

1

# **Optimal control project**

2

Gregor-Fausto Siegmund, Stephen Ellner, Monica Geber

3

Last updated: June 8, 2021

# 1 Introduction

Life history theory is a framework for understanding how evolution generates and responds to tradeoffs among growth, survival, and reproduction over the course of an organisms' life cycle. A central tenet of life history theory is that selection maximizes fitness by favoring trait combinations that optimally balance different parts of the life cycle [Cole \(1954\)](#); [Lande and Arnold \(1983\)](#). Theoretical and empirical studies typically assume that organisms must allocate a limited pool of resources to competing functions such as growth versus survival. While this may be an appropriate assumption for animals, plants are modular organisms.

Plants grow and reproduce via meristems, tissues that are made up of undifferentiated cells and are analogous to stem cells in animals (reviewed in [McSteen and Leyser \(2005\)](#); [Wang et al. \(2018\)](#)). Individual meristems can grow vegetatively, become an inflorescence meristem, or remain undifferentiated. Each vegetative meristem may generate additional meristems with the potential to differentiate into one of these three types. A meristem that differentiates into an inflorescