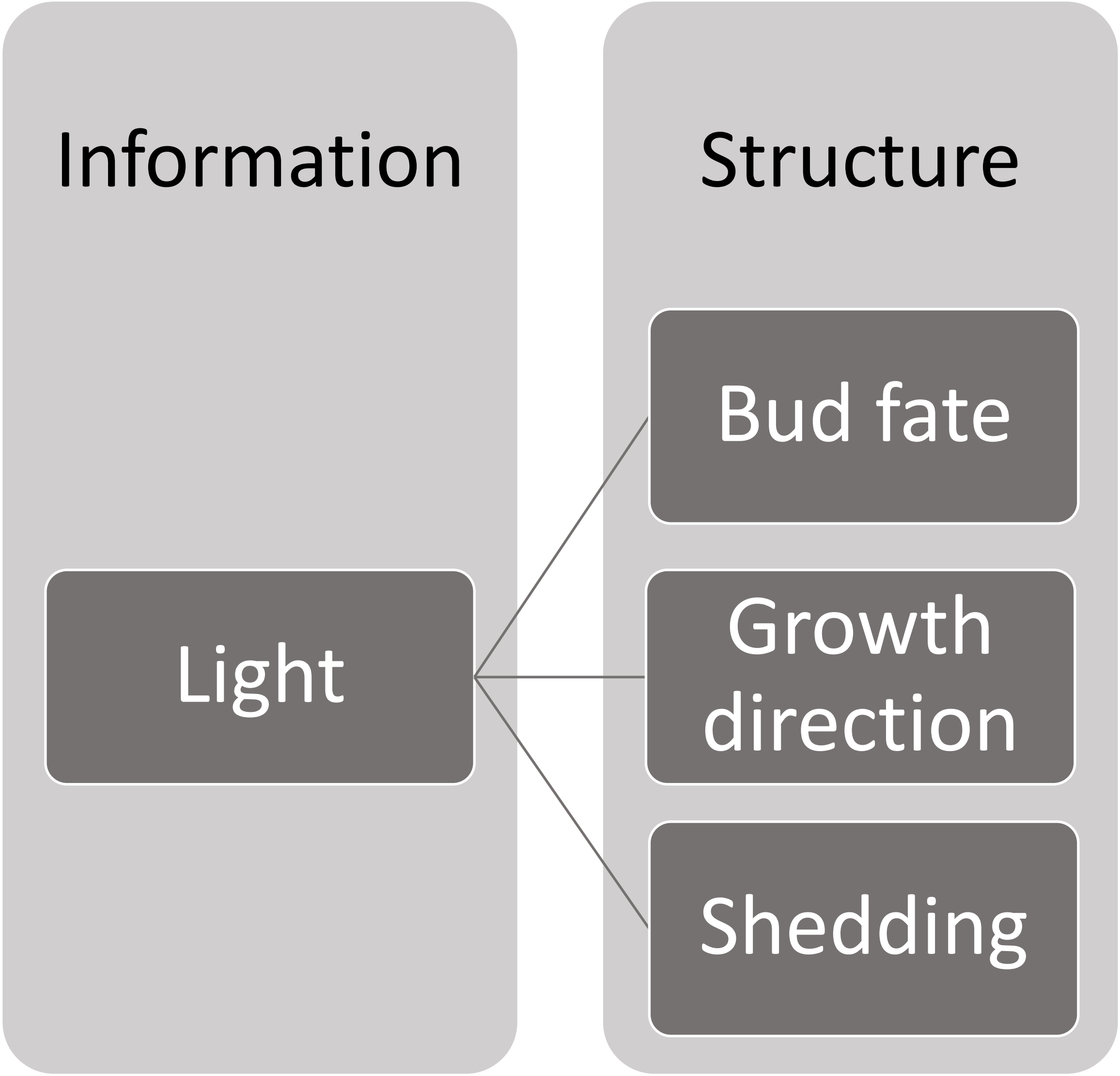
Branch orientation



Calculating Growth Direction






Information
Structure
Bud fate
Light
Growth direction
Shedding

Model controlled by competition for light only

Architectural models

Hallé, Oldeman, Tomlinson 1978

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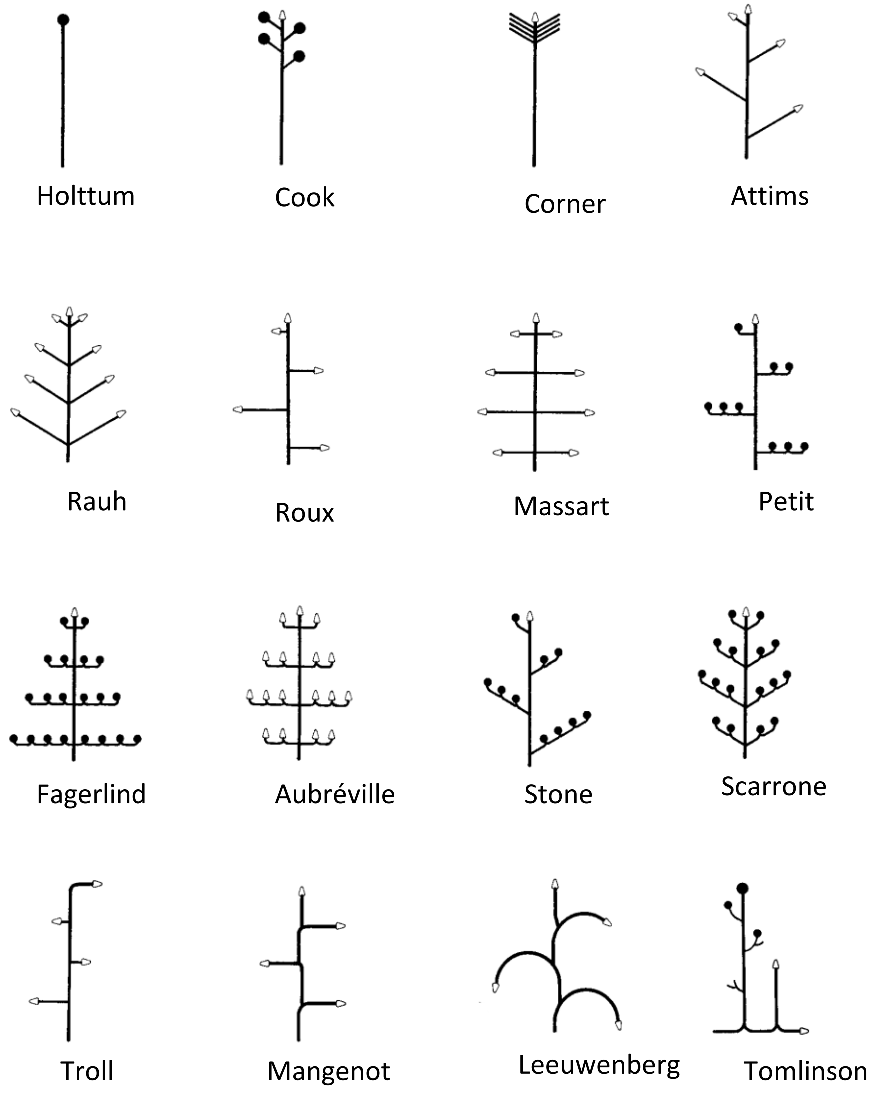
This program is disrupted by environmental factors.”



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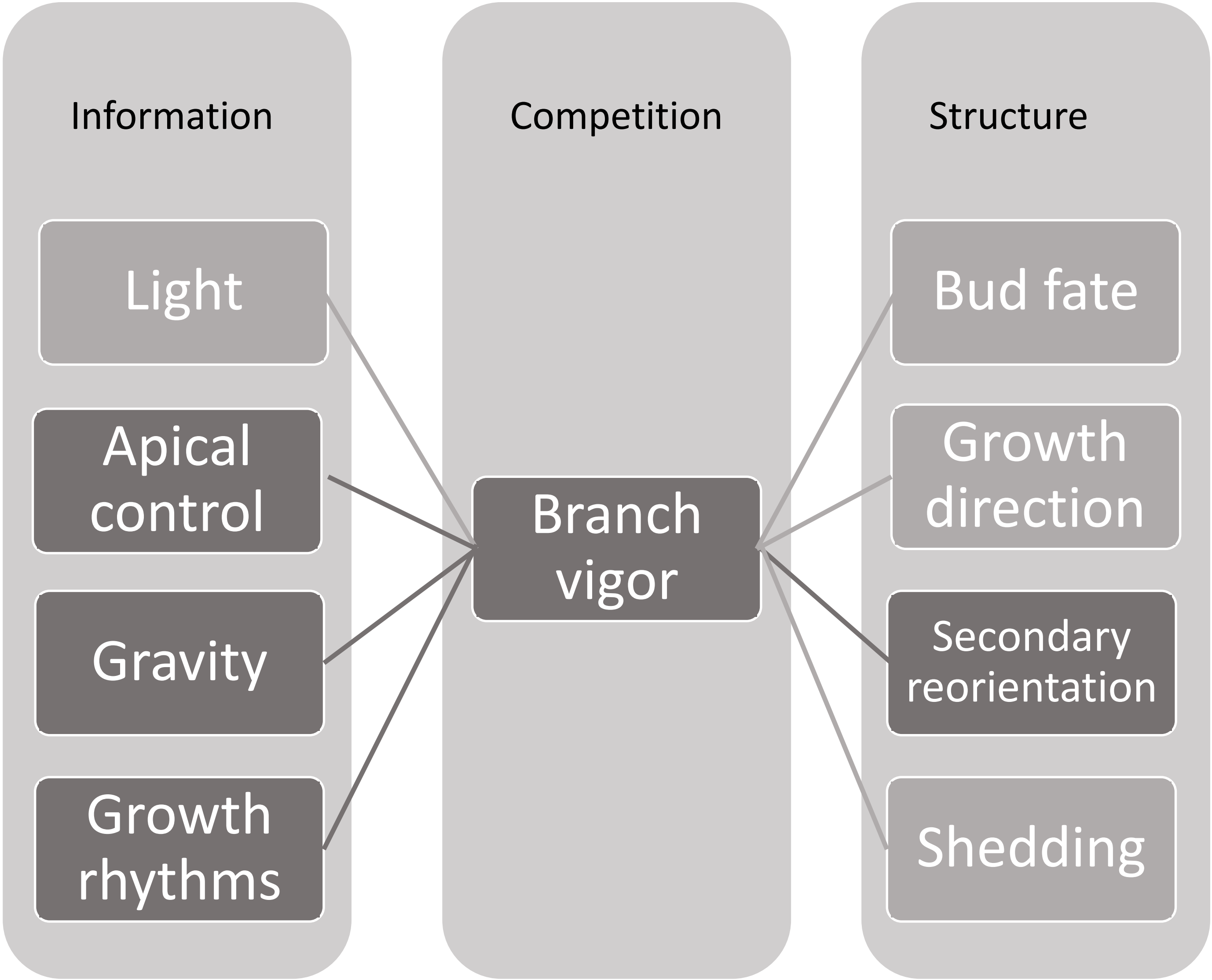
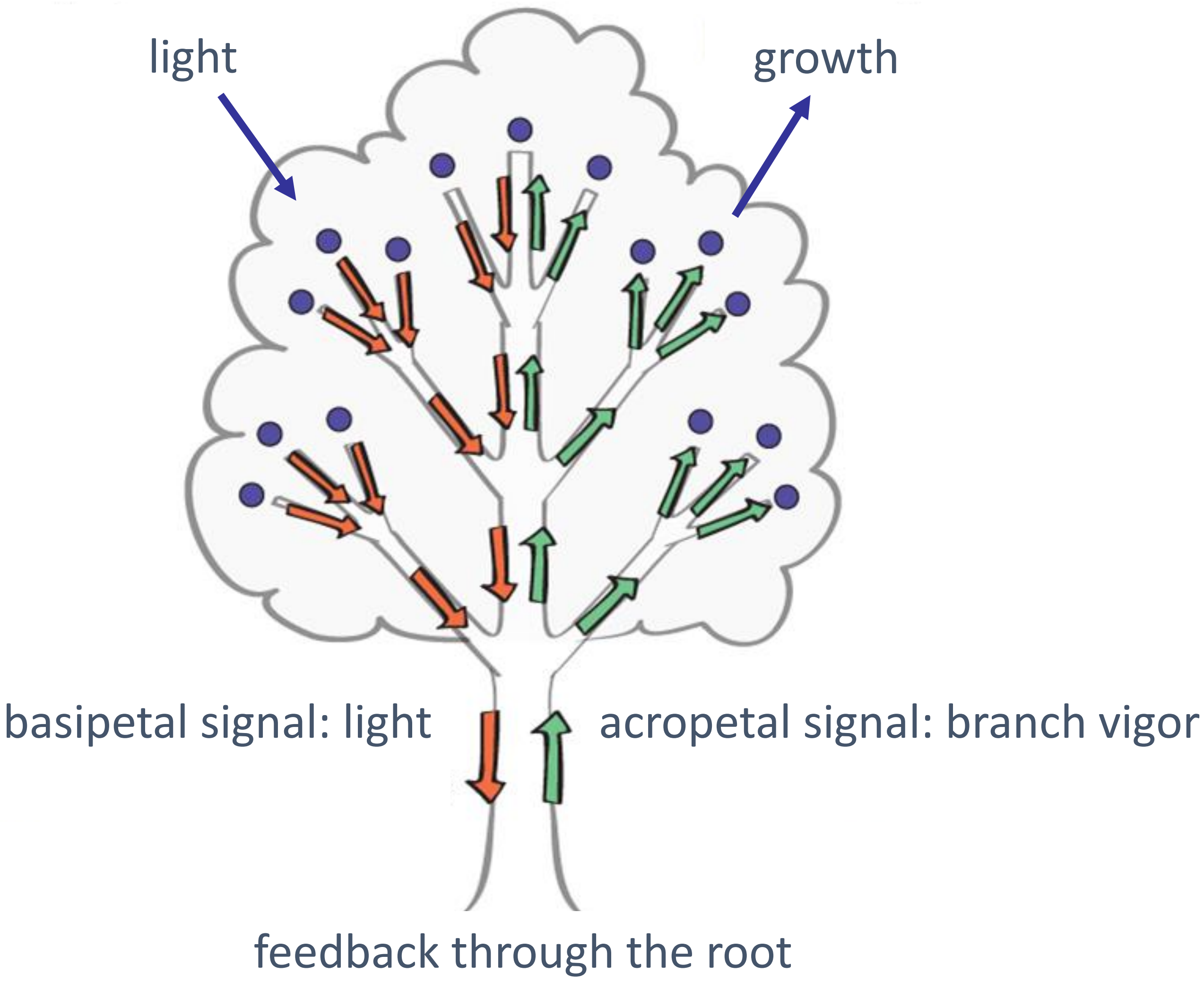
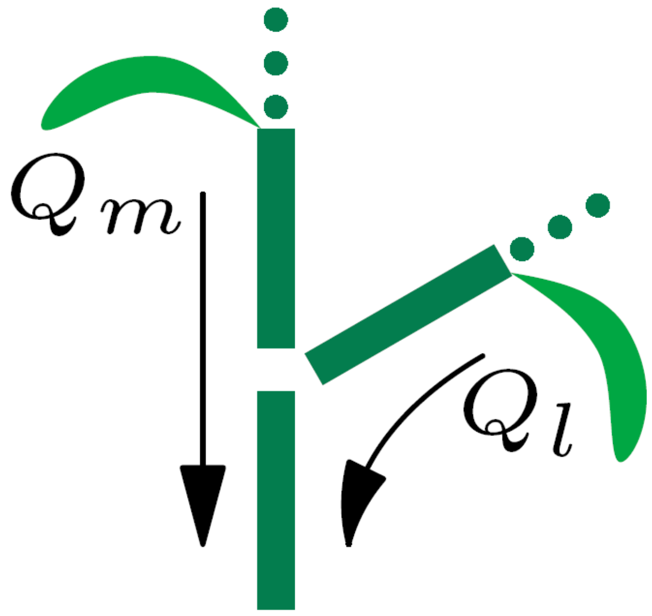

Information
Competition
Structure
Light
Apical control
Gravity
Growth rhythms
Branch vigor
Bud fate
Growth direction
Secondary reorientation
Shedding

Overview: How to compute branch vigor



Internal Signals as Flux

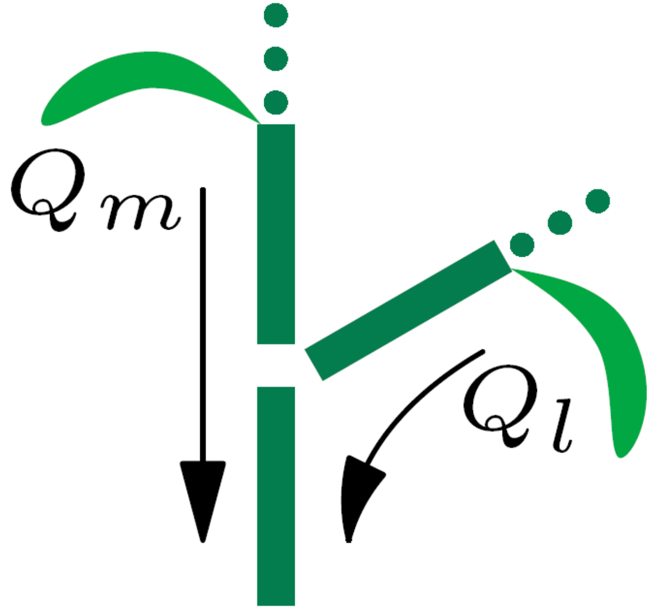
Light flux Q



$$Q = Q_m + Q_l$$

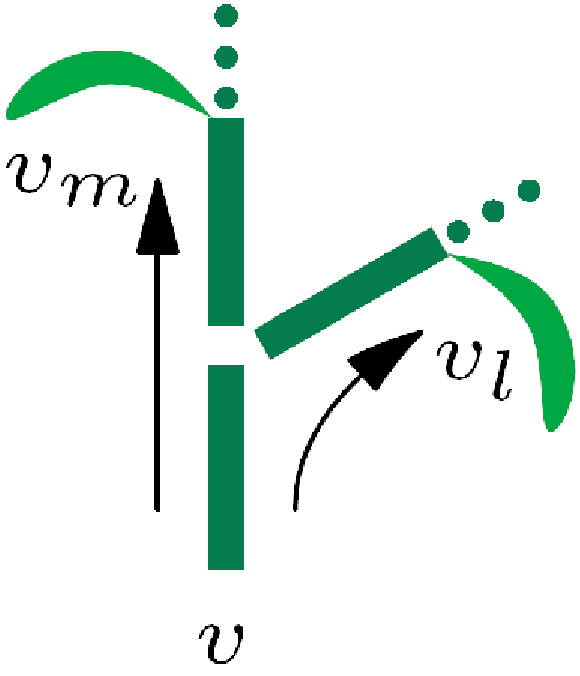
R. Borchert & H. Honda (1984): Control of development in the bifurcating branch system of Tabebuia rosea. *Botanical Gazette* 145 (2), 184-195.

Internal Signals as Flux



$$Q = Q_m + Q_l$$

Light flux Q

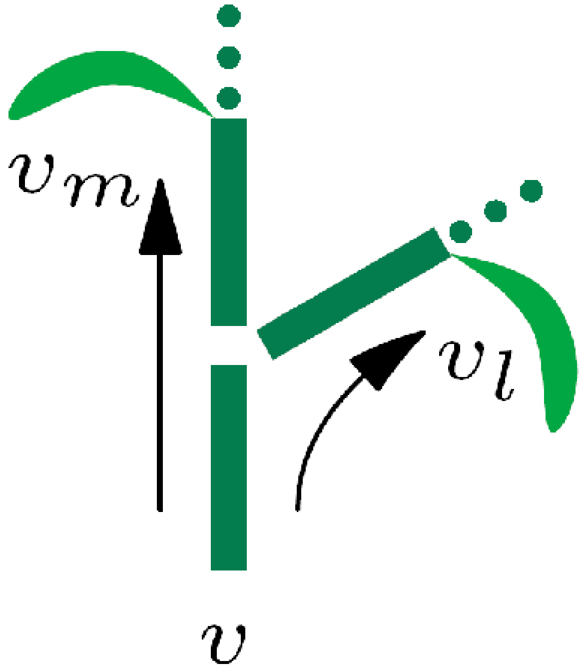


Vigor flux v

Vigor Flux Function

$$(1)\quad v_m = v\frac{\lambda Q_m}{\lambda Q_m + (1-\lambda)Q_l}$$

$$(2)\quad v_l = v\frac{\lambda Q_l}{\lambda Q_m + (1-\lambda)Q_l}$$



Vigor flux v

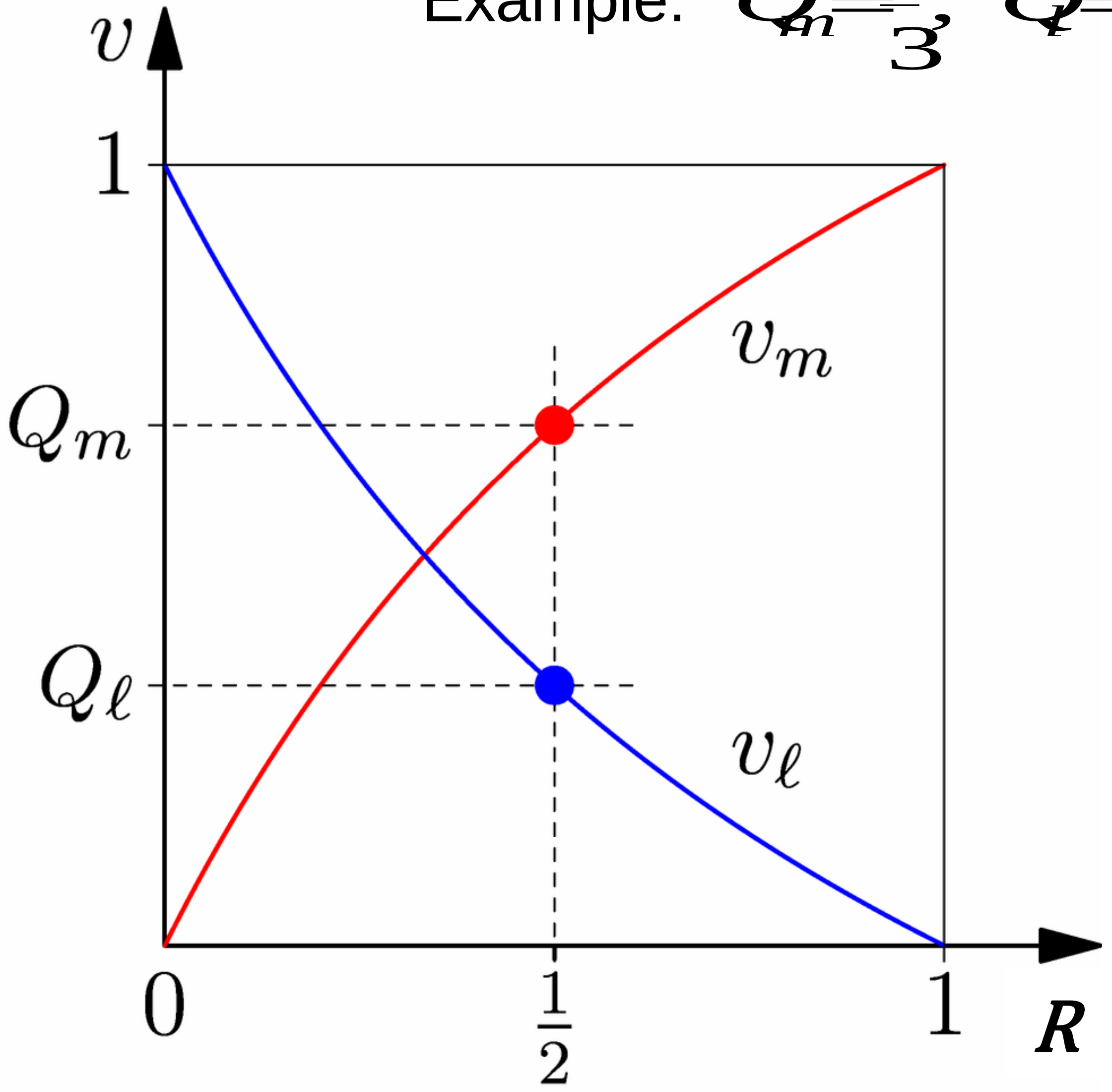
λ – Branch lineage

$$\lambda = \boldsymbol{R}\,[\mathrm{a}x^2 + b((y+c)^2)] \quad a, b \in [0,1];\; c \in [-1,1]$$

- Parameter ***R*** conceptualizes the relation between parent branch and child branch.
- A high value for parameter ***R*** favors parent branches, a low value child branches.

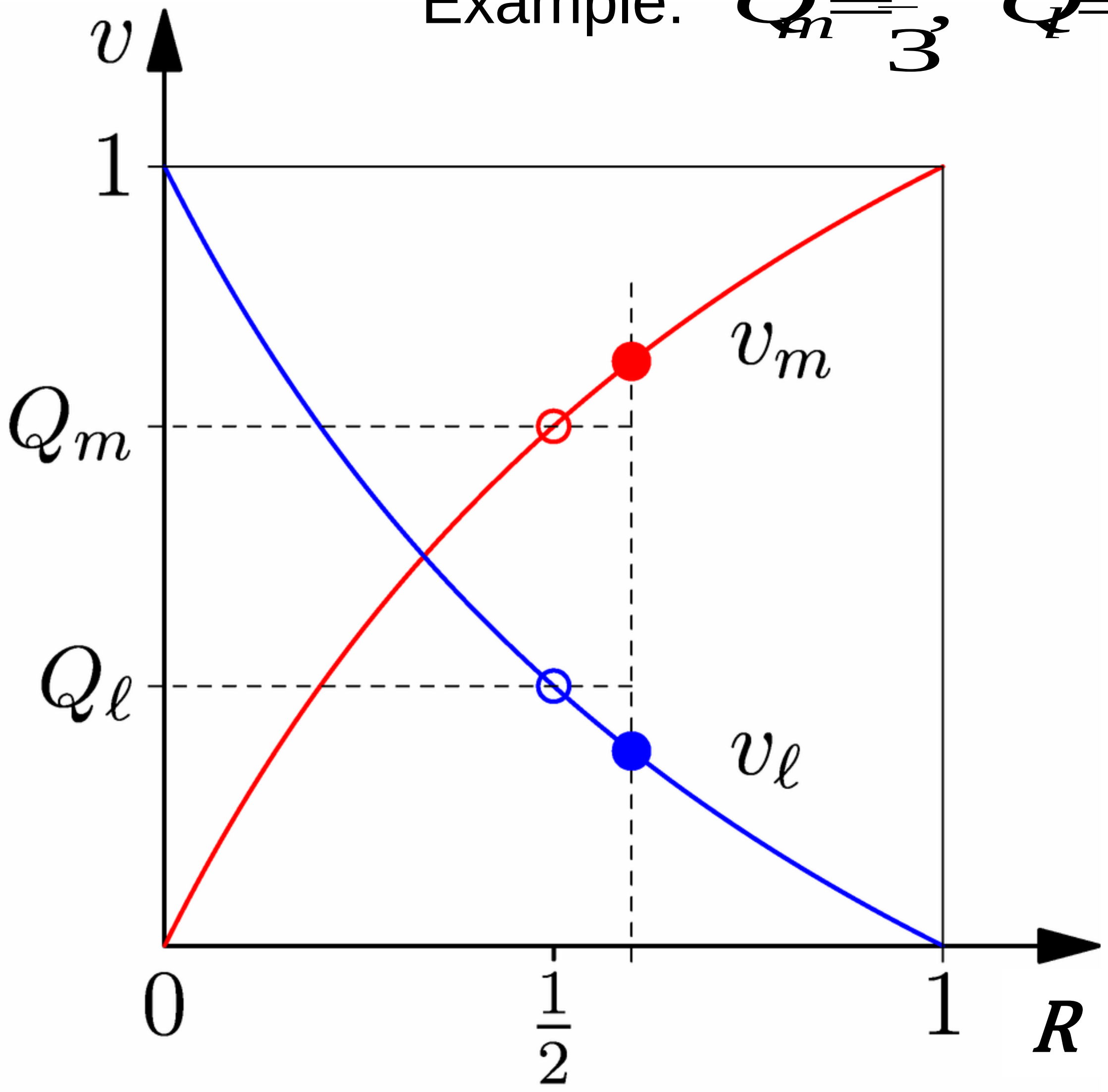
The meaning of R

Example: $Q_m = \frac{2}{3},\ Q_\ell = \frac{1}{3}$



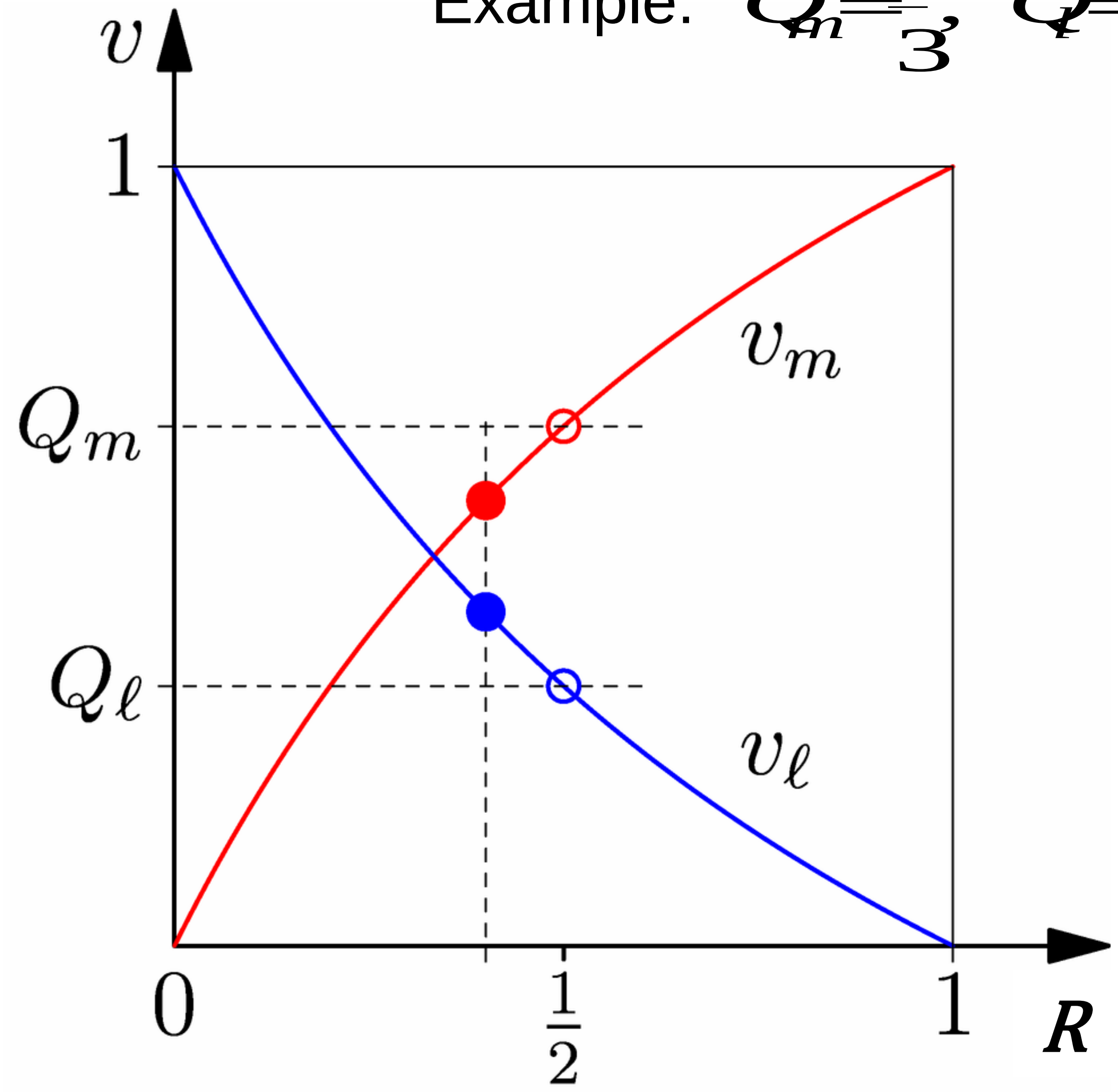
The meaning of R

Example: $Q_m = \frac{2}{3},\ Q_\ell = \frac{1}{3}$

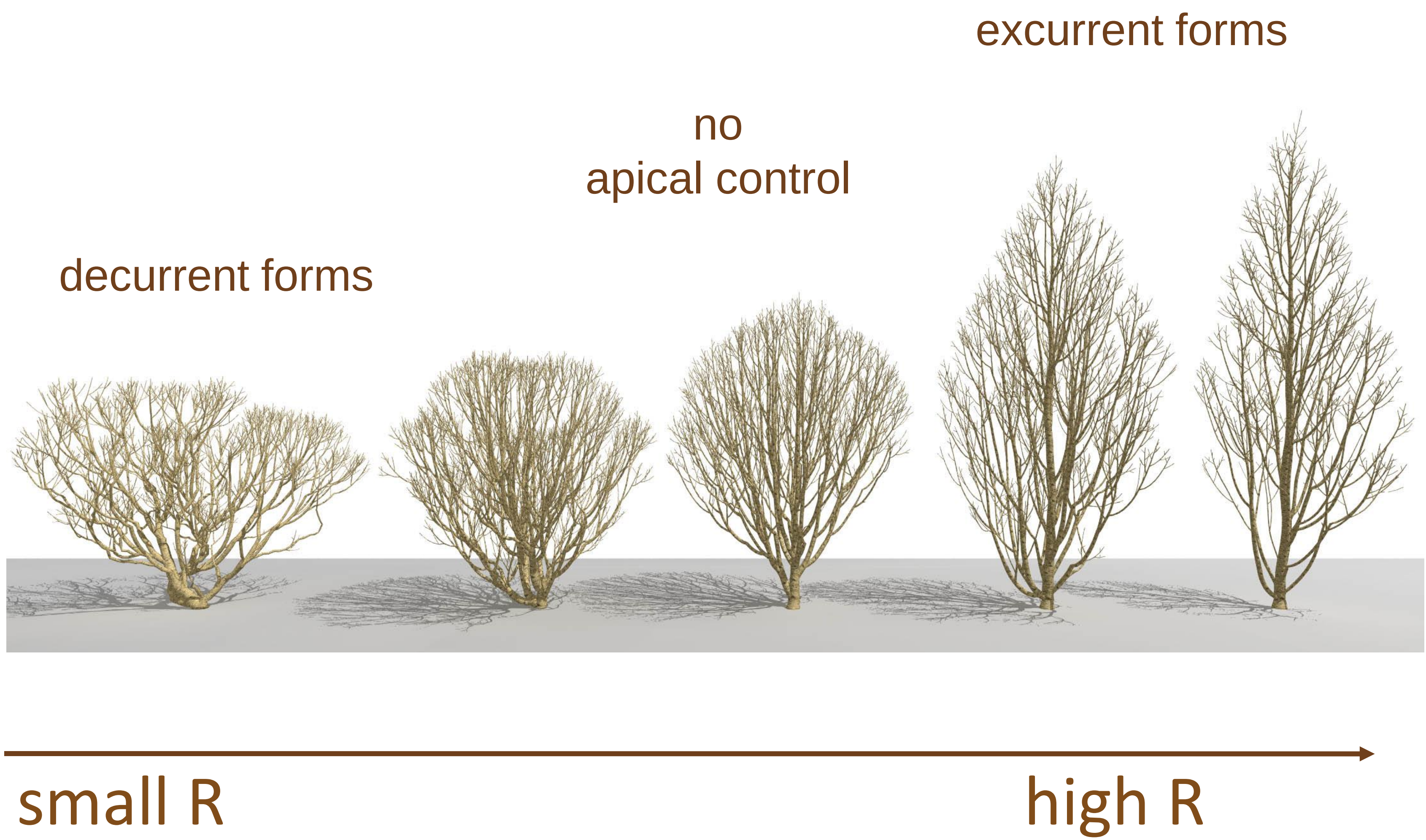


The meaning of R

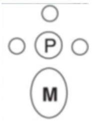
Example: $Q_m = \frac{2}{3}, \; Q_\ell = \frac{1}{3}$



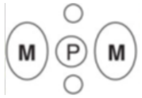
Apical control



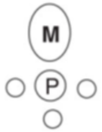
Gravimorphism



Hypotony (sympodial)



Amphitony

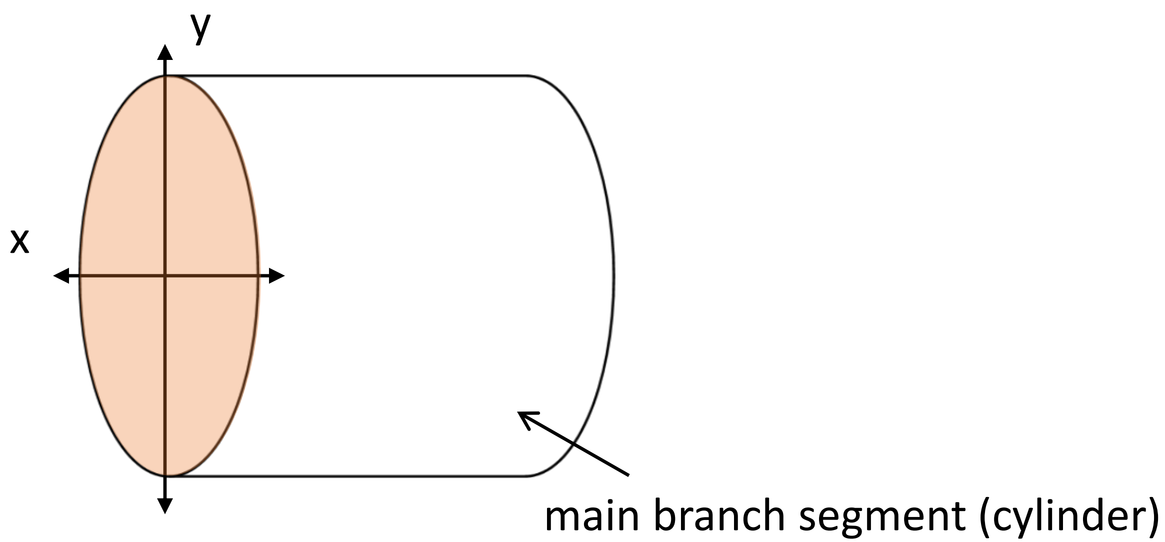


Epitony

λ – Preferential development of lateral axes (Gravimorphism)

$$\lambda = R\,[\mathbf{a}x^2 + \boldsymbol{b}((y + \boldsymbol{c})^2)] \quad a, b \in [0,1];\ c \in [-1,1]$$

- *x* and *y* denote the location of a lateral branch

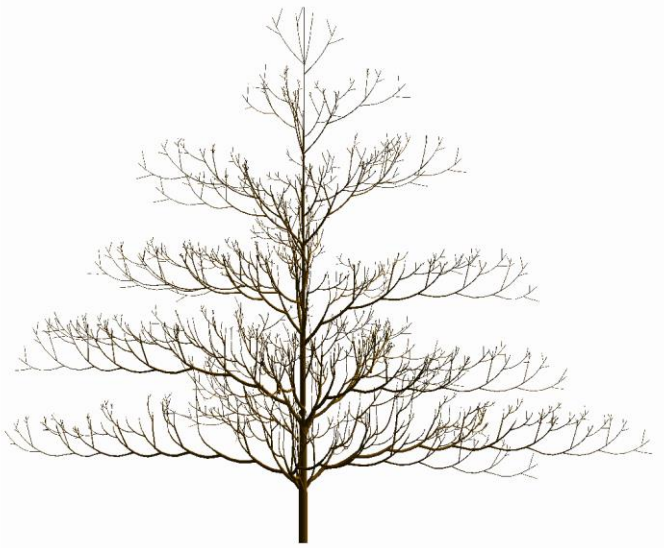


λ – Preferential development of lateral axes (Gravimorphism)

$$\lambda = R\,[\mathbf{a}x^2 + \boldsymbol{b}((y + \boldsymbol{c})^2)] \quad a, b \in [0,1];\ c \in [-1,1]$$

- *x* and *y* denote the location of a lateral branch
- Parameter ***a*** defines preference for buds located at the sides of a branch (**Amphitony**)
- Parameter ***b*** defines preference for buds located at the upper and lower surface of a branch
- Parameter ***c*** defines a preference for buds located at either upper or lower surface of a branch (**Epitony/Hypotony**)

Gravimorphism - Examples



orthotropism ↑
\+
hypotony (high c)

plagiotropism ↔
\+
amphitony (high a)

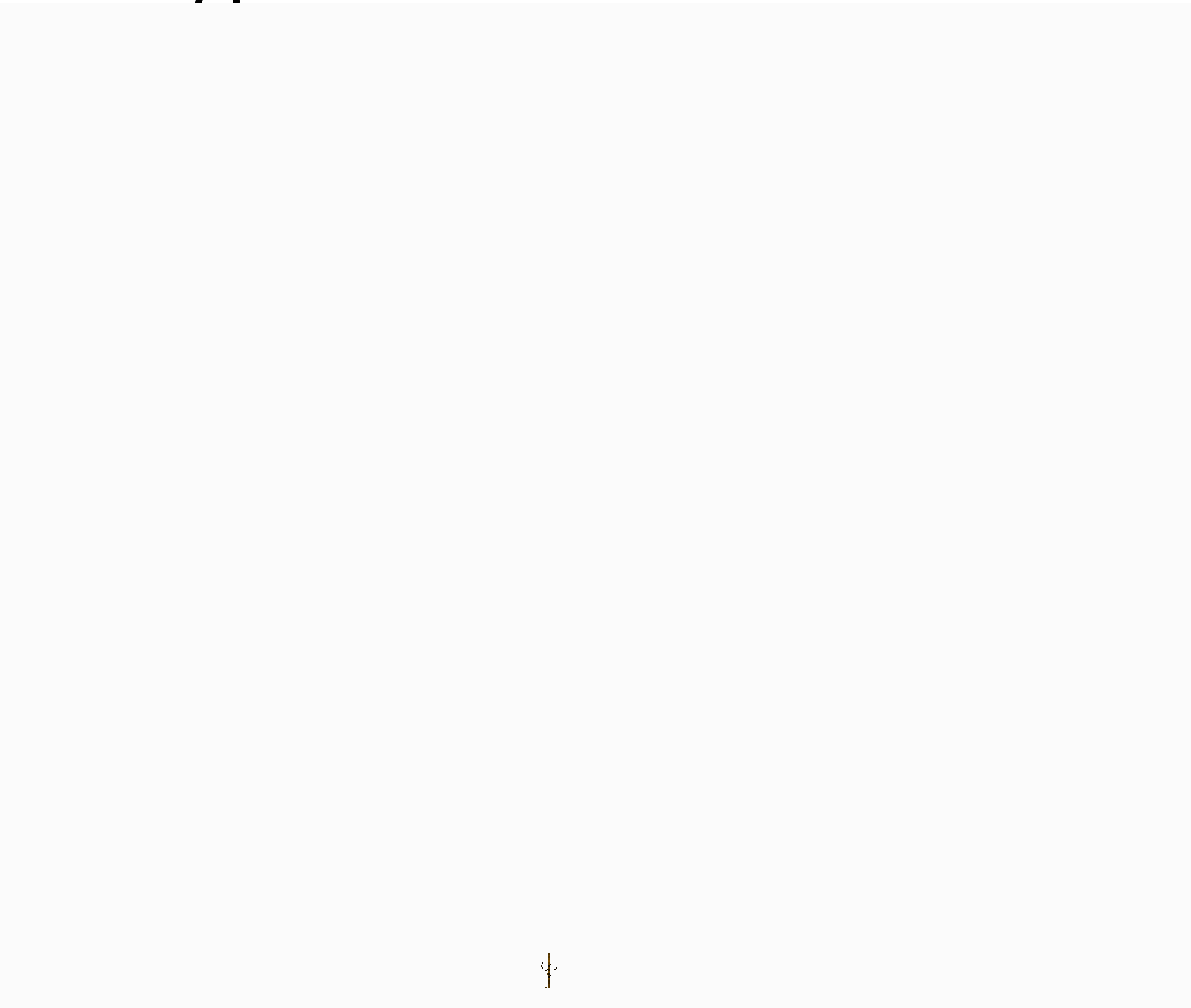
orthotropism ↓
\+
epitony (low c)

Branch Bending

- **Elasticity theory** – branches as elastic circular rods composed of isotropic and homogenous material (no stretching)
- Solve static equilibrium of gravity and forces resulting from growth
- Torque–based model

J. Taylor-Hell (2005): Incorporating Biomechanics into Architectural Tree Models. *Proceedings of the XVIII Brazilian Symposium on Computer Graphics and Image Processing.*

Branch Bending - Animation



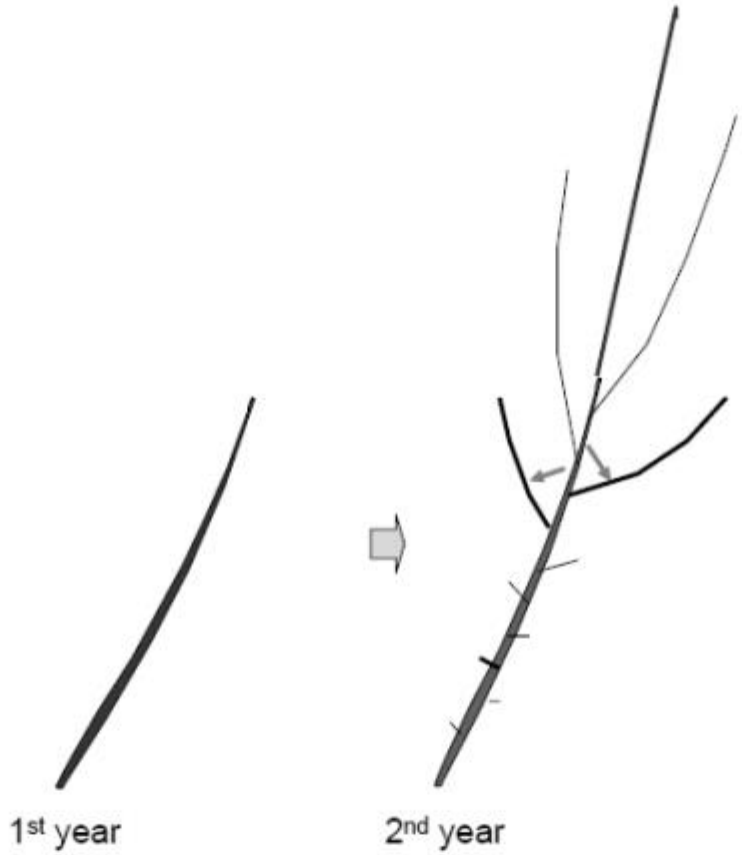
Growth Rhythms

Growth Rhythms

Growth Rhythms

Growth Rhythms

Proleptic growth



Growth Rhythms

- Shoot growth determined by shoot to root relation *(Borchert 1973)*

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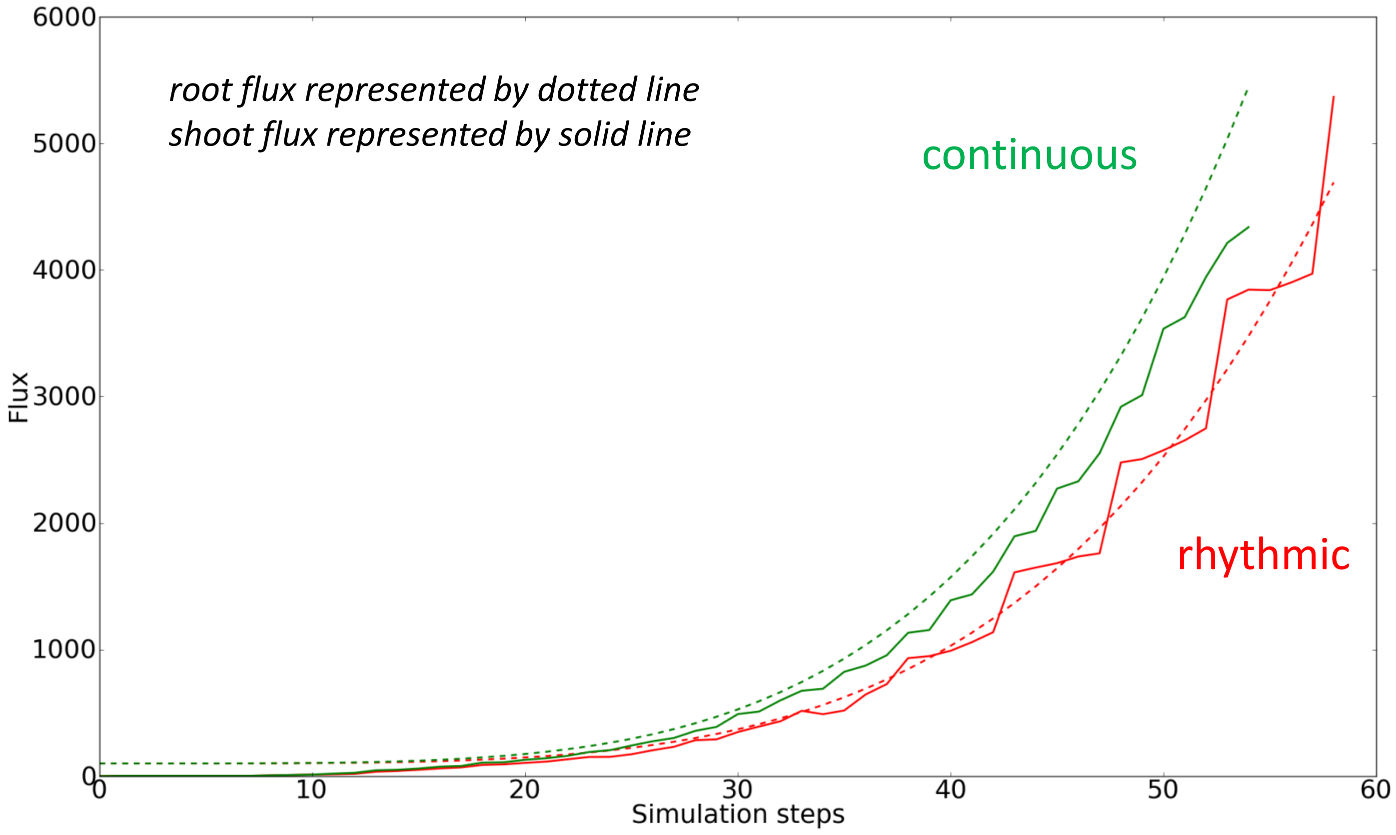
  - Decrease length of branch segments
  - Increase bud activation threshold
  - Increase branch shedding threshold
- If $Q_{total} \leq R_{total}$ → *grow*
  - Increase length of branch segments until maximum
  - Decrease bud activation until minimum
  - Decrease branch shedding threshold

Growth Rhythms - Example



Root and shoot flux development in continuous example and rhythmic example

Growth Rhythms - Close up

Continuous development

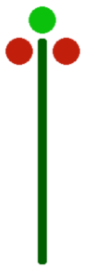
Rhythmic development

Bud Fate – Dormant, Flowering and Active

- Buds which satisfy the inequality **flux < flowering threshold** become a flower and are removed from the simulation
- Threshold affects only **active buds**

Active bud

Dormant bud



Before calculating flux

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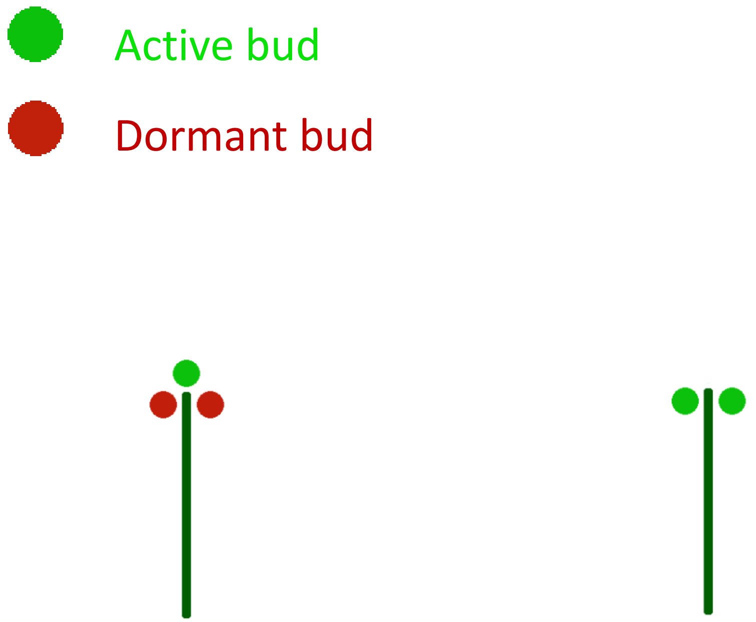

Before calculating flux   After calculating flux

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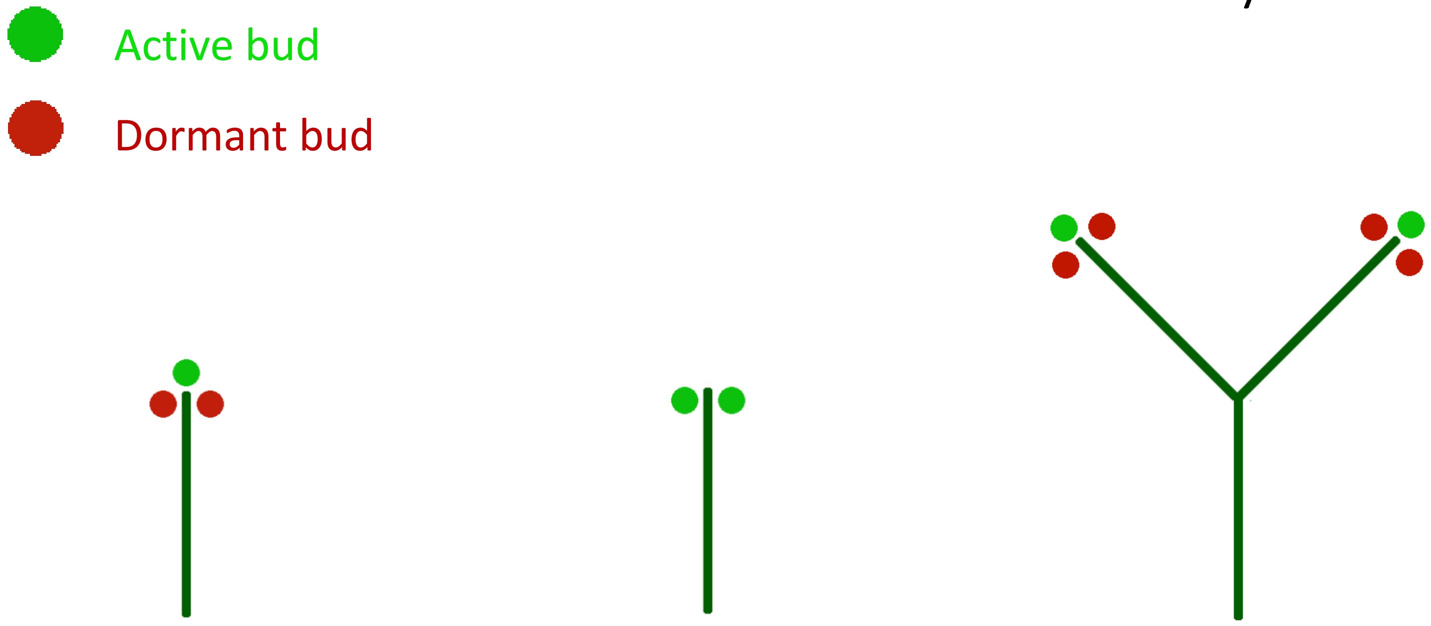


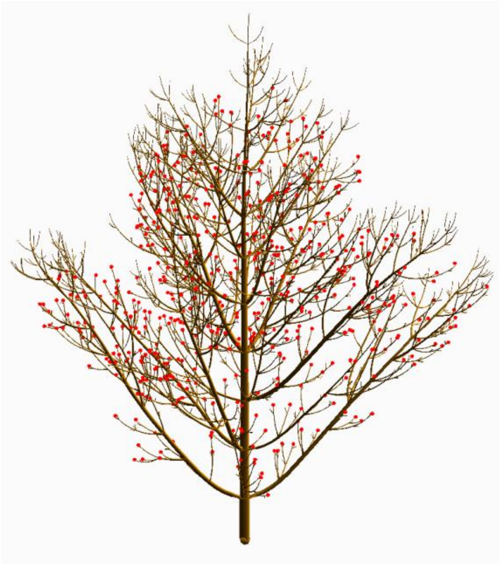
Before calculating flux | After calculating flux | After growth phase

Flowering and Architectural Models

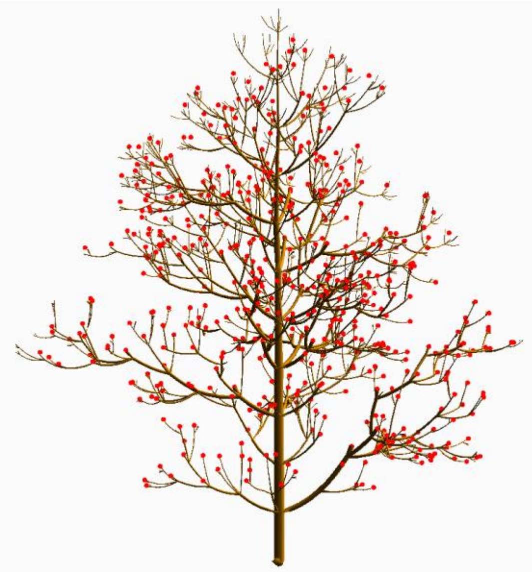
Flowering threshold

(pronounced parent child bias)

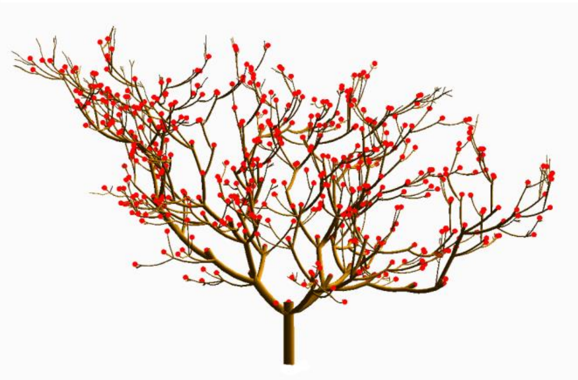
Flowering and Architectural Models



Rauh



Scarrone

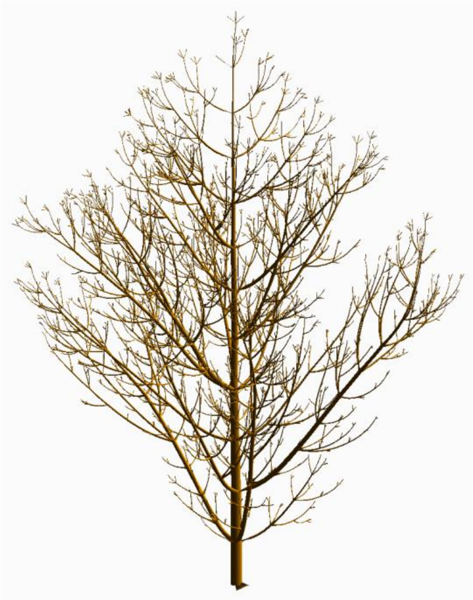


Leeuwenberg

Flowering threshold

(pronounced parent child bias)

Plagiotropy and Architectural Models



Rauh

Plagiotropy threshold

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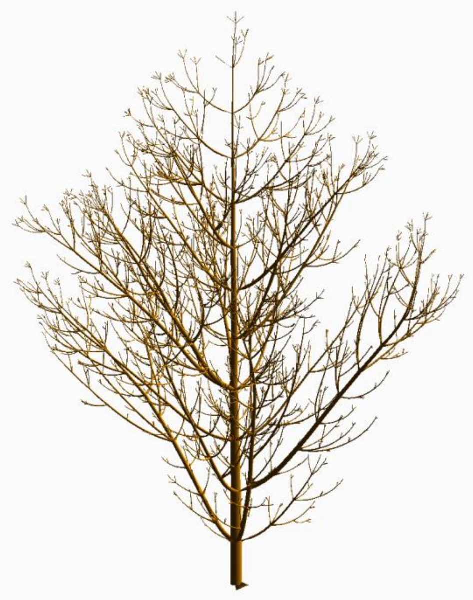
Plagiotropy and Architectural Models



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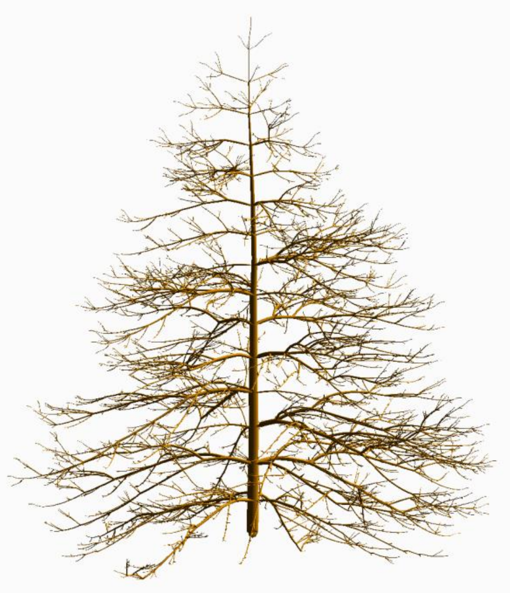
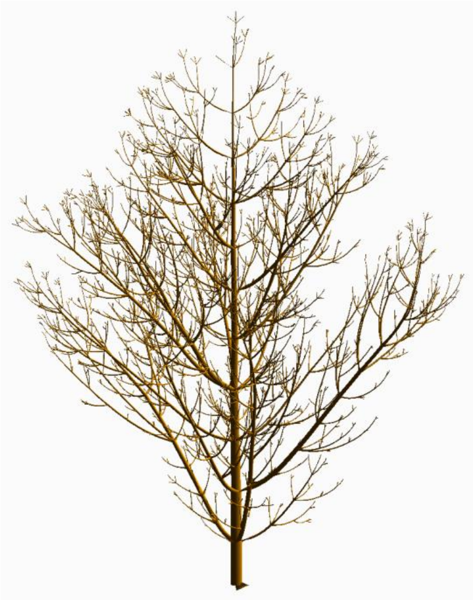


Massart

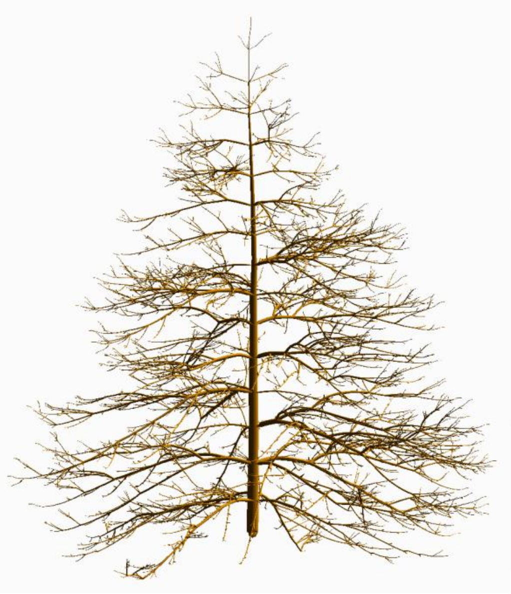
Plagiotropy threshold

(pronounced parent child bias)

Plagiotropy and Architectural Models



Rauh

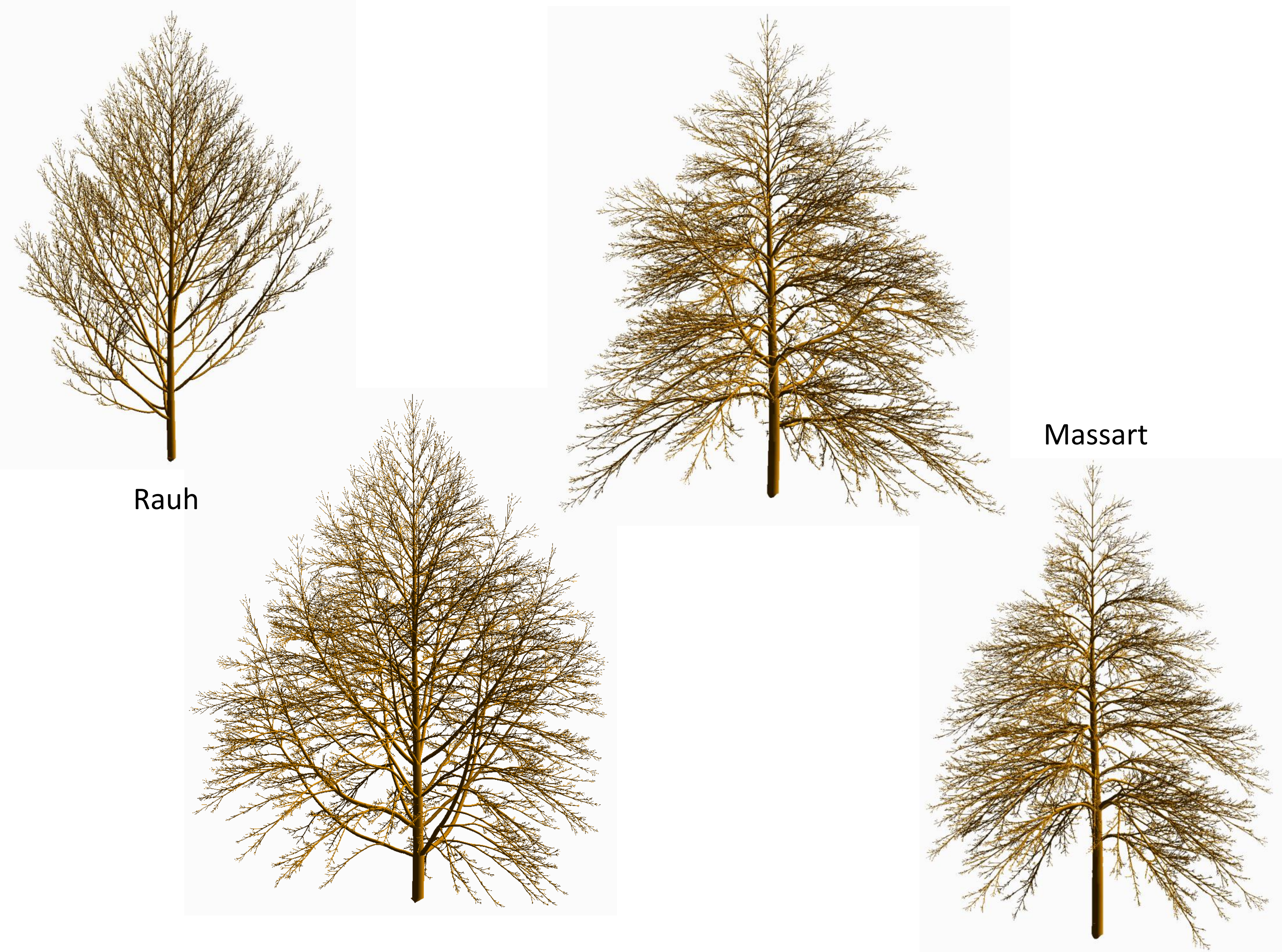


Massart

Troll

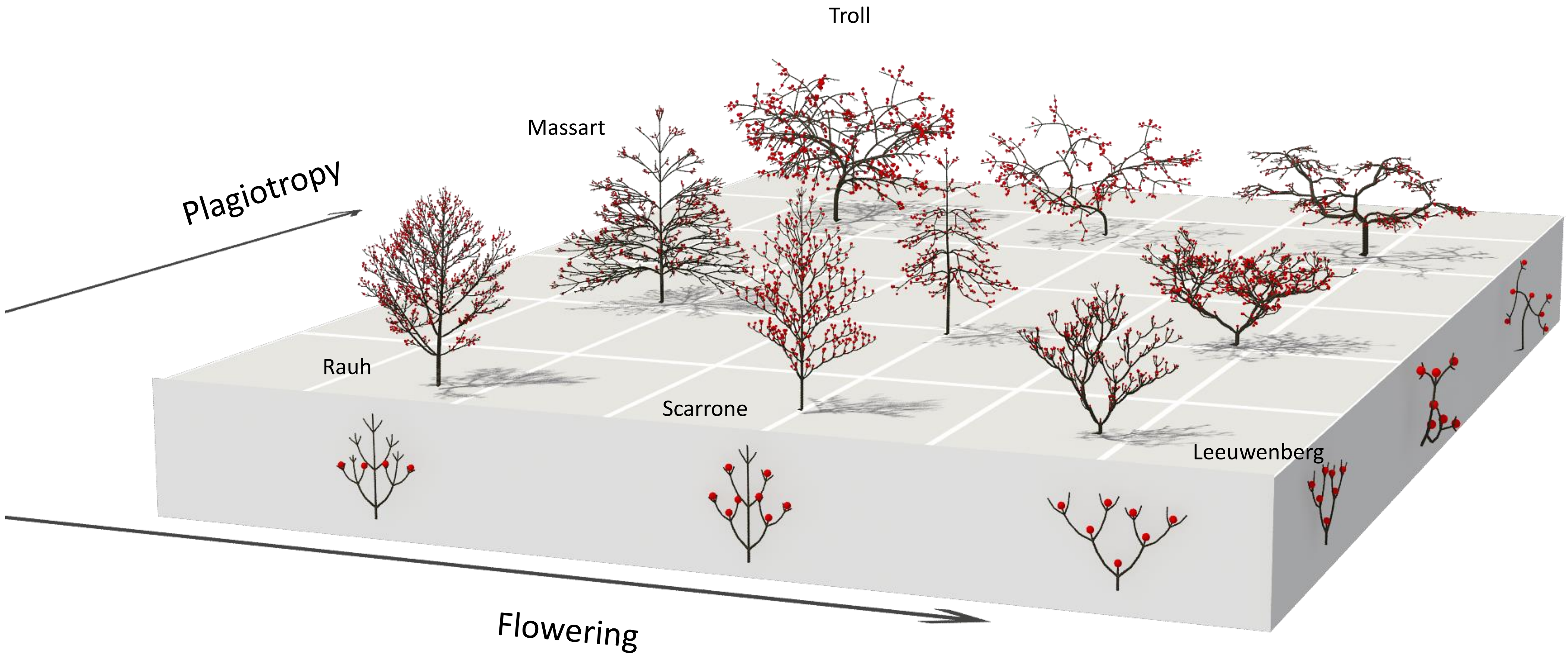
Plagiotropy threshold

(pronounced parent child bias)

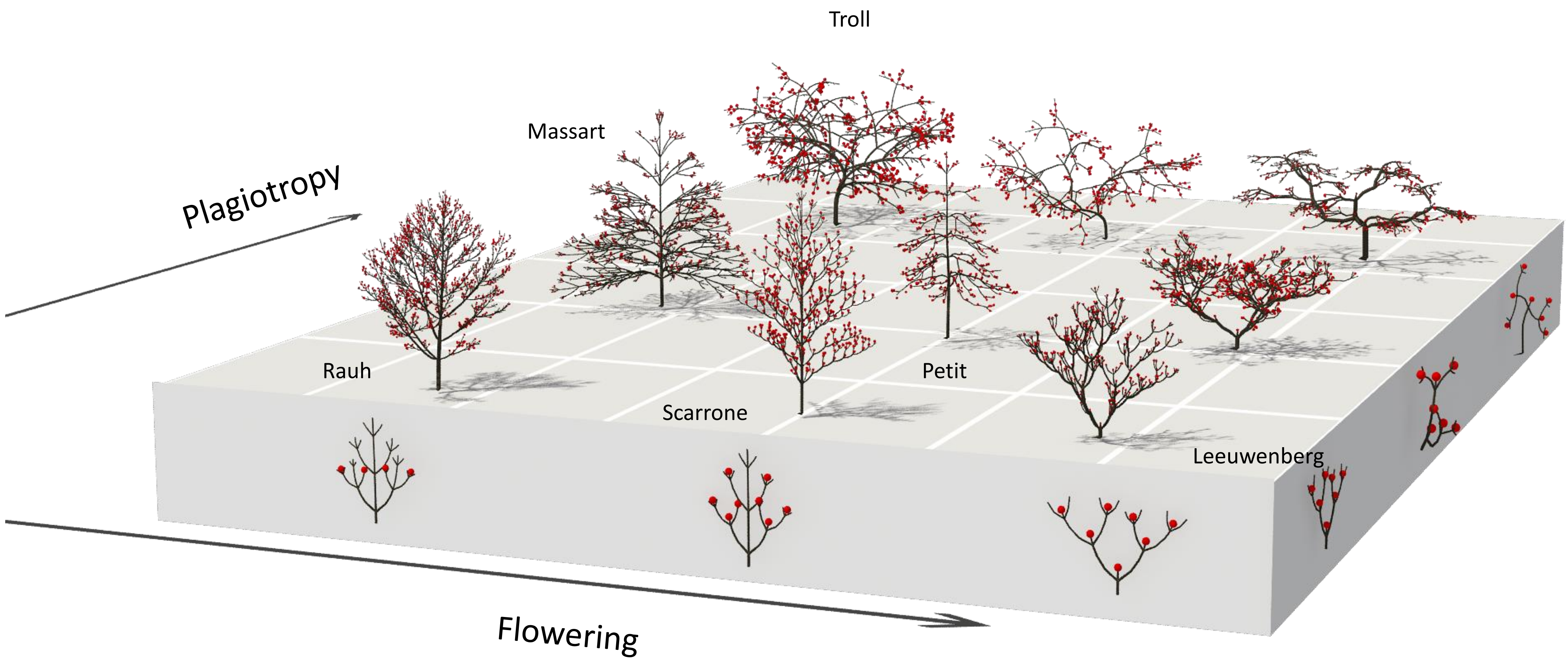

Rauh
Massart

Morphospace containing the Architectural Models

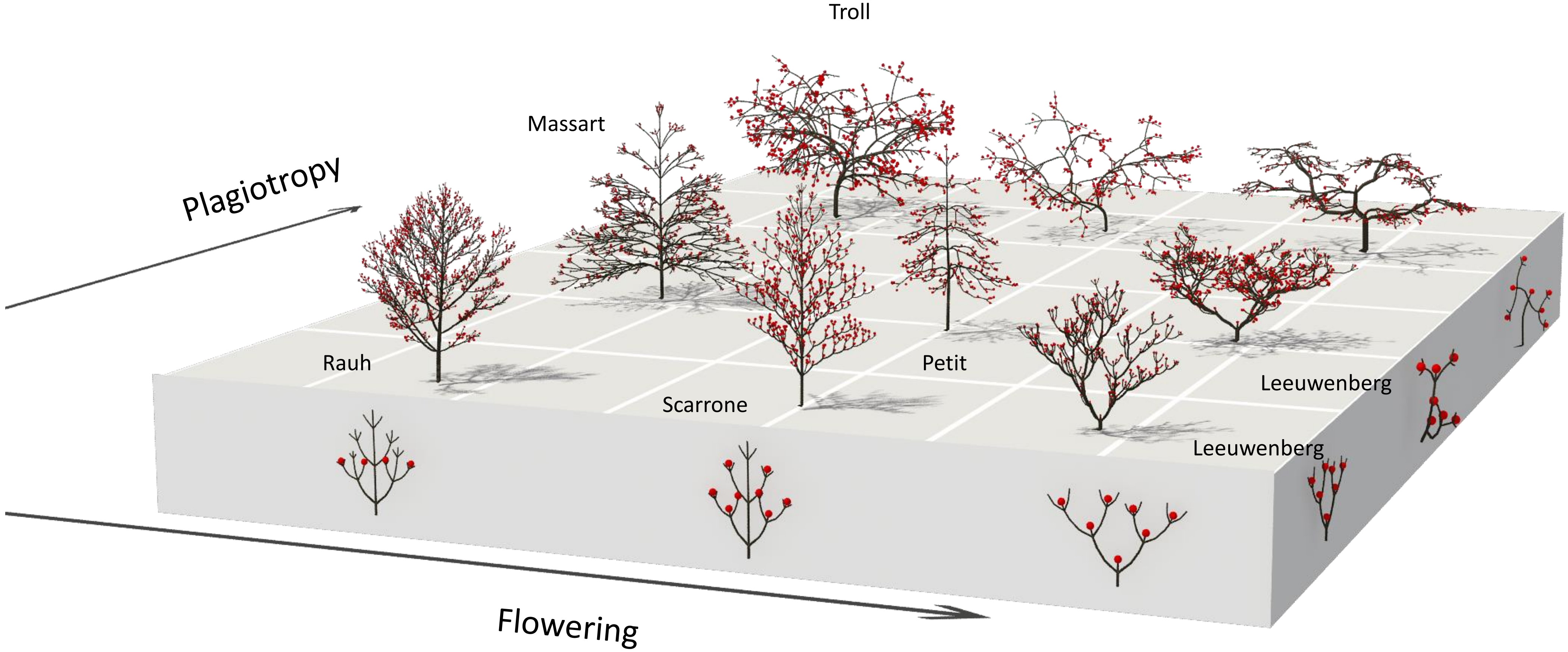
Plagiotropy x Flowering



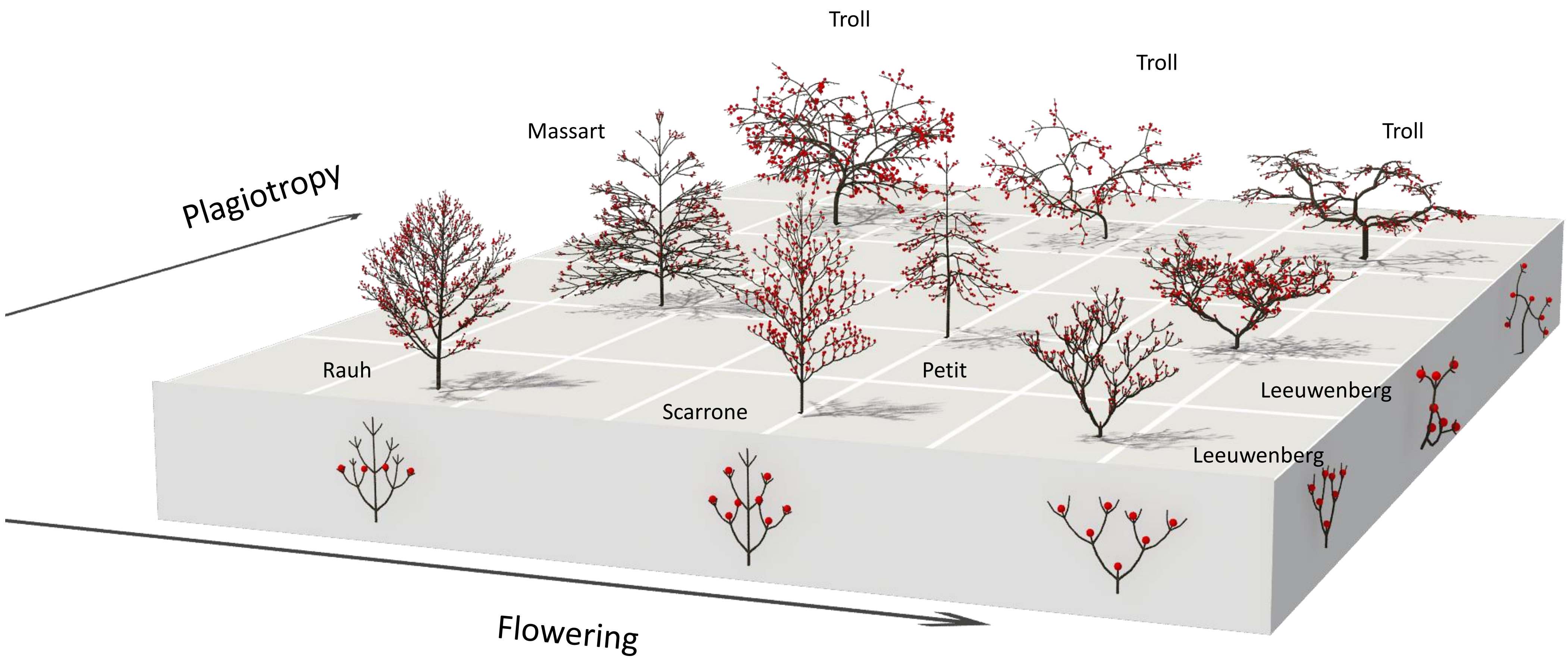
Plagiotropy x Flowering



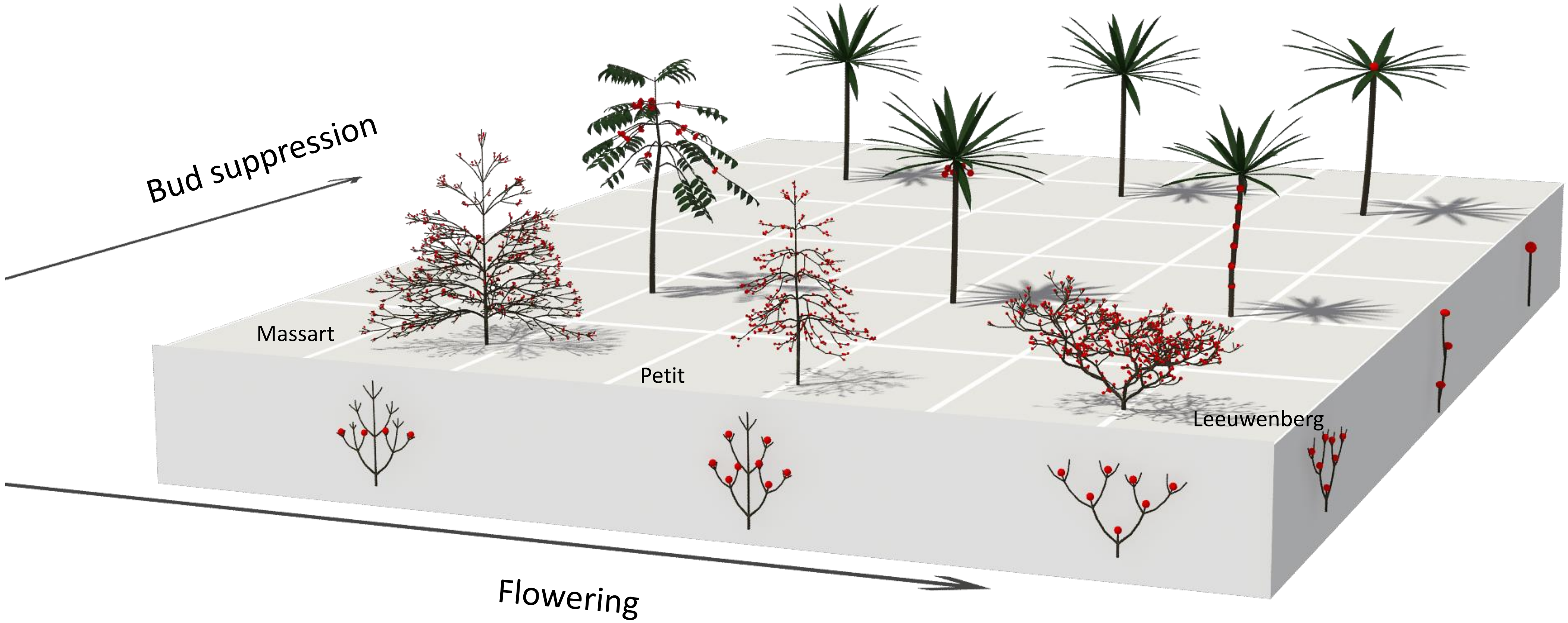
Plagiotropy x Flowering



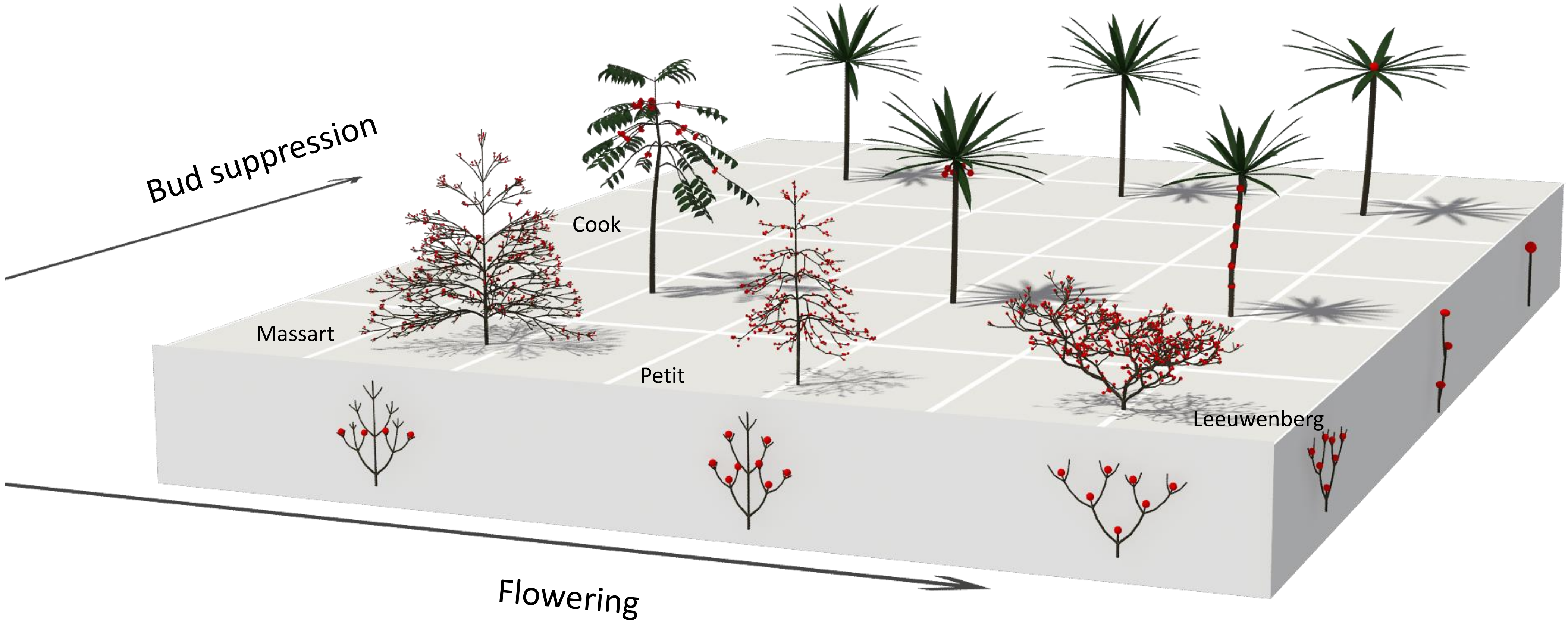
Plagiotropy x Flowering



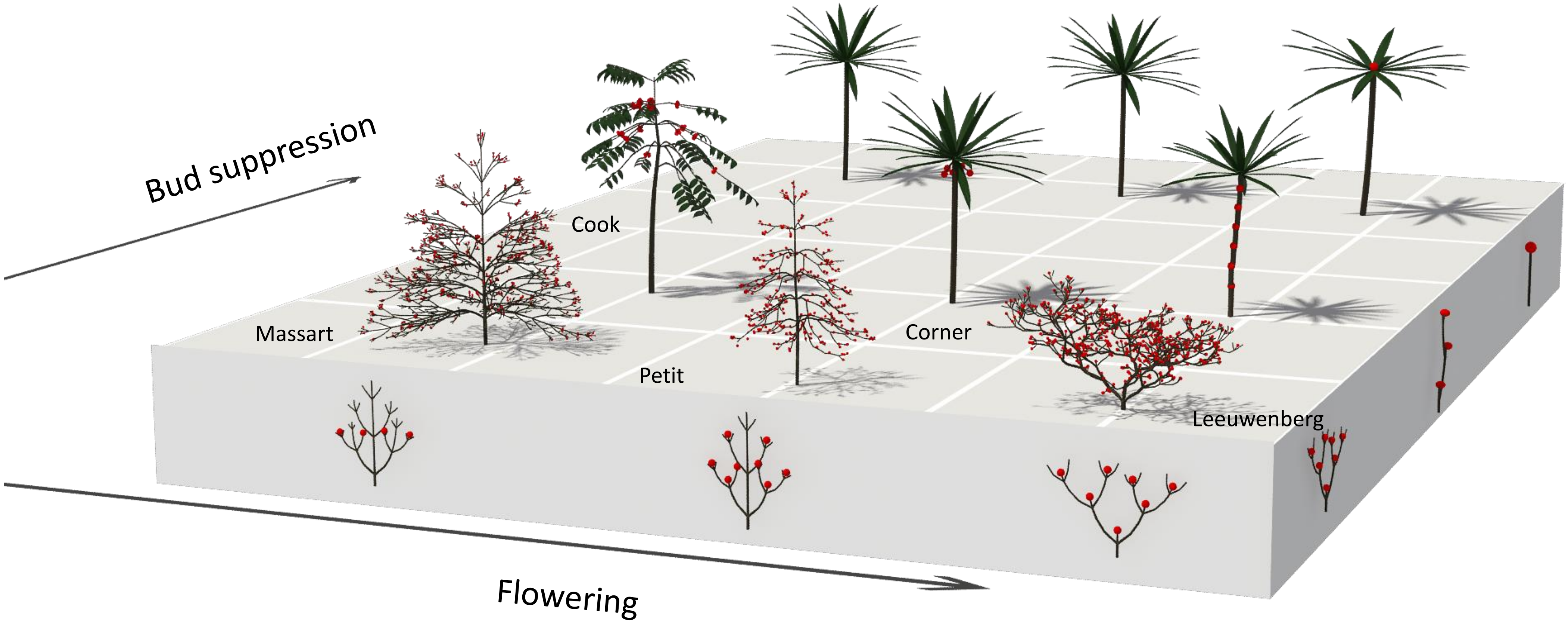
Bud Suppression x Flowering



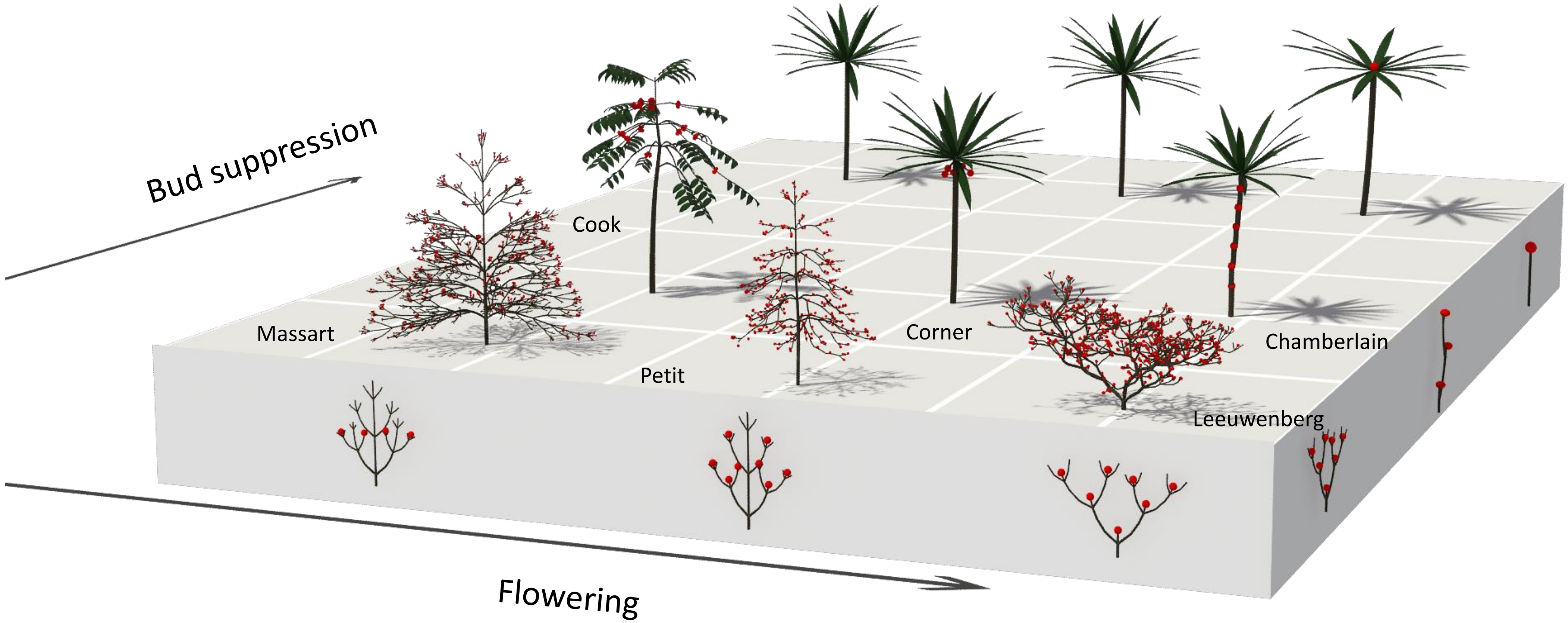
Bud Suppression x Flowering



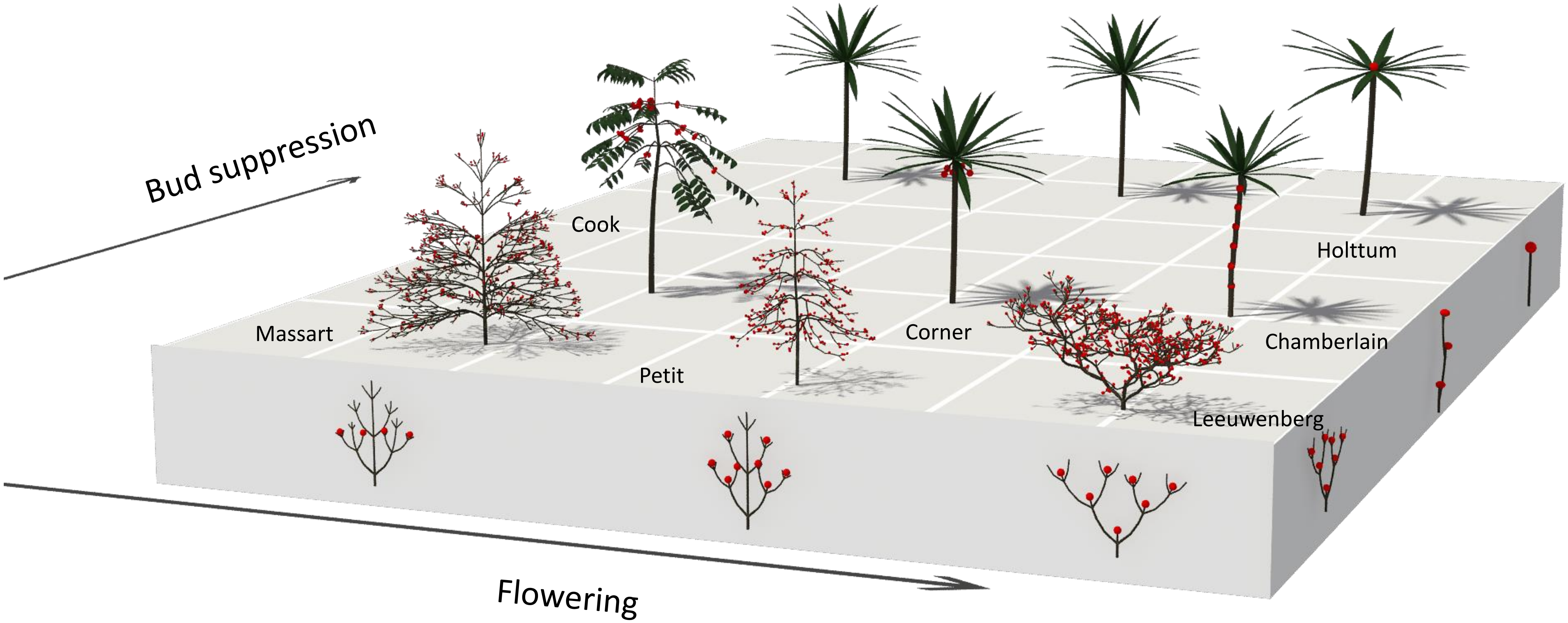
Bud Suppression x Flowering



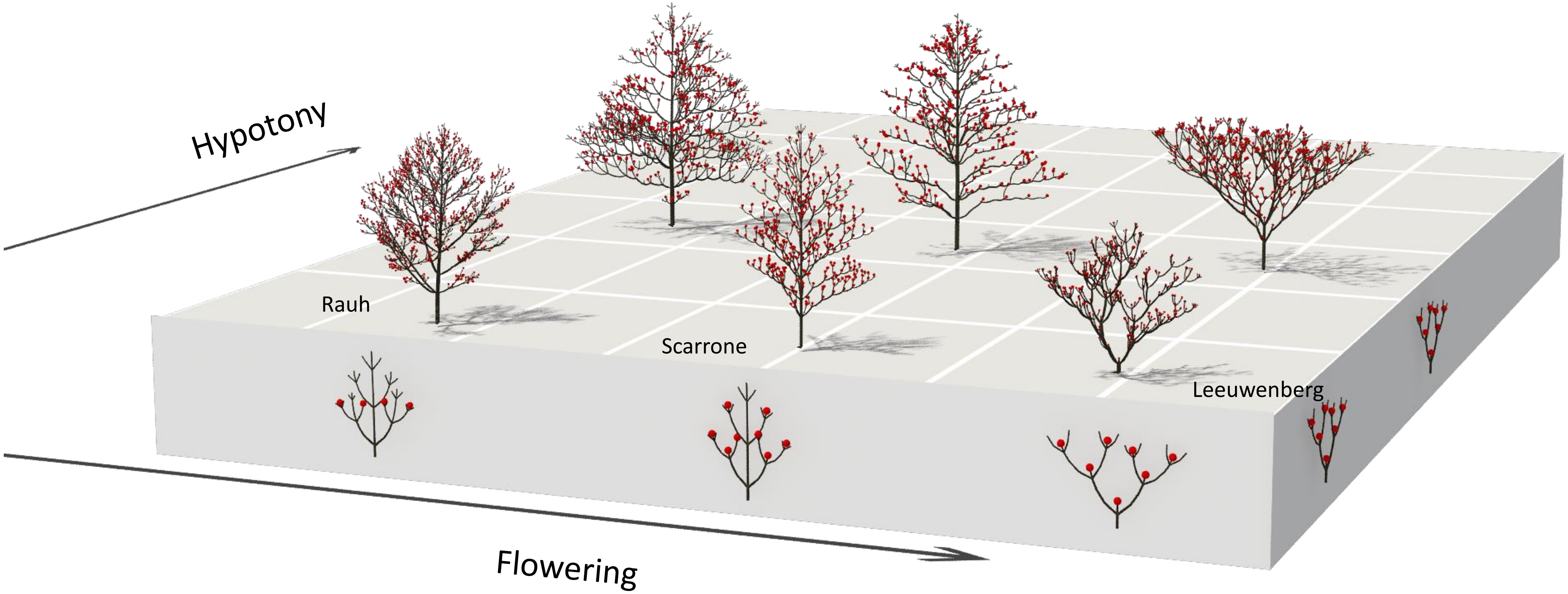
Bud Suppression x Flowering



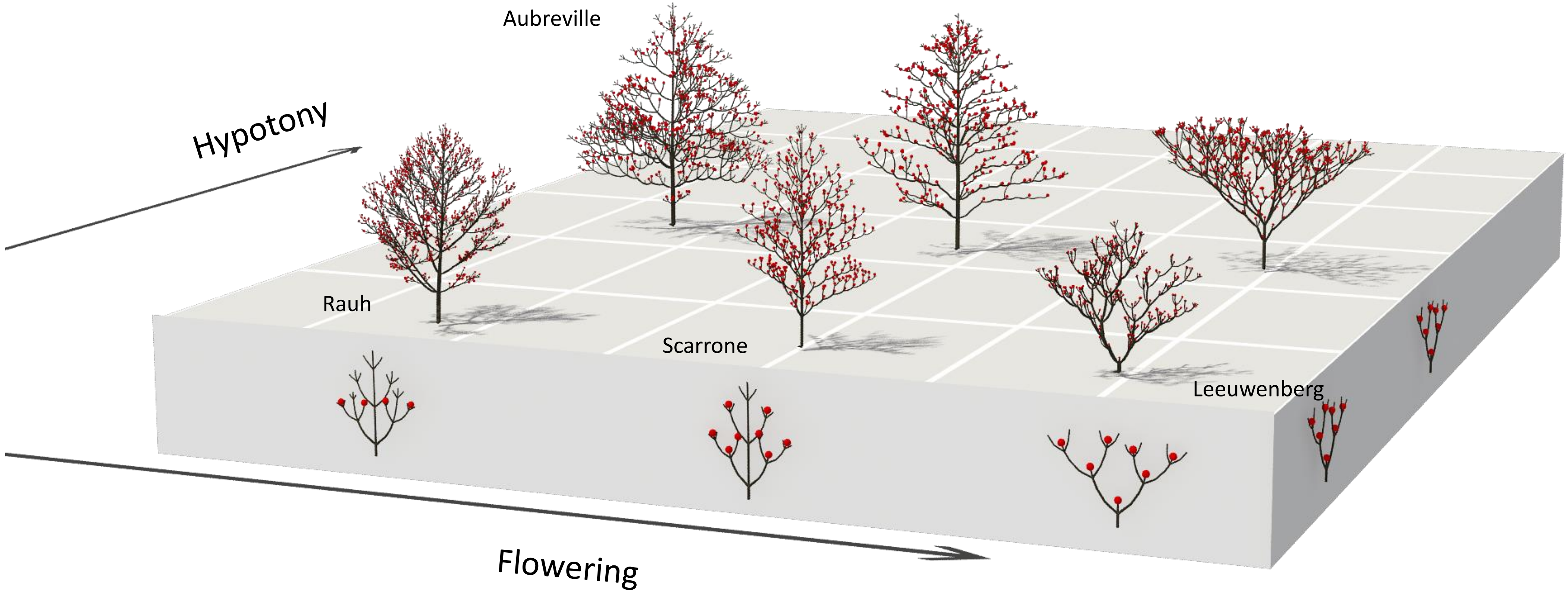
Bud Suppression x Flowering



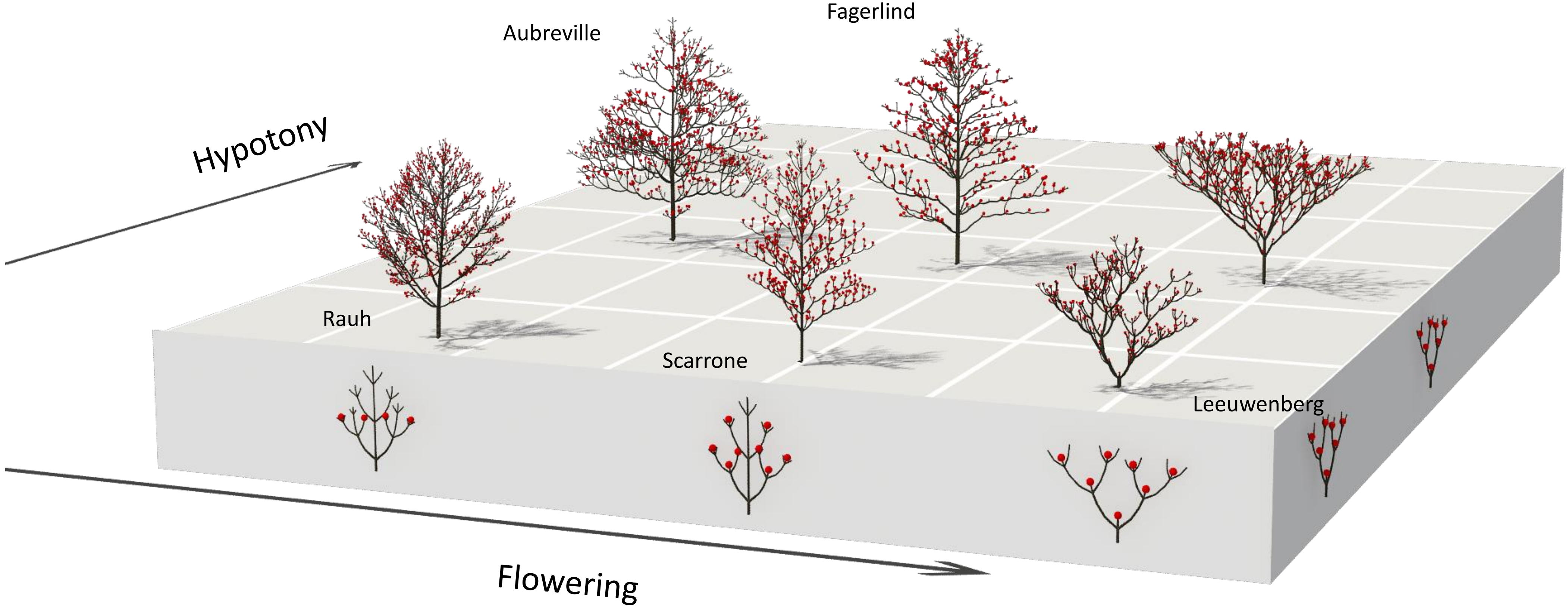
Hypotony x Flowering



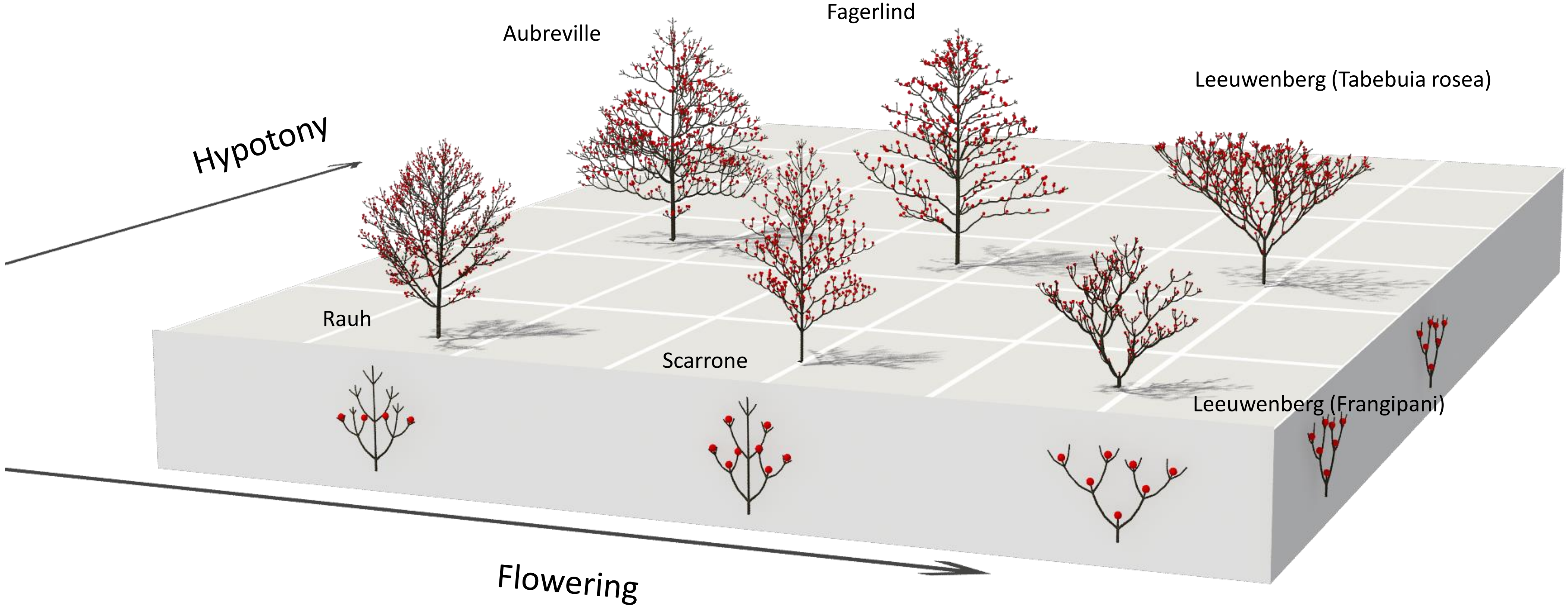
Hypotony x Flowering



Hypotony x Flowering



Hypotony x Flowering



Observations

- 20 Architectural Models are captured with the growth model
- Self-organization is fundamental for understanding plant architecture
- Highlights the key plant processes to describe a variety of different tree forms, presented in a mechanistic model of development

Comparison to real trees

Tabebuia rosea (Model of Leeuwenberg)

Comparison to real trees

Tabebuia rosea (Model of Leeuwenberg)

Sequoia sempervirens (Model of Massart)

Comparison to real trees

Phellodendron chinense (Model of Scarrone)

Tabebuia rosea (Model of Leeuwenberg)

Sequoia sempervirens (Model of Massart)

Comparison to real trees

Tabebuia rosea (Model of Leeuwenberg)

Phellodendron chinense (Model of Scarrone)

Delonix regia (Model of Troll)

Sequoia sempervirens (Model of Massart)

Modeling with Differential Equations

Differential equation

- Equations of the form $\frac{dx(t)}{dt} = f\ (x(t), t)$
- when x is a 1D function we call the above an **ordinary differential equation** otherwise a **partial differential equation**

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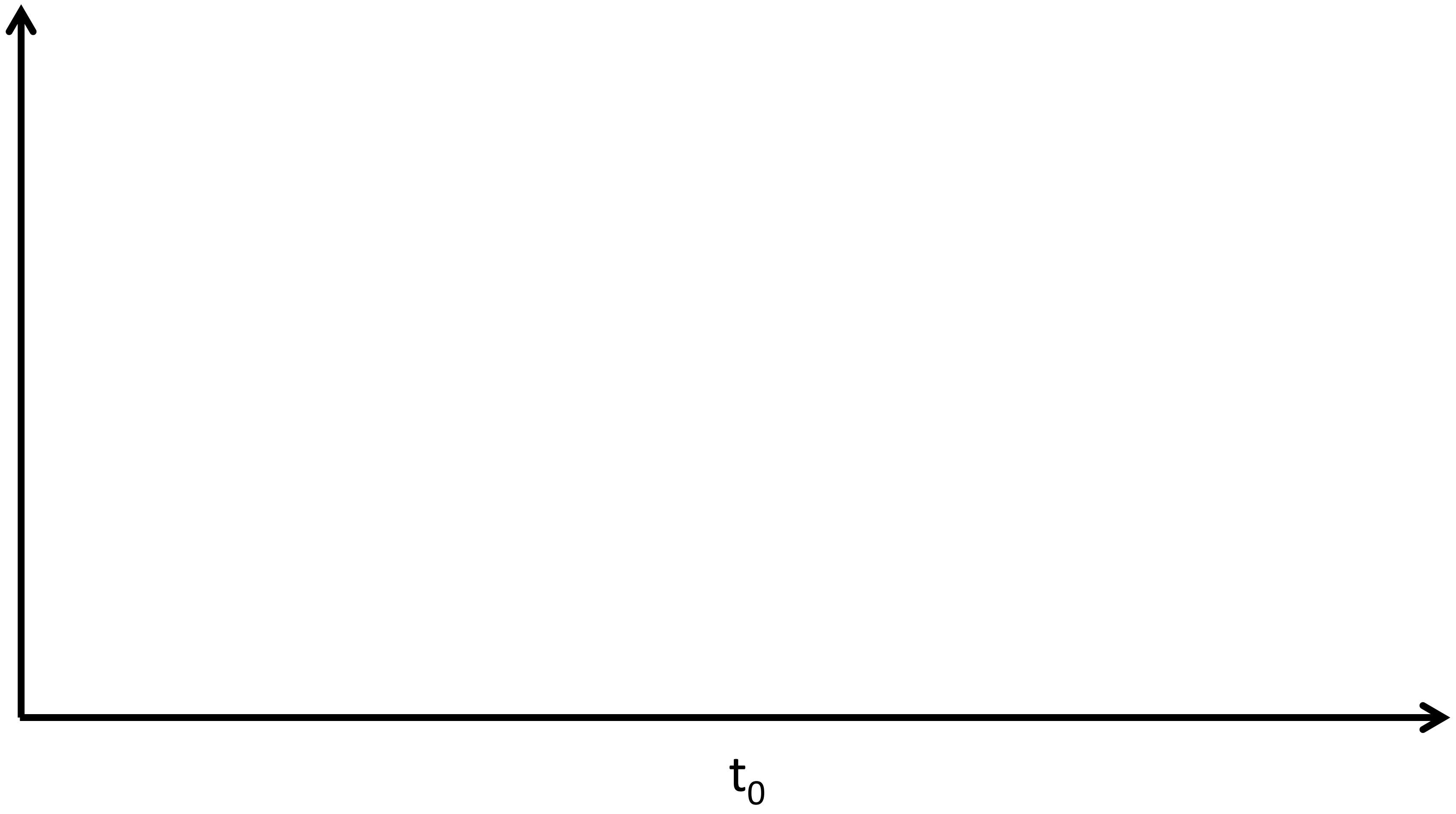
- $\frac{dx(t)}{dt}$ or $\frac{dx}{dt}$ or $x'(t)$ is read as "**the rate of change of x over t**"
- f is the function that computes the derivative of x with respect to t
- The solution to a differential equation is a **function x** that satisfies the equation

Geometric Interpretation (1st order ODE)



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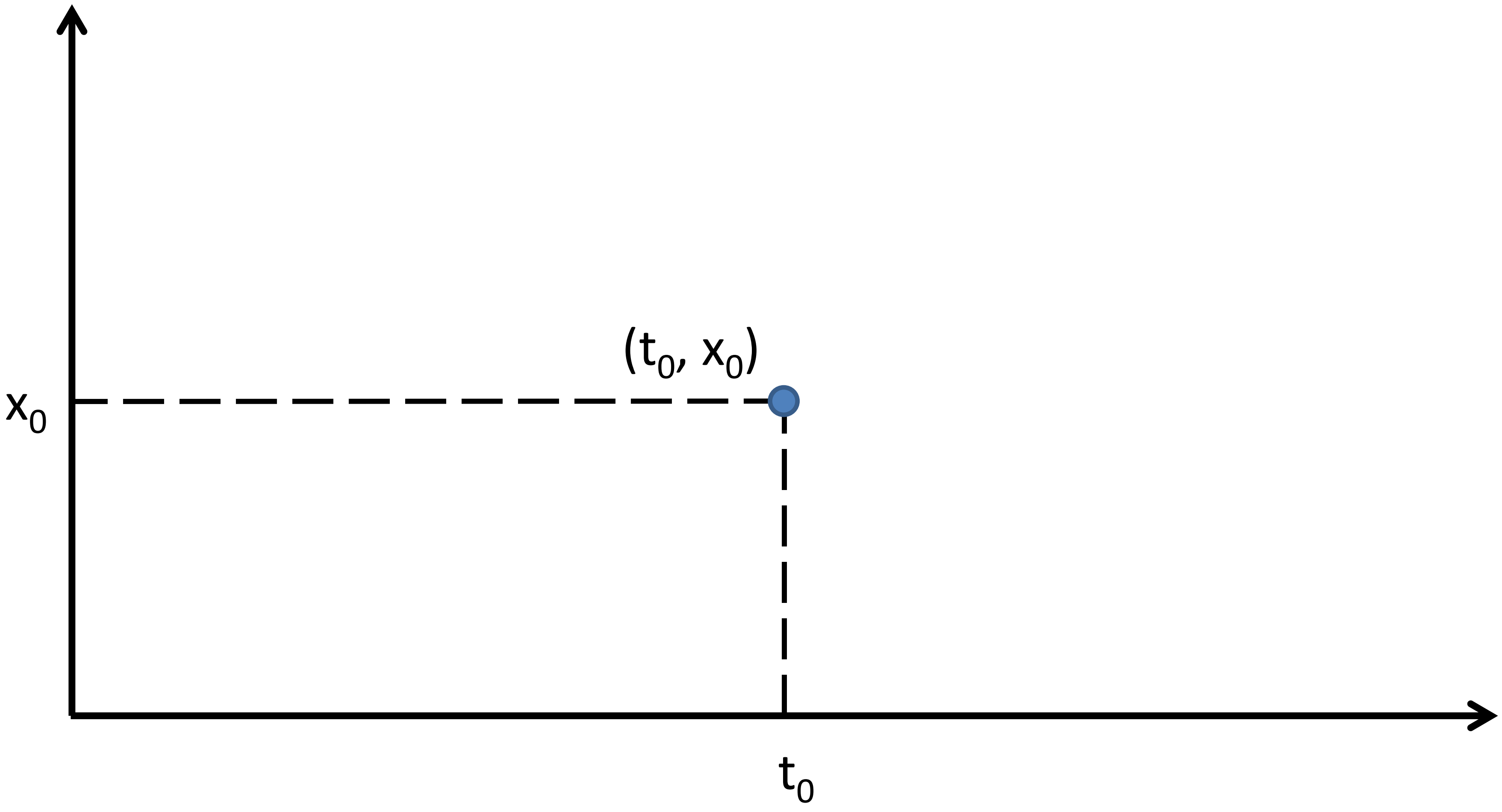

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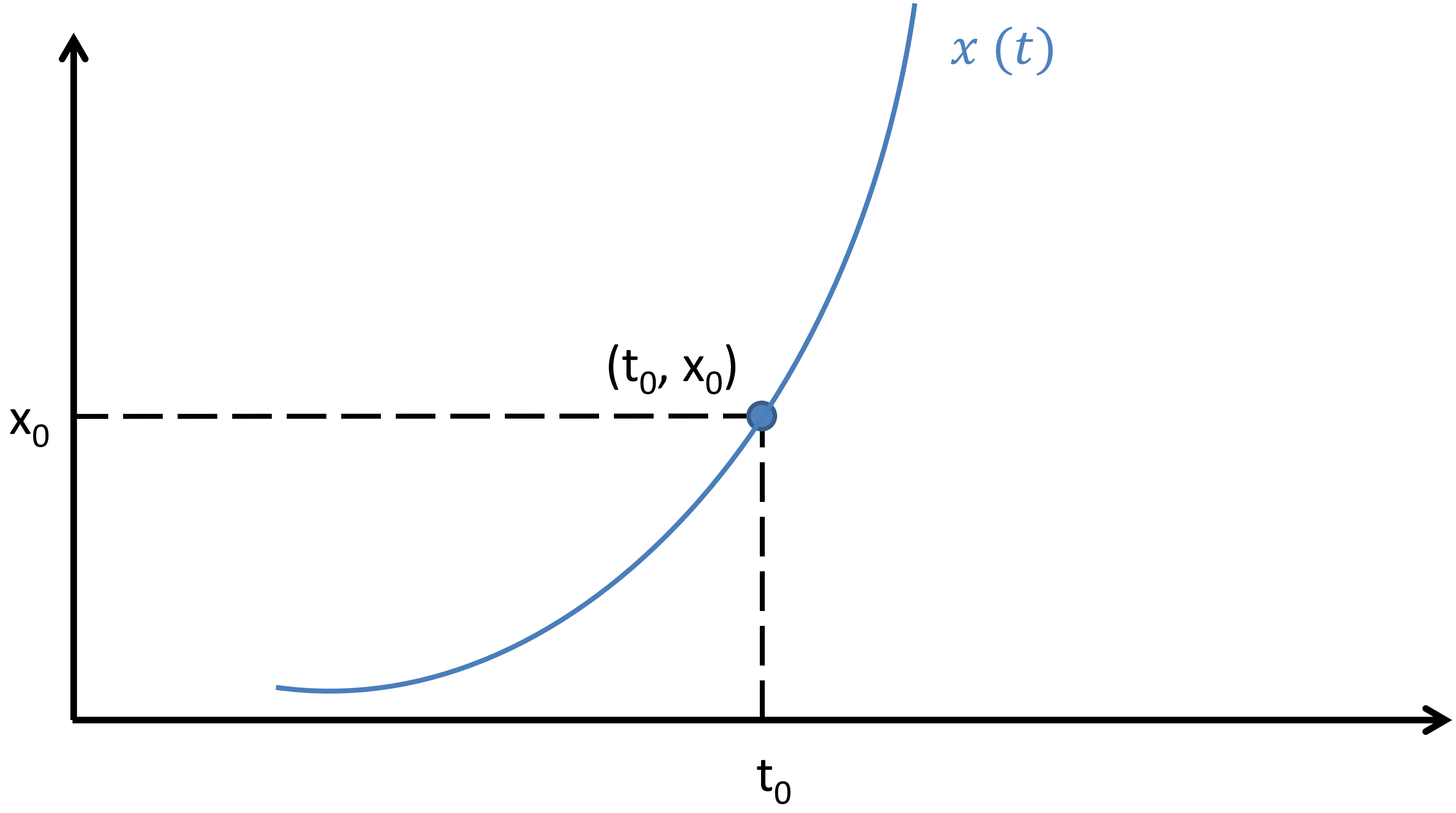

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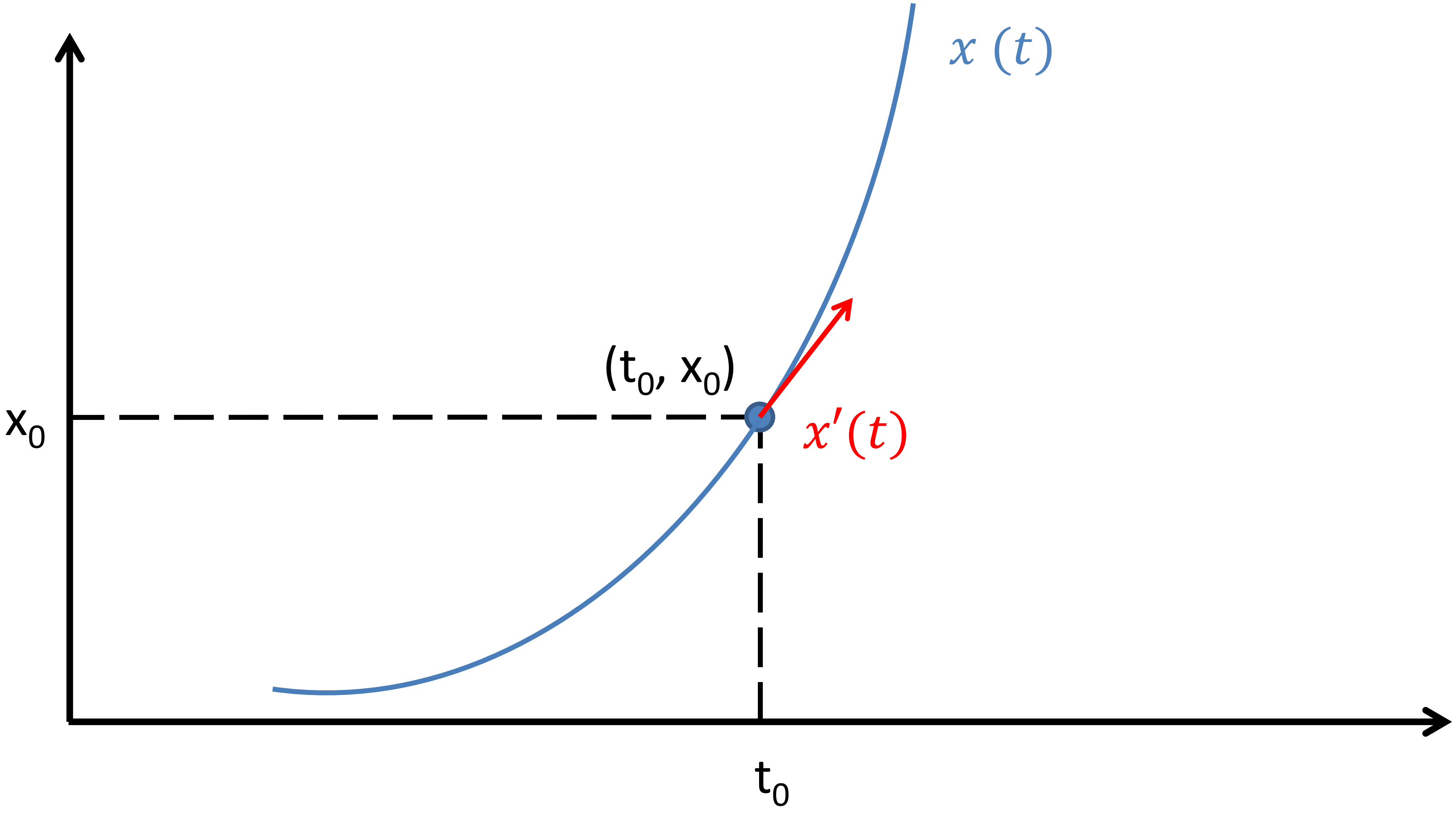

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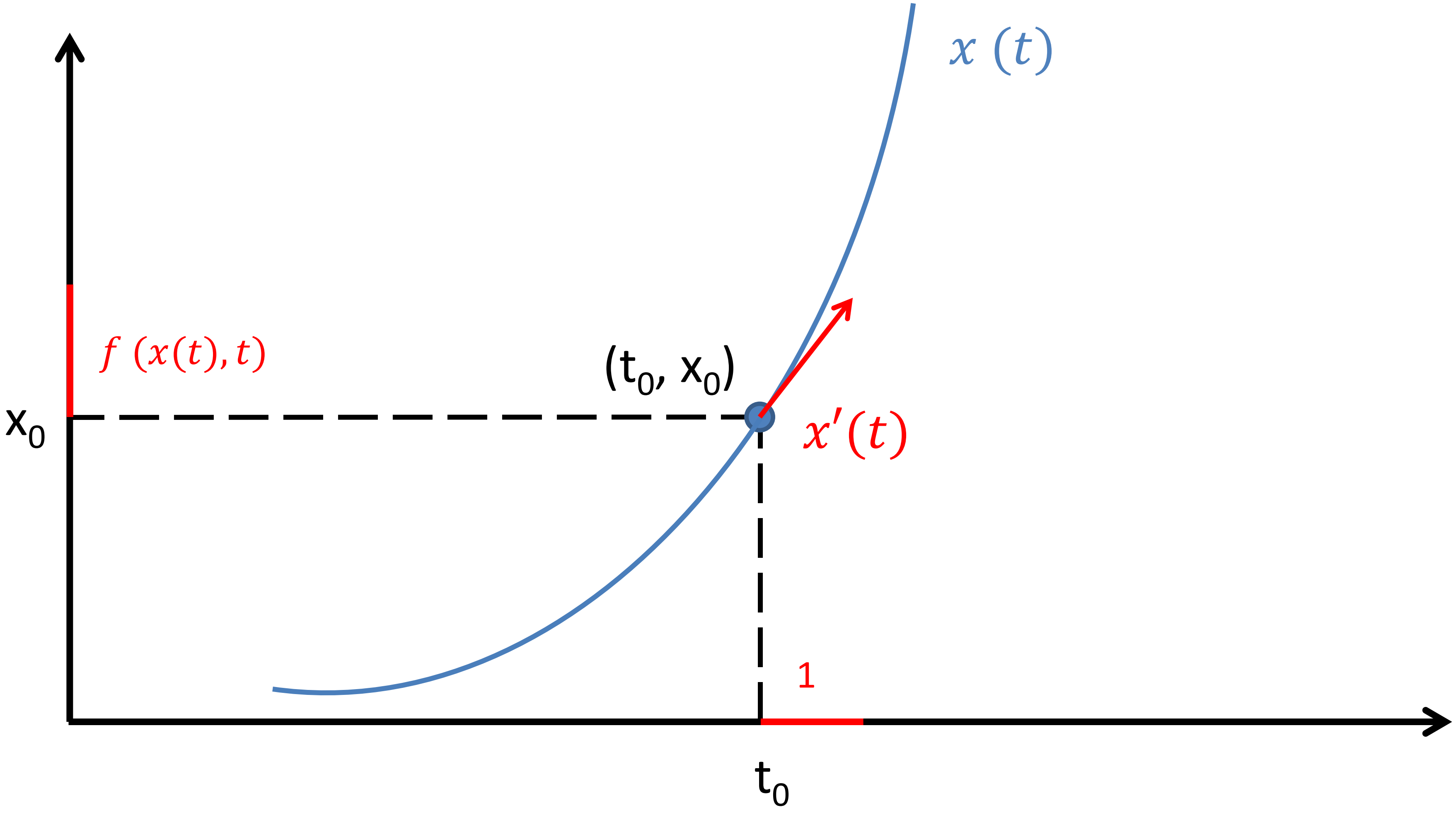
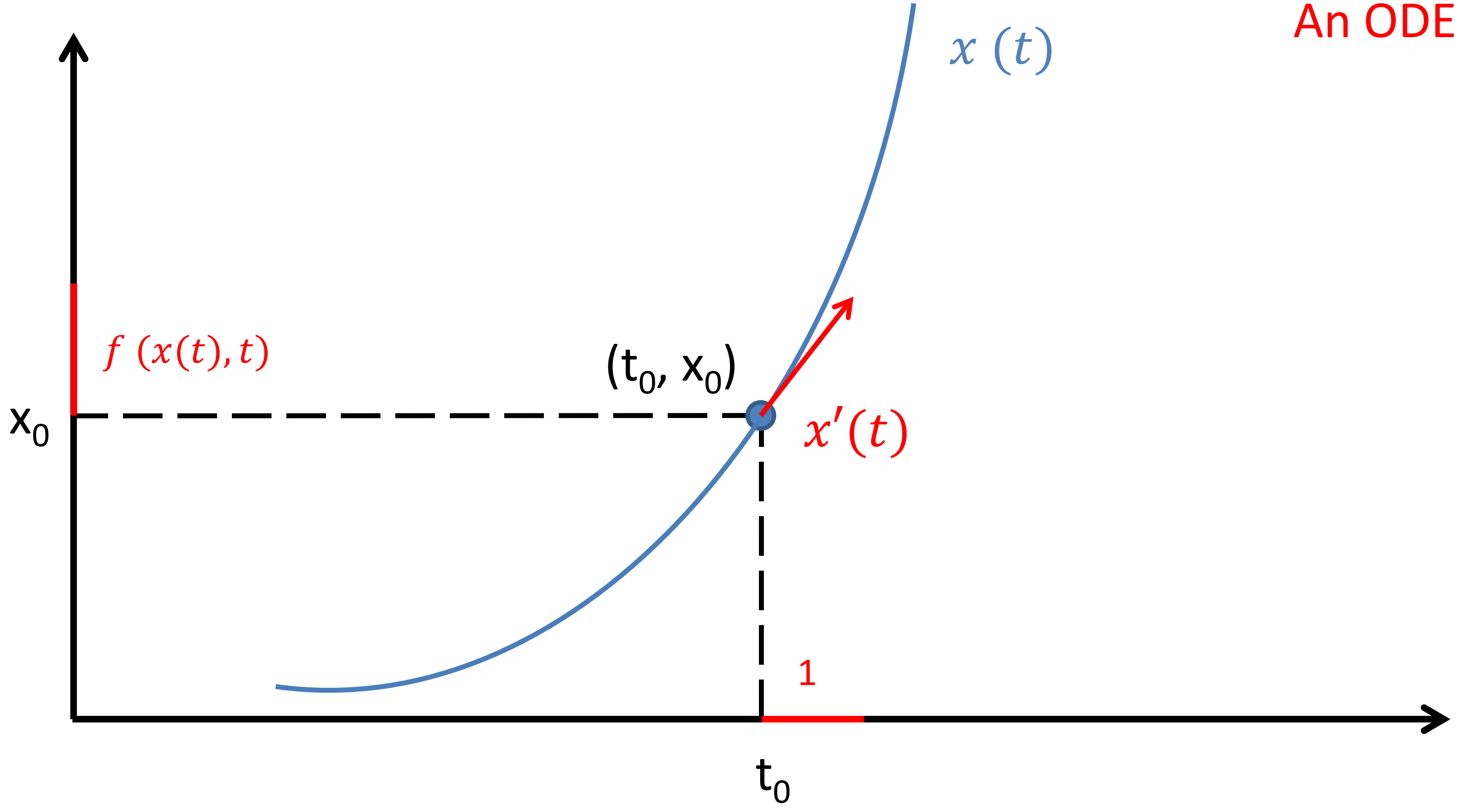
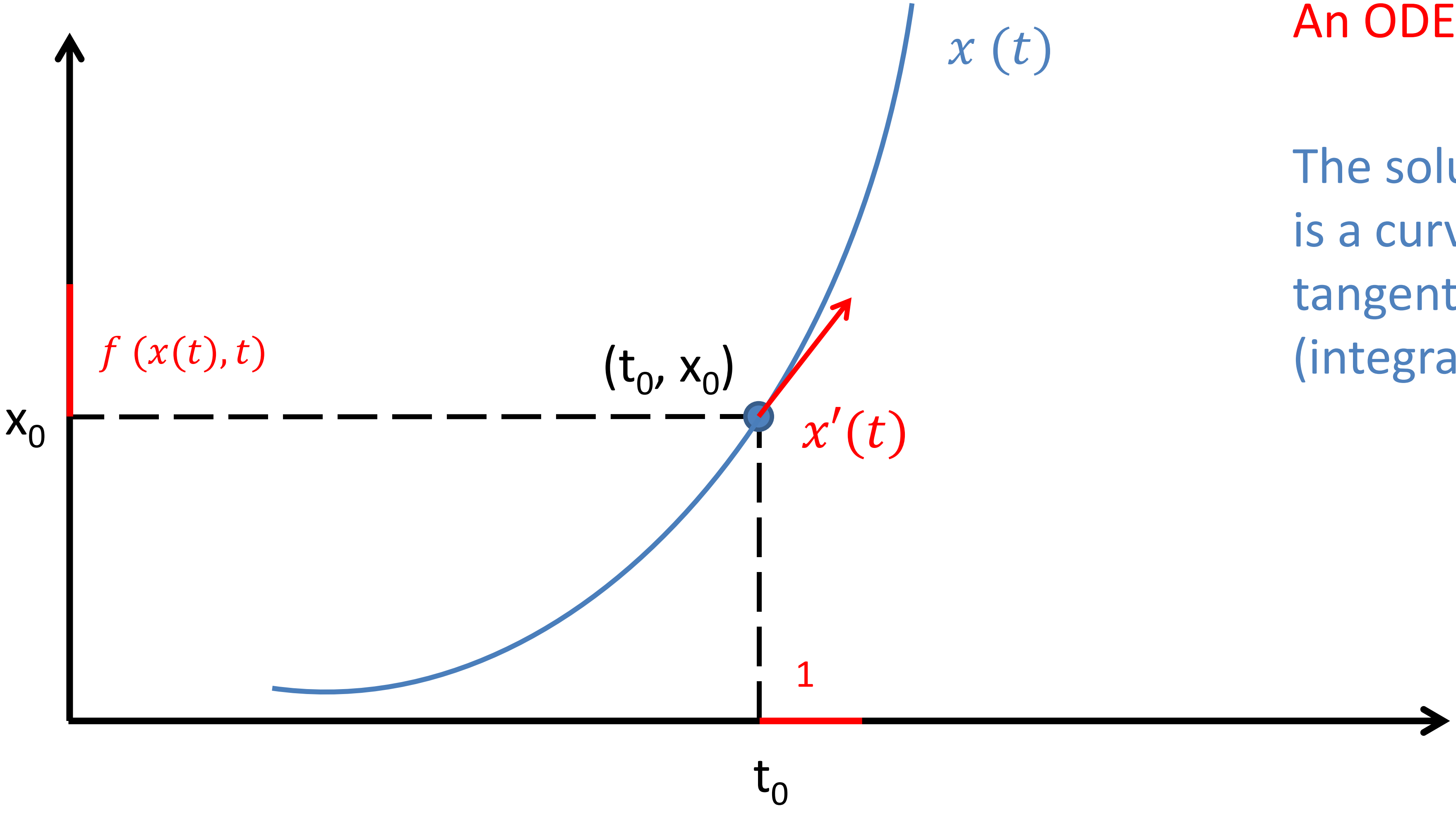


Geometric Interpretation (1st order ODE)

An ODE is a vector field



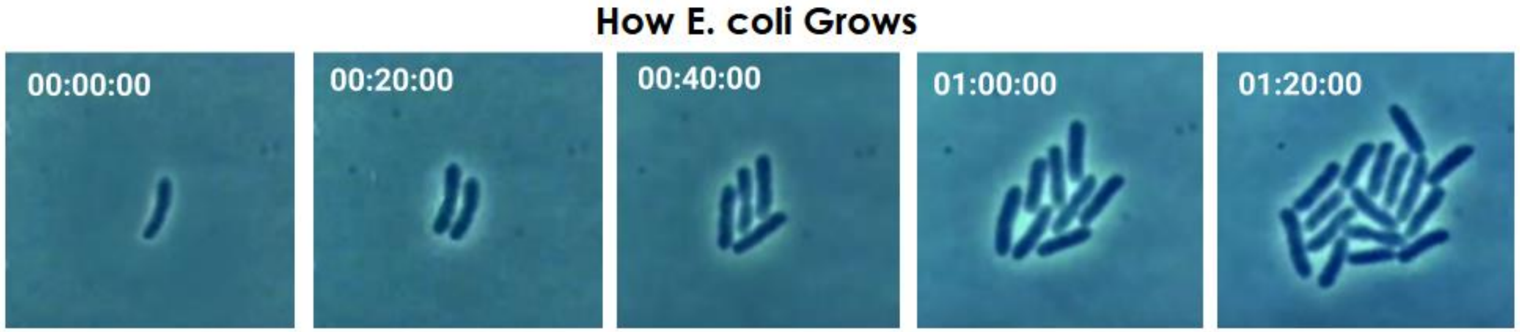
Geometric Interpretation (1^{st} order ODE)



An ODE is a vector field

The solution to an ODE is a curve which is tangential at all points, (integral curve)

Bacterial Growth



1 2 4 8 16

Modeling with differential equations

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- $\frac{1}{P}\frac{dP}{dt} = K$

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- $ln|P| = Kt + C_1$

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- $ln|P| = Kt + C_1$
- $|P| = e^{Kt+C_1}$

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Modeling with differential equations

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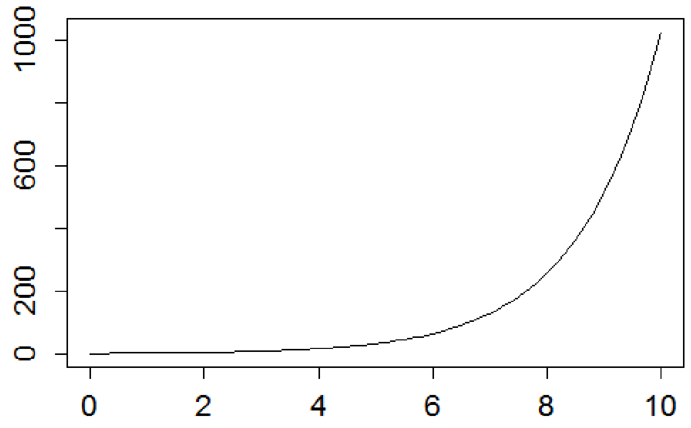
- $ln|P| = Kt + C_1$
- $|P| = e^{Kt+C_1} = e^{Kt}e^{C_1} = Ce^{Kt}$

Exponential Growth

- P = population, t = time(days)
- $\frac{dP}{dt} = KP$
- $\frac{1}{P}\frac{dP}{dt} = K$
- $\frac{1}{P}dP = Kdt$
- $\int \frac{1}{P}dP = \int Kdt$
- $ln|P| = Kt + C_1$
- $|P| = e^{Kt+C_1} = e^{Kt}e^{C_1} = Ce^{Kt}$

$$P(t) = Ce^{Kt}$$

SOLUTION



Verification

$P'(t) = (Ce^{Kt})'$

Verification

$$P'(t) = (Ce^{Kt})' = KCe^{Kt}$$

Verification

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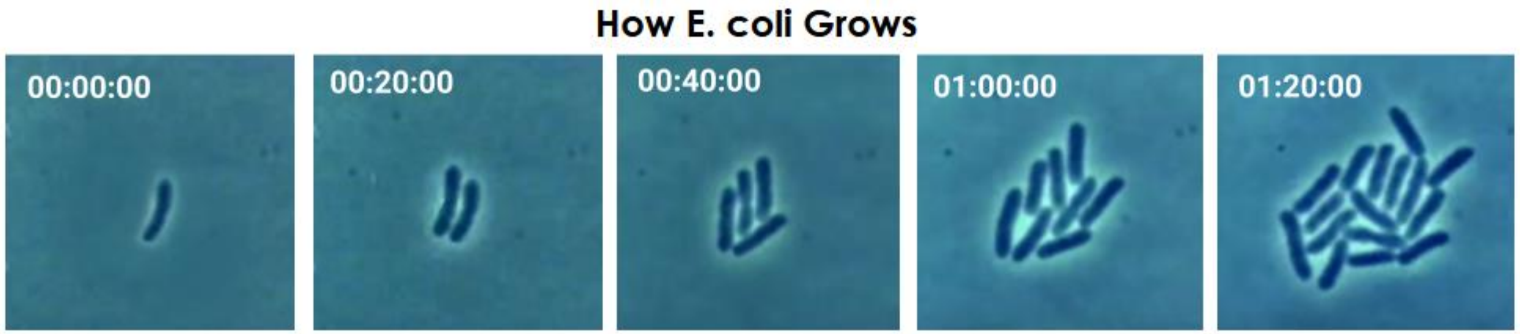
Verification

$$P'(t) = (Ce^{Kt})' = KCe^{Kt} = KP(t) = KP$$

Example

$$\boxed{P = Ce^{Kt}}$$

- $t = 0 \qquad P = 1$
- $t = 80 \quad P = 16$



Example

$$\boxed{P = Ce^{Kt}}$$

- $t = 0 \qquad P = 1 \qquad 1 = Ce^{0}$
- $t = 80 \quad P = 16$

Example

$$\boxed{P = Ce^{Kt}}$$

- $t = 0 \qquad P = 1 \qquad 1 = Ce^0 = C$
- $t = 80 \quad P = 16$

Example

$$\boxed{P = Ce^{Kt}}$$

- $t = 0 \qquad P = 1 \qquad 1 = Ce^0 = C$
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Example

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- $\qquad ln16 = 80K$

Example

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- $t = 0 \qquad P = 1 \qquad 1 = Ce^{0} = C$
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- $ln16 = 80K$
- $K = \frac{ln16}{80}$

Example

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$$\boxed{P(t) = e^{\frac{ln16}{80}t}}$$

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$$\boxed{P(t) = e^{\frac{ln16}{80}t}}$$

C → Population at time 0

Example

$$P = Ce^{Kt}$$

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- $t = 80 \qquad P = 16 \qquad 16 = e^{80K}$
- $ln16 = 80K$
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$$P(t) = e^{\frac{ln16}{80}t}$$

C → Population at time 0

K → coefficient of growth

Example

$$P = Ce^{Kt}$$

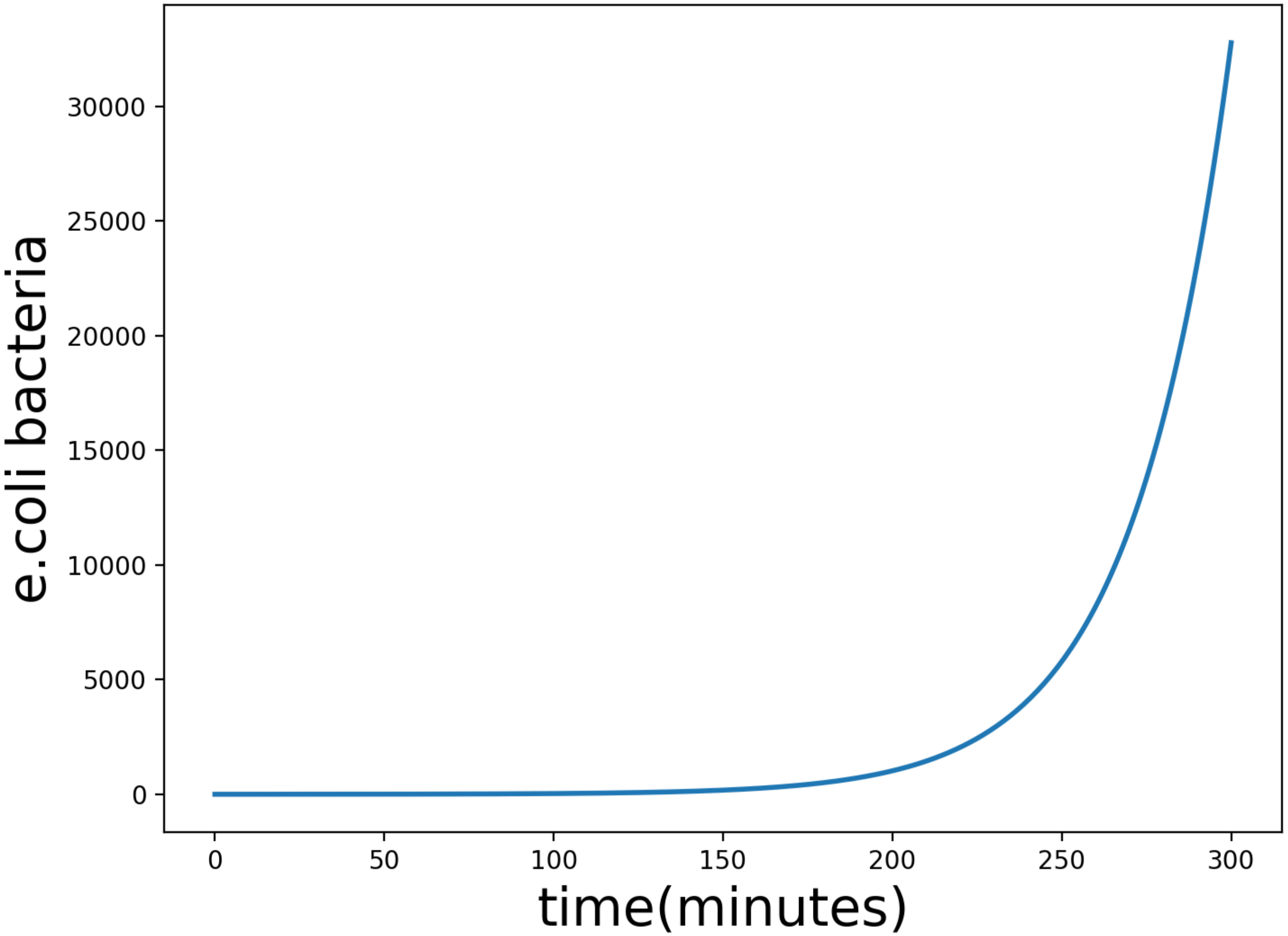
- $t = 0 \quad P = 1 \quad 1 = Ce^0 = C$
- $t = 80 \quad P = 16 \quad 16 = e^{80K}$
- $ln16 = 80K$
- $K = \frac{ln16}{80}$

$$P(t) = e^{\frac{ln16}{80}t}$$

C → Population at time 0

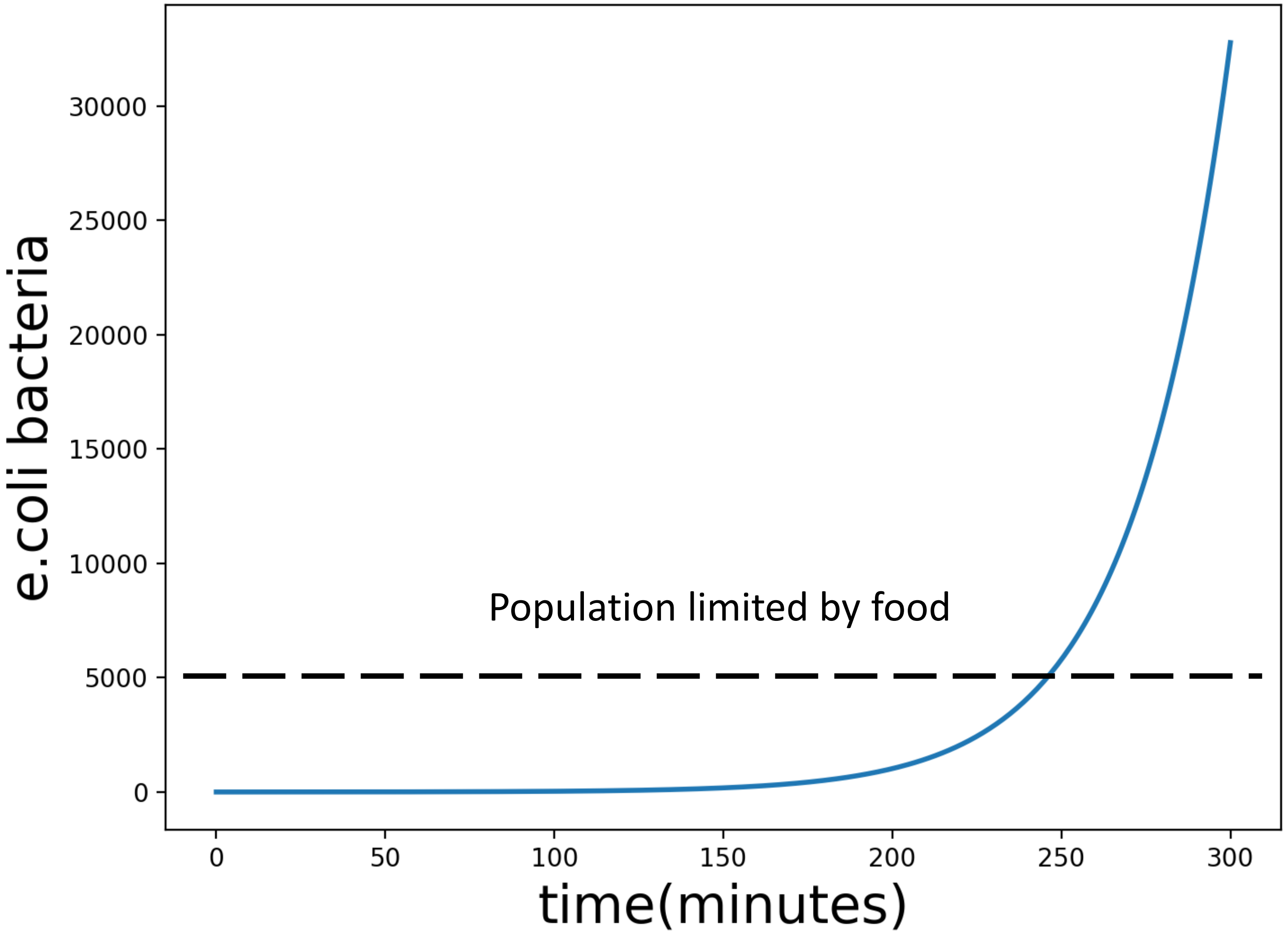
K → coefficient of growth (unit is 1/t)

Mathematical Model of e.coli Growth



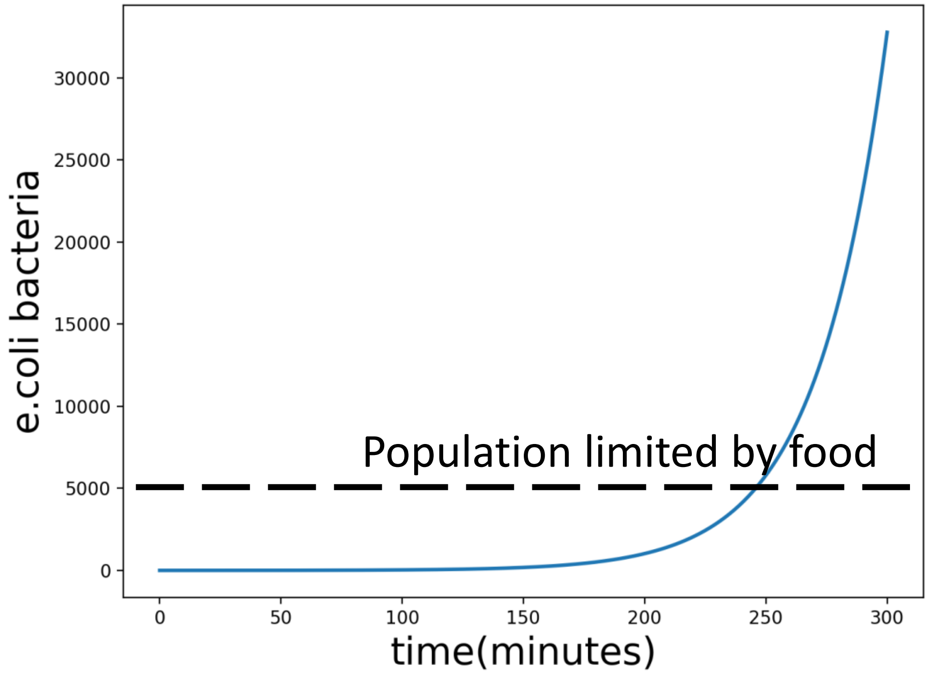
*also used to compute compound interest rates

Population growth N relative to food C



Population growth N relative to food C

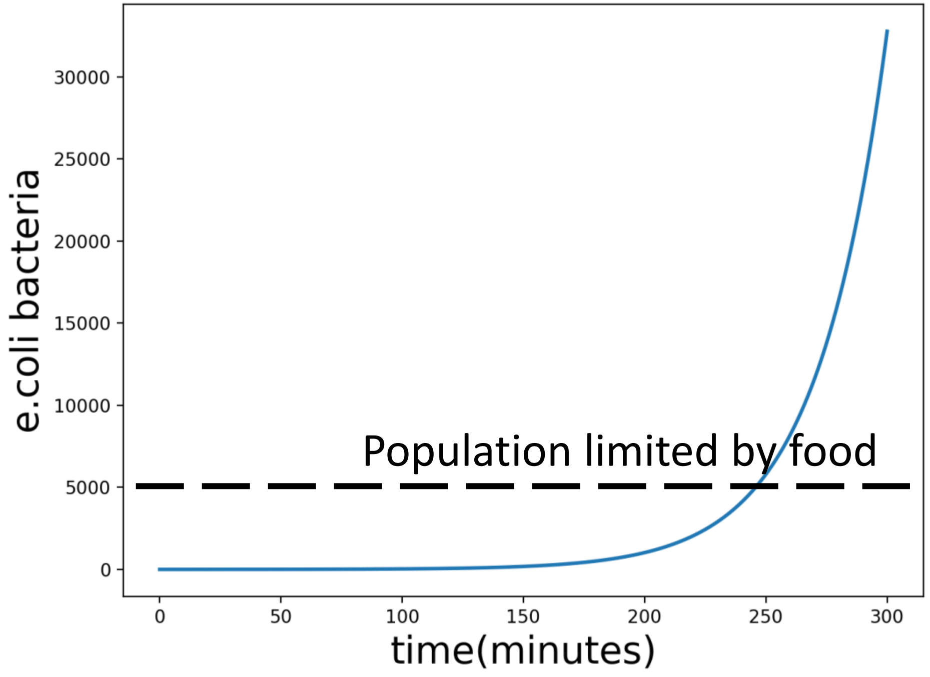
- $N' = K(C)N$



Population growth N relative to food C

- $N' = K(C)N$

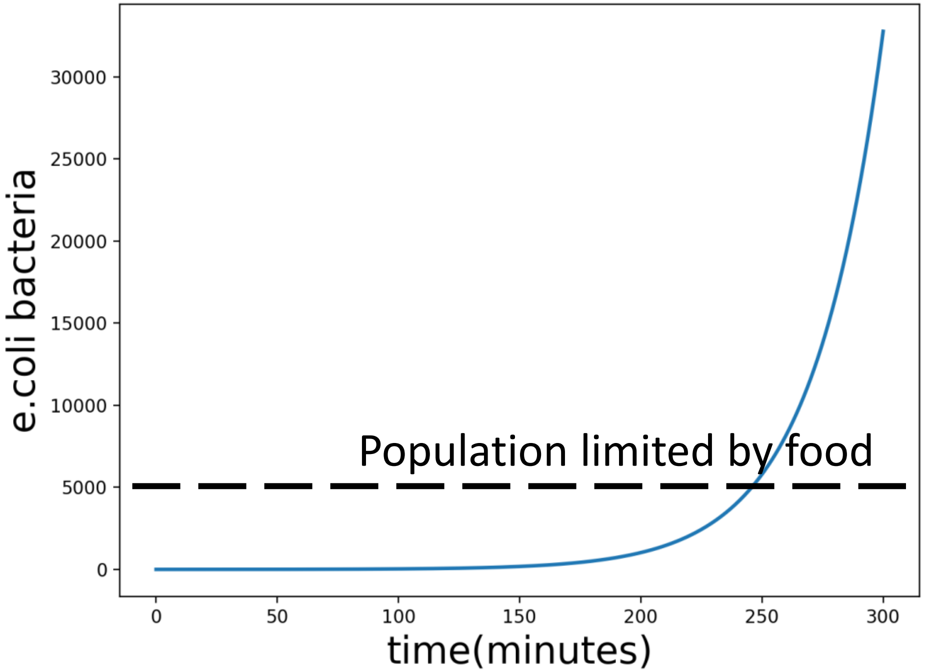
K is a function of how food is converted to growth



Population growth N relative to food C

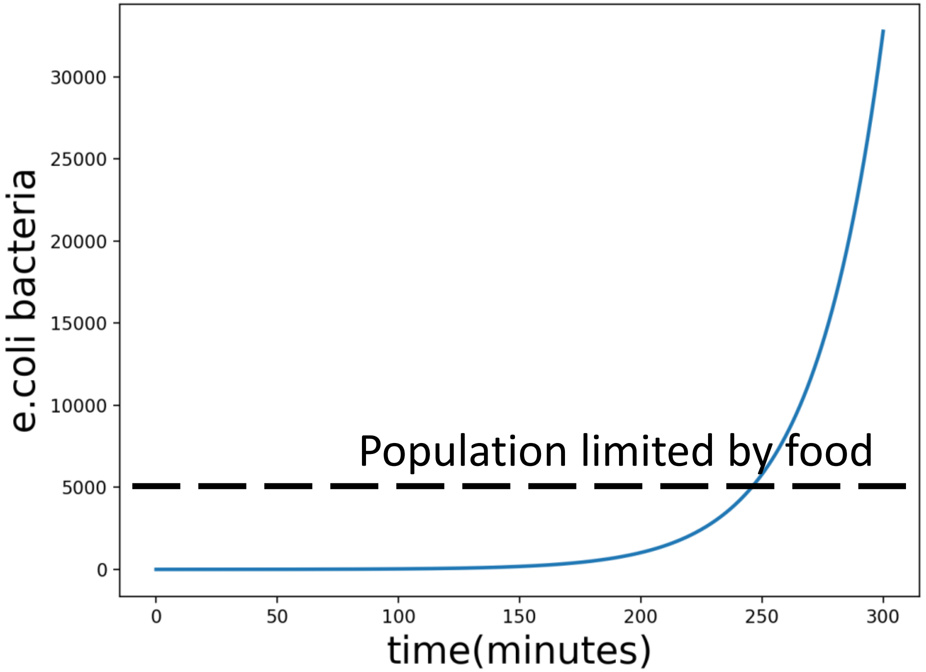
- $N' = K(C)N$

C(t) is food concentration



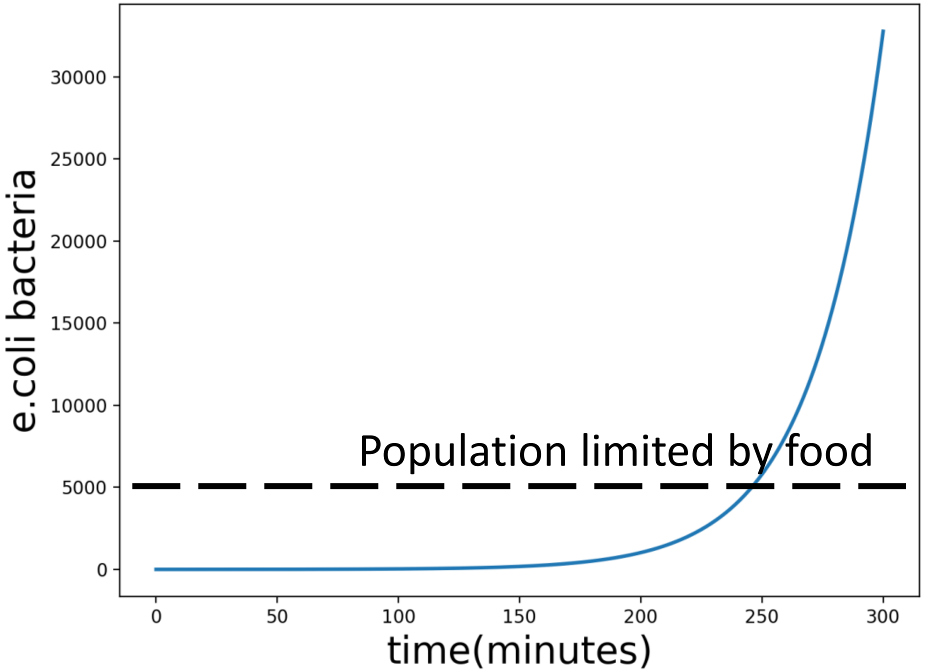
Population growth N relative to food C

- $N' = K(C)N$
- $C' =$



Population growth N relative to food C

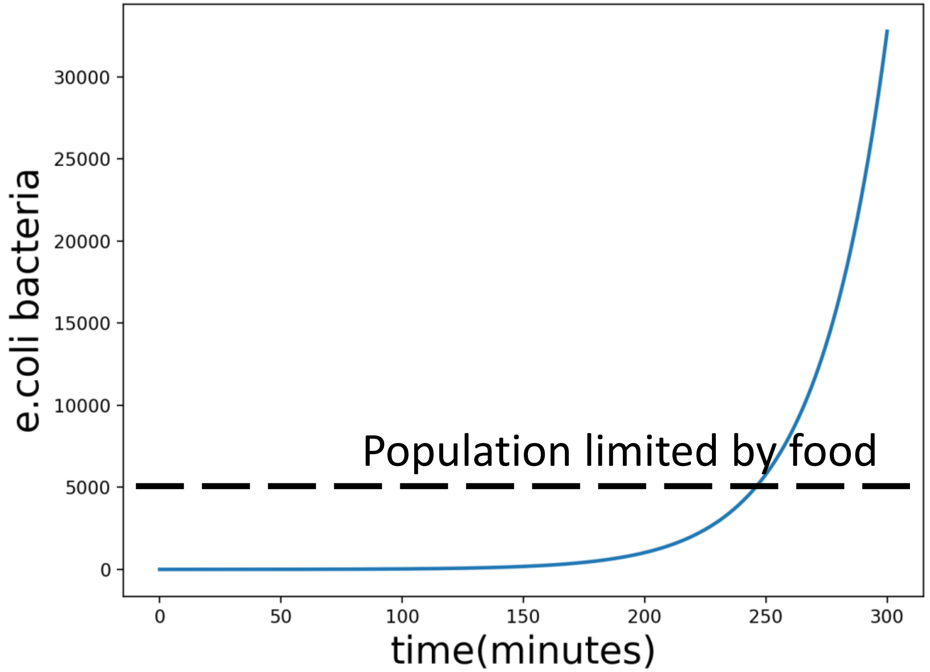
- $N' = K(C)N$
- $C' = -\alpha N'$



Population growth N relative to food C

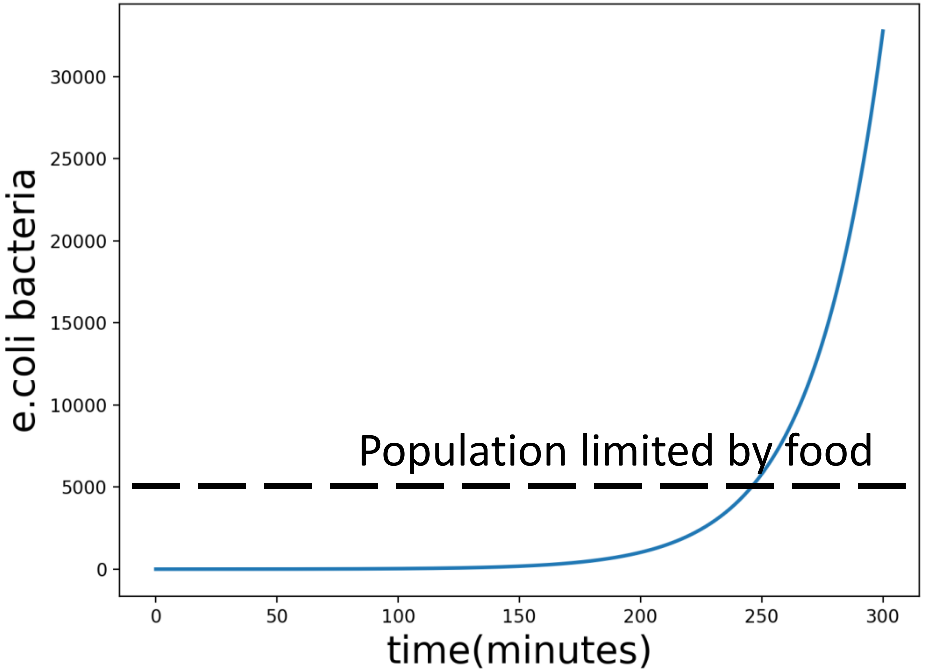
- $N' = K(C)N$
- $C' = -\alpha N'$

α: constant describing consumption of food by each new bacterium



Population growth N relative to food C

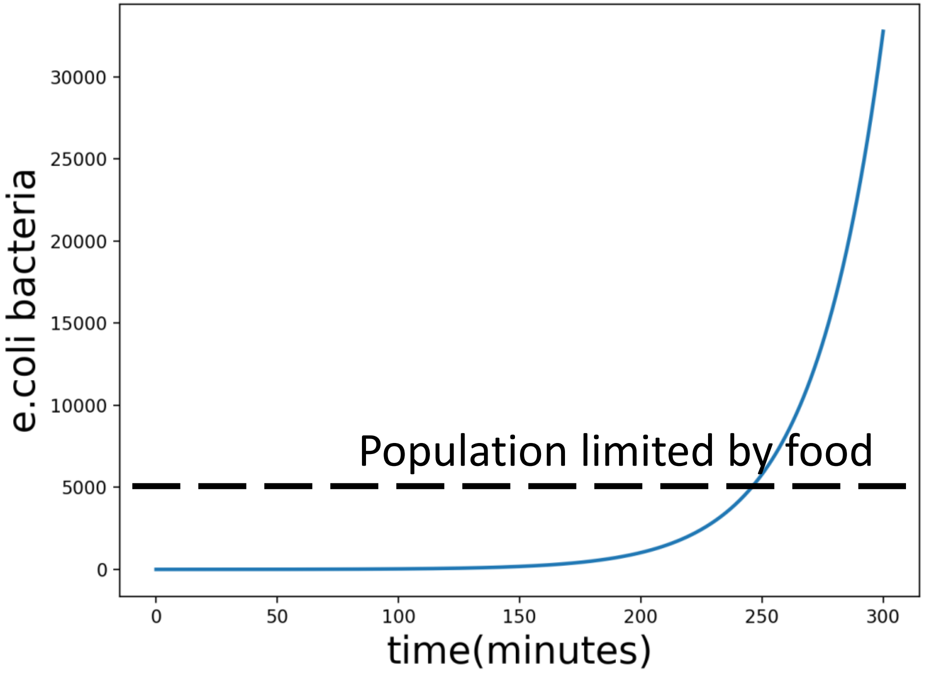
- $N' = K(C)N$
- $C' = -\alpha K(C)N$



Population growth N relative to food C

- $N' = K(C)N$
- $C' = -\alpha K(C)N$

If $K(C) = kC$

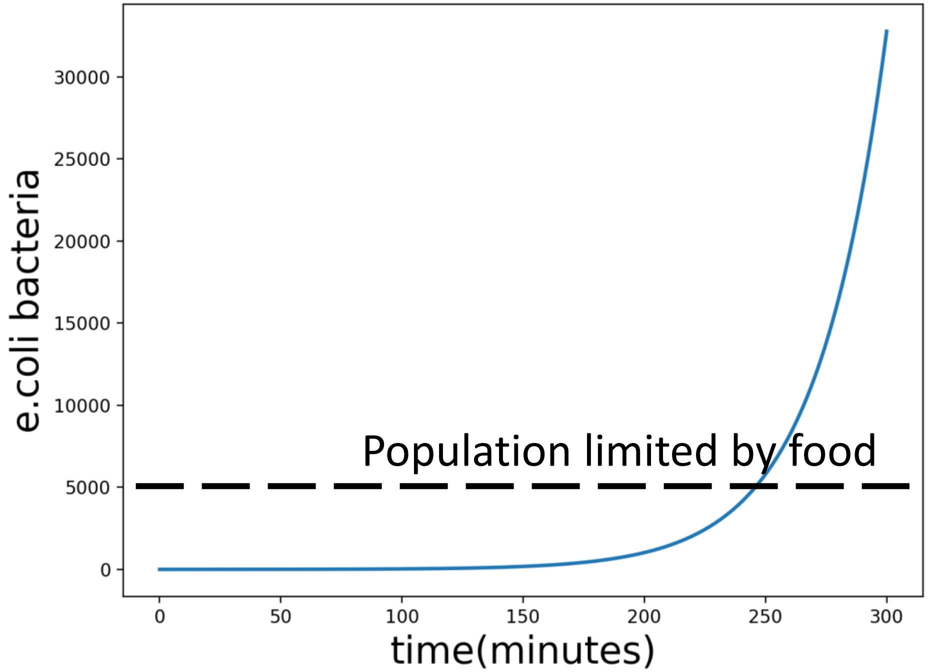


Population growth N relative to food C

- $N' = K(C)N$
- $C' = -\alpha K(C)N$

If $K(C) = kC$

- $C' = -\alpha N'$

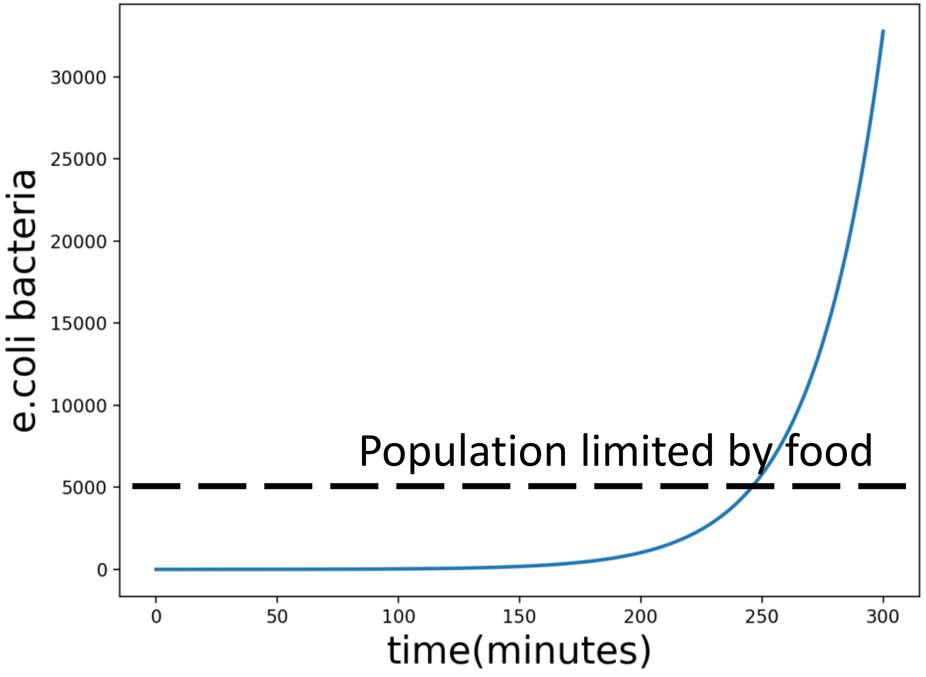


Population growth N relative to food C

- $N' = K(C)N$
- $C' = -\alpha K(C)N$

If $K(C) = kC$

- $C' = -\alpha N'$
- $C = -\alpha N + C_0$

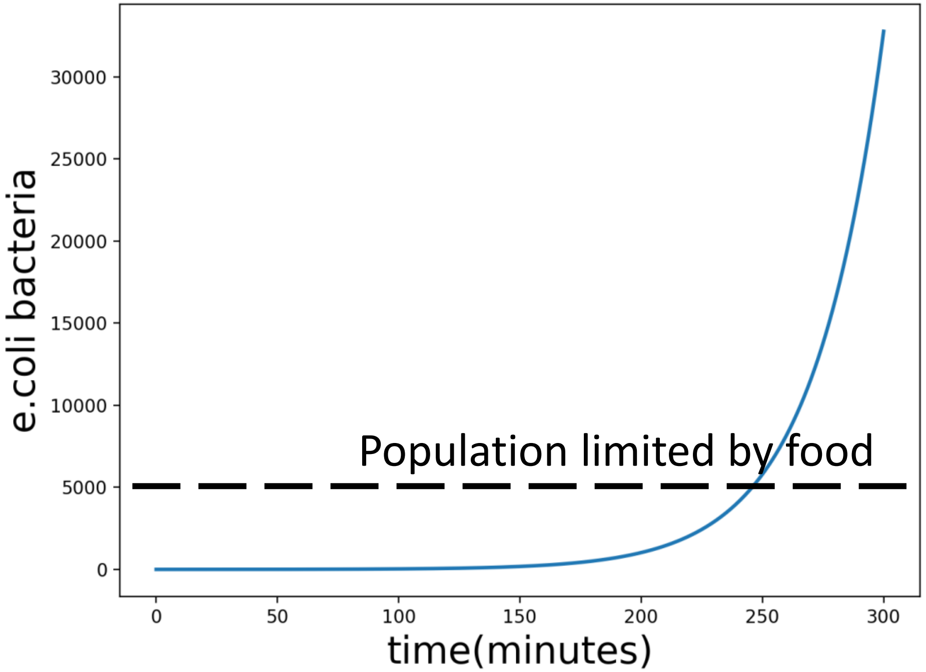


Population growth N relative to food C

- $N' = K(C)N$
- $C' = -\alpha K(C)N$

If $K(C) = kC$

- $C' = -\alpha N'$
- $C = -\alpha N + C_0$
- $N' = k(C_0 - \alpha N)N$



Population growth N relative to food C

- $N' = K(C)N$
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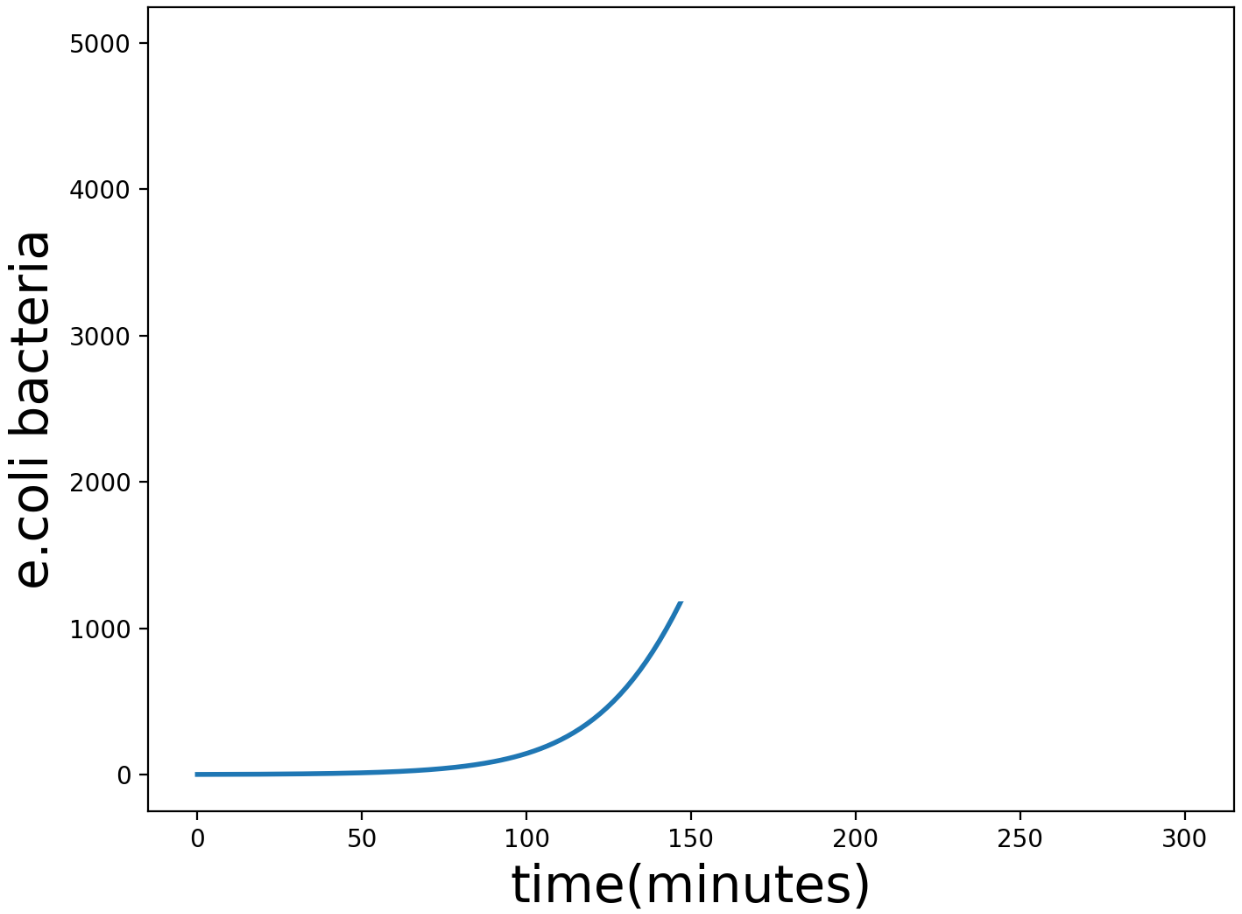
- $C' = -\alpha N'$
- $C = -\alpha N + C_0$
- $N' = k(C_0 - \alpha N)N$



Population growth N relative to food C

- $N' = K(C)N$
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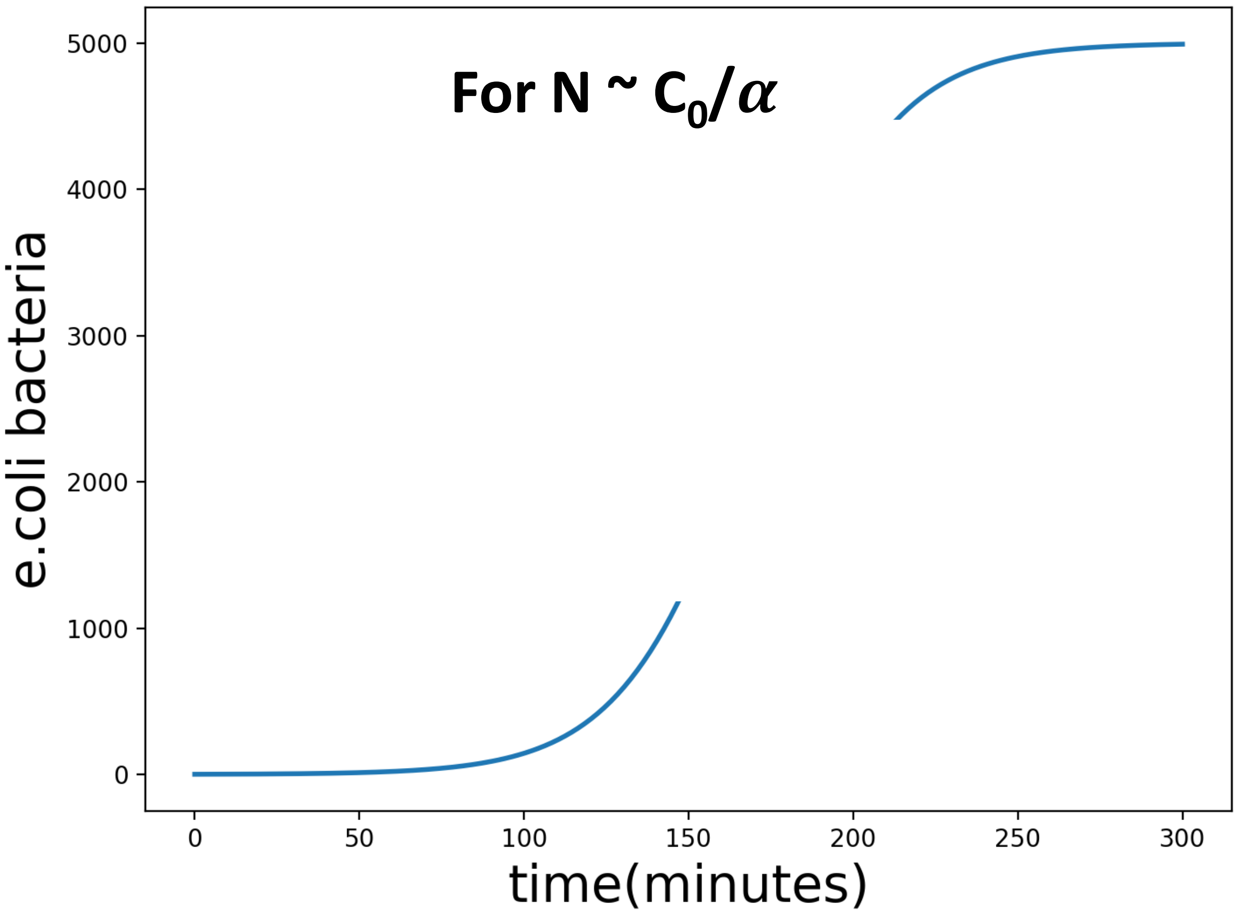
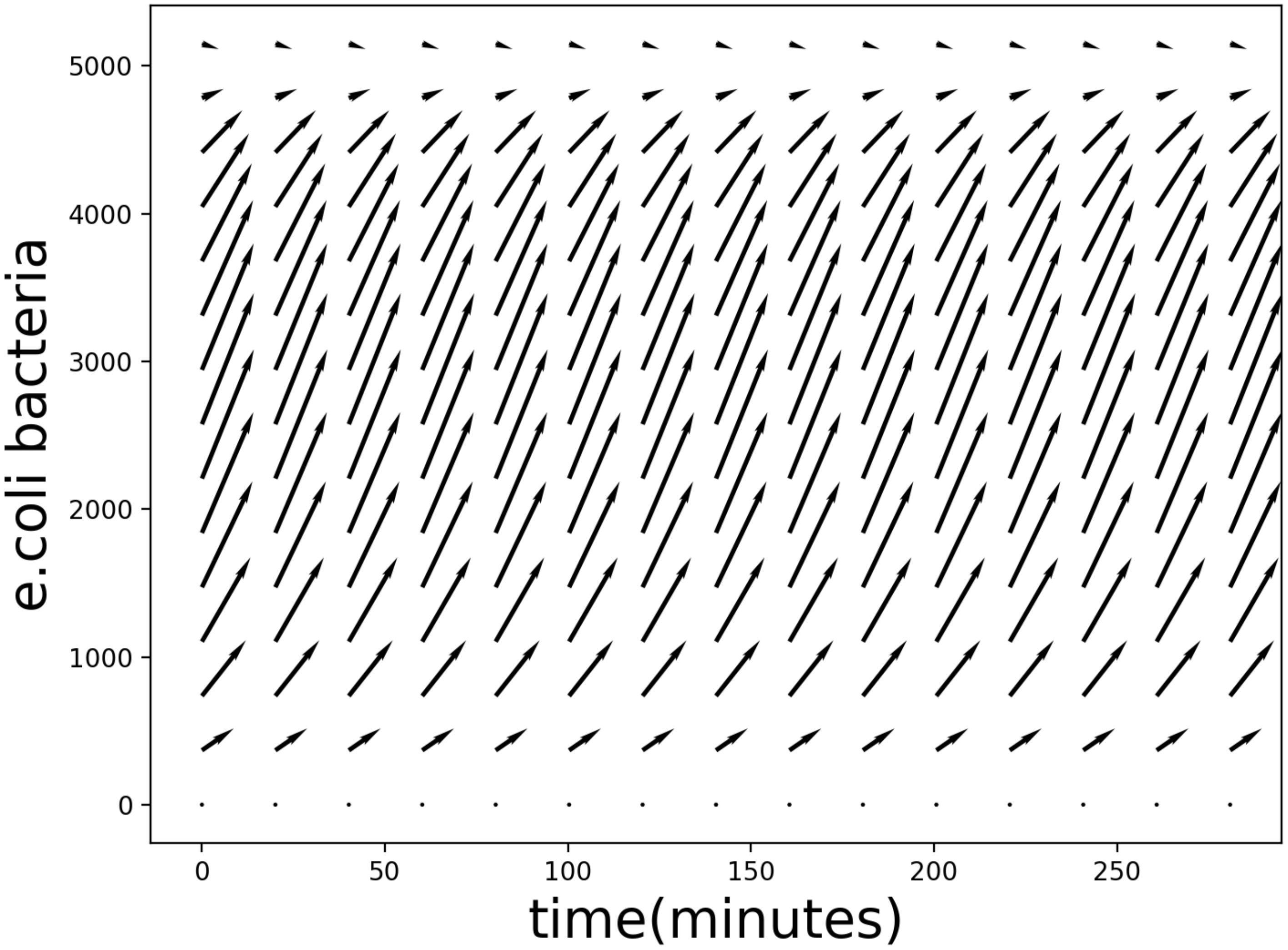
- $C = -\alpha N + C_0$
- $N' = k(C_0 - \alpha N)N$



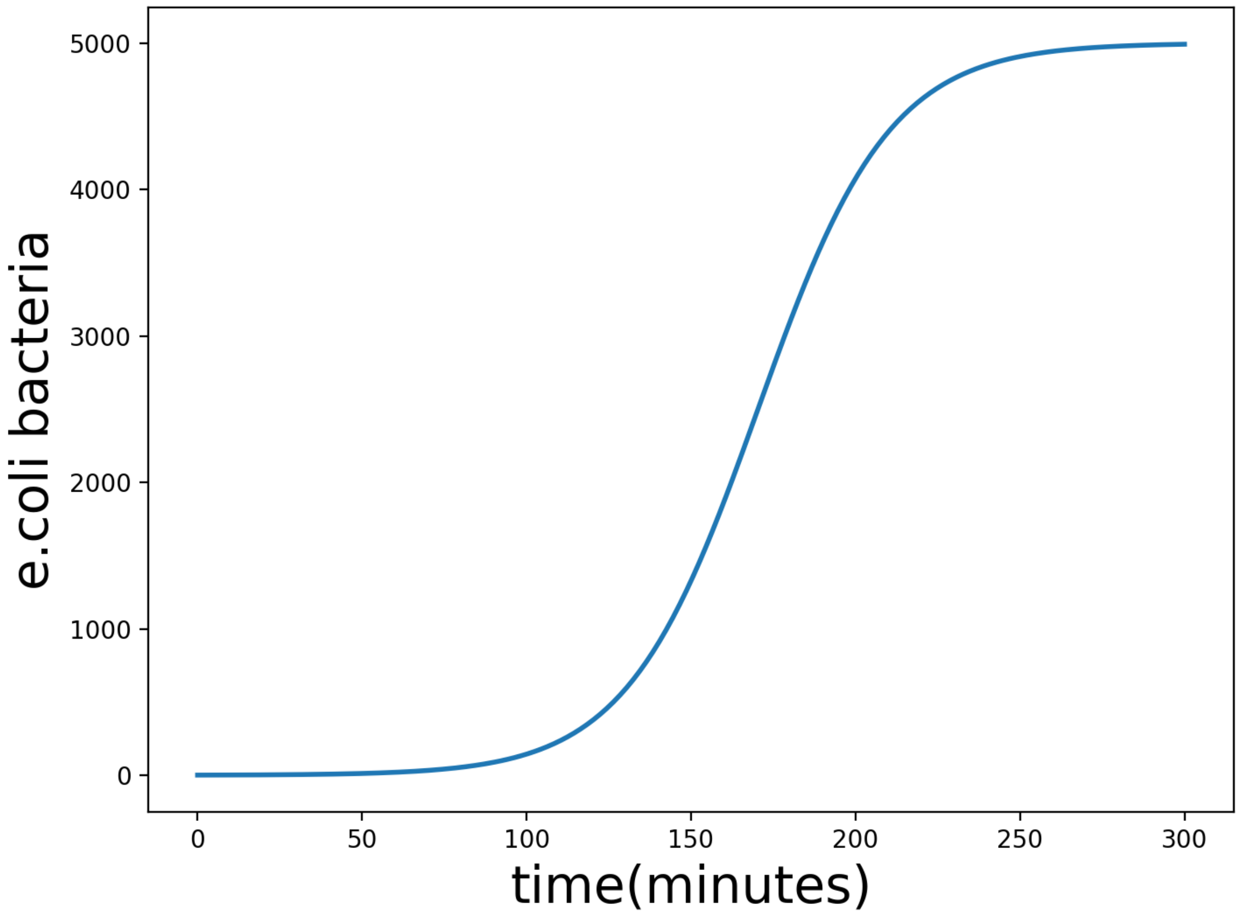
Vector Field



Logistic Growth Function

$$N(t) = \frac{N_0 B}{N_0 + (B - N_0)e^{-rt}}$$

$$N_0 = N(0), B = \frac{C_0}{\alpha}, r = kC_0$$



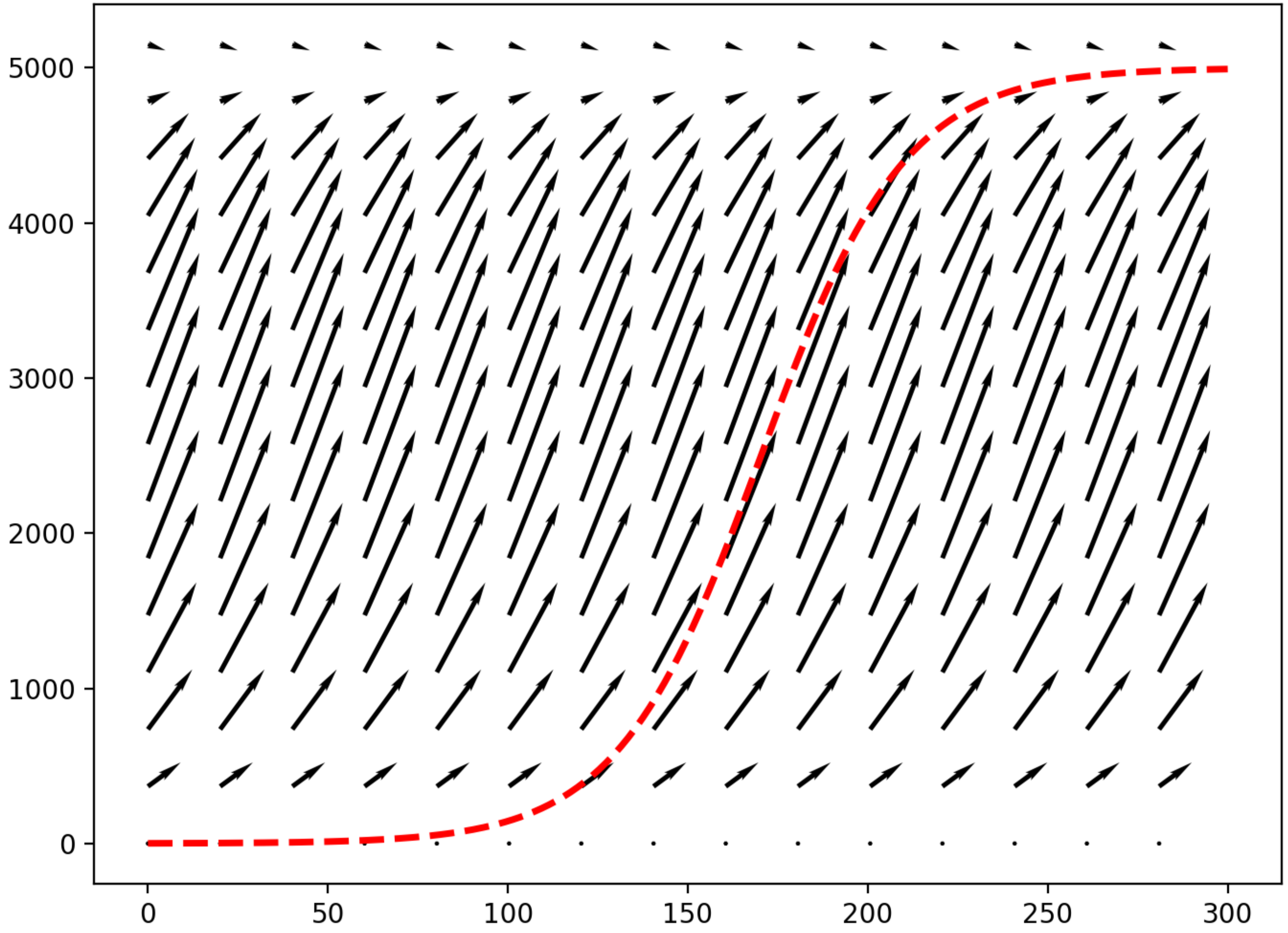
Numerical solutions

- There is usually **no closed form solution** for a system of differential equations, unless the problem is really simple
- We look therefore for an **approximate** solution

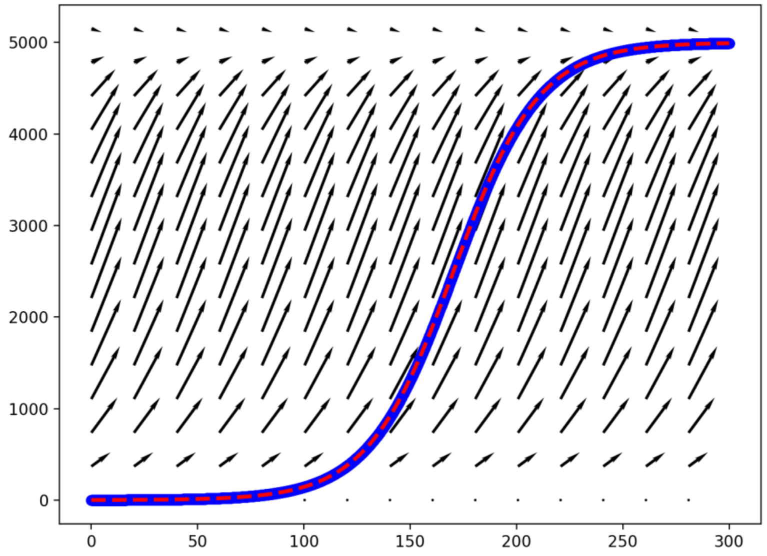
Field of derivatives

- We know how to compute f
- This means that we can compute the **vector/slope field** of x

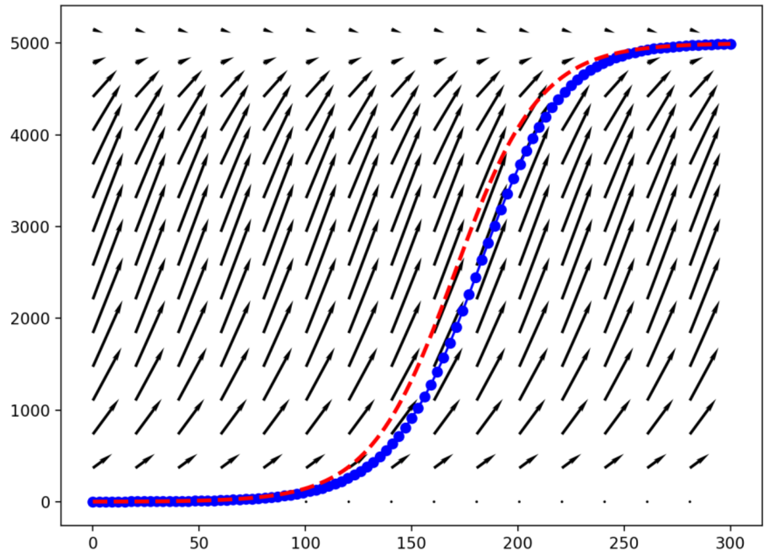
Vector/Slope field



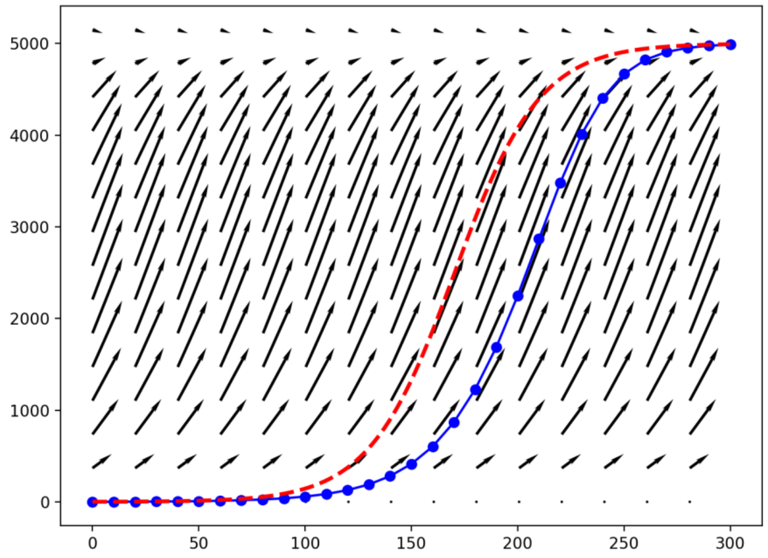
Forward Euler Numerical Solution



dt = 0.1



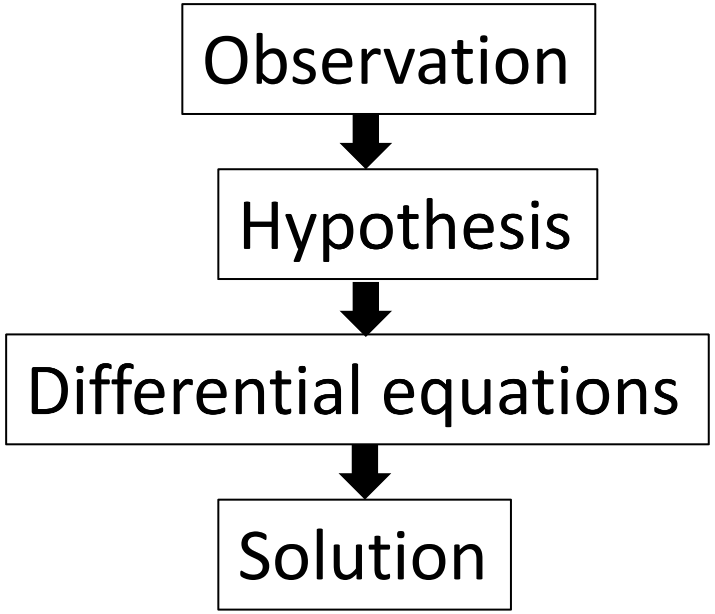
dt = 3



dt = 10

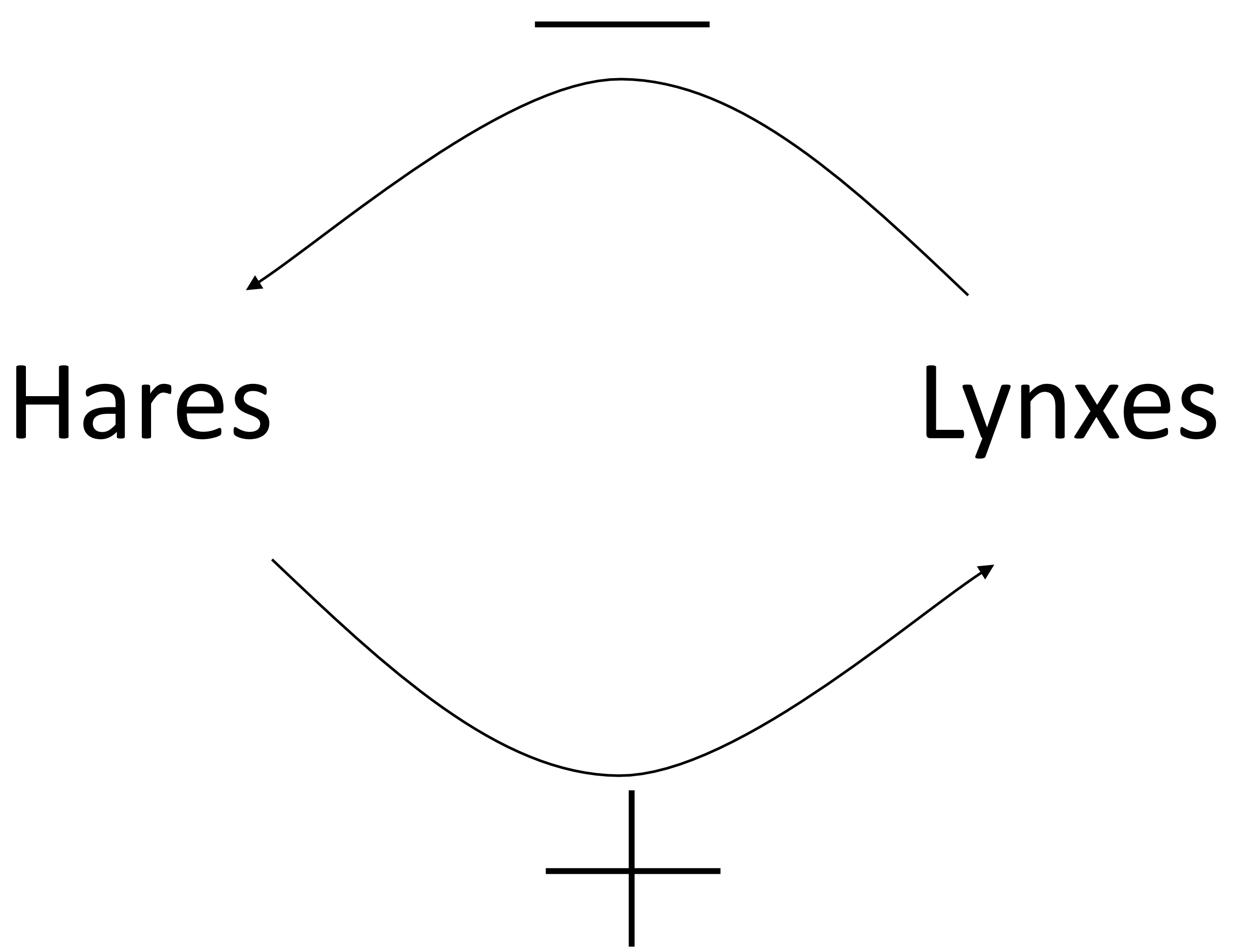
Follow the vector field: `x[n+1] = x[n] + dt*f(x[n], t[n])`

Modeling Process



Hares and Lynxes Population Growth Model

Predator – Prey Relation



Hares and Lynxes Population Growth Model

- Population y (lynxes) changes in time due to reproduction limited by population x (hares)

Hares and Lynxes Population Growth Model

- Population y (lynxes) changes in time due to reproduction limited by population x (hares)

$$\frac{dy}{dt} = dx$$

Hares and Lynxes Population Growth Model

- Population y (lynxes) changes in time due to reproduction limited by population x (hares)

$$\frac{dy}{dt} = dxy$$

Hares and Lynxes Population Growth Model

- Population y (lynxes) changes in time due to reproduction limited by population x (hares)
- Some die due to age

$$\frac{dy}{dt} = dxy$$

Hares and Lynxes Population Growth Model

- Population y (lynxes) changes in time due to reproduction limited by population x (hares)
- Some die due to age

$$\frac{dy}{dt} = dxy - cy$$

Hares and Lynxes Population Growth Model

Lynxes: $\frac{dy}{dt} = dxy \ - cy$

Hares: $\frac{dx}{dt} =$

Hares and Lynxes Population Growth Model

Lynxes: $\frac{dy}{dt} = dxy \ - cy$

Hares: $\frac{dx}{dt} = axx$

Hares and Lynxes Population Growth Model

Lynxes: $\frac{dy}{dt} = dxy\ - cy$

Hares: $\frac{dx}{dt} = ax - bxy$

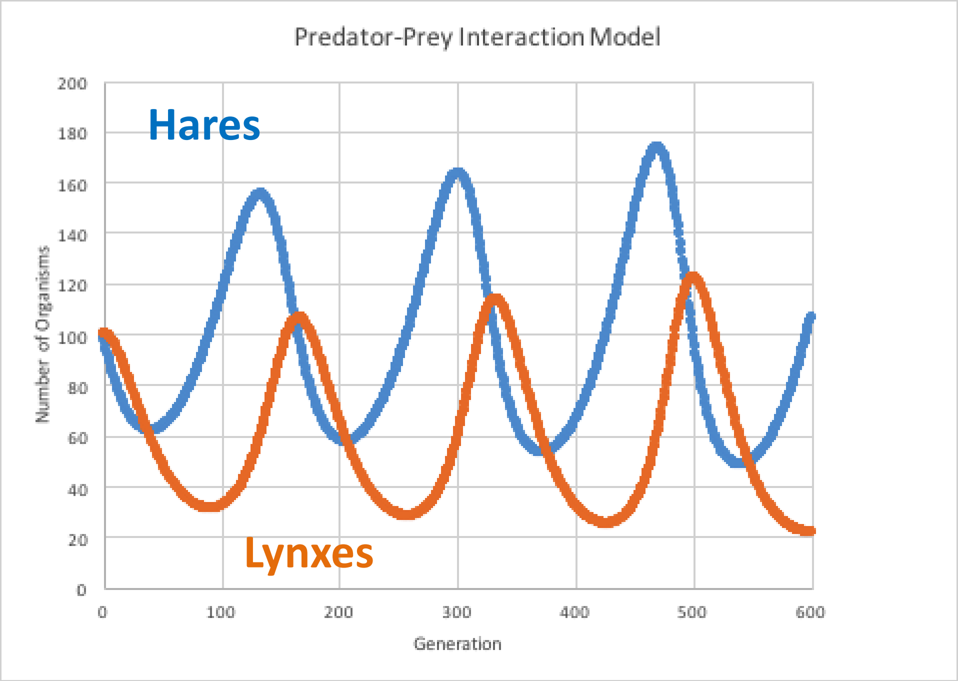
Hares and Lynxes Population Growth Model

Lynxes: $\frac{dy}{dt} = dxy\ - cy$

Hares: $\frac{dx}{dt} = ax - bxy$

Multiply by lynxes to reflect effects of predation

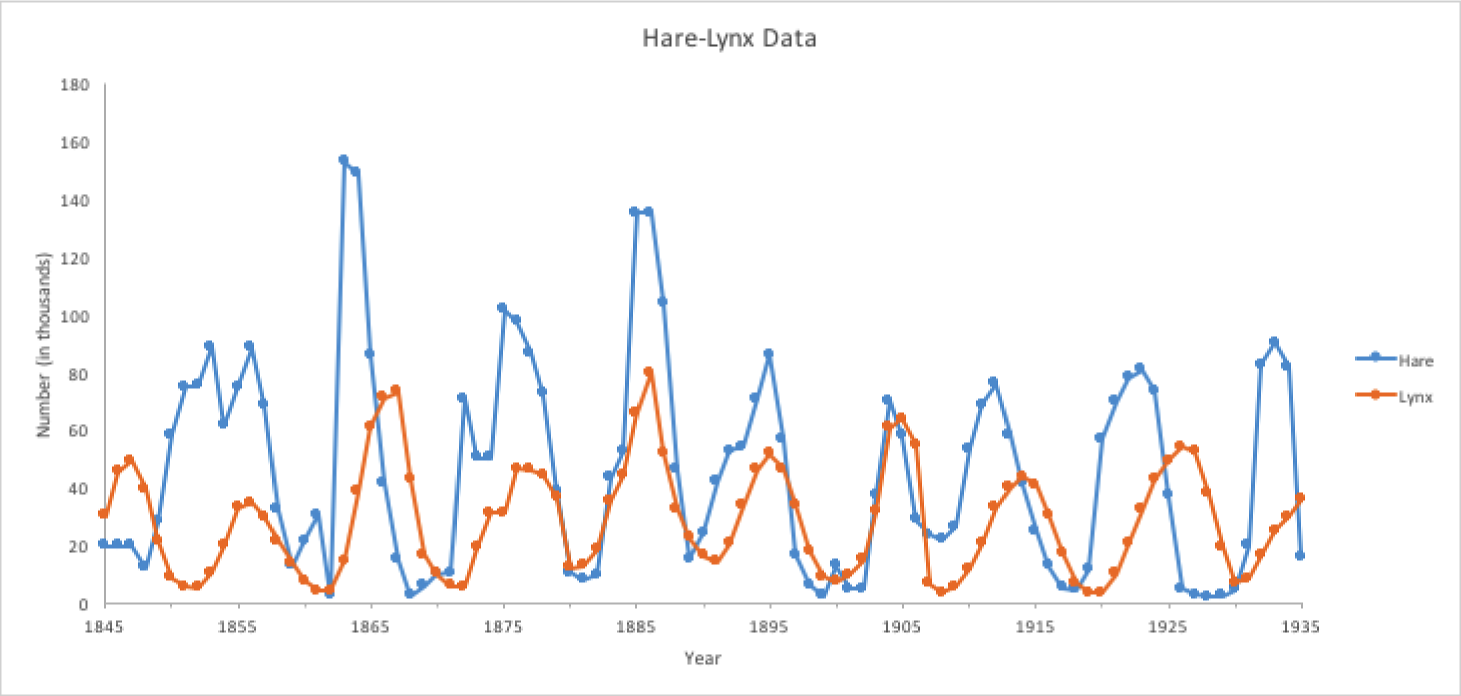
Example Model Solution



Lynxes: $\frac{dy}{dt} = dxy \ - cy$

Hares: $\frac{dx}{dt} = ax - bxy$

Real World



Hare-Lynx Data
180
160
140
120
100
80
60
40
20
0
Number (in thousands)
1845
1855
1865
1875
1885
1895
1905
1915
1925
1935
Year
Hare
Lynx

Lotka-Volterra Predator-Prey Model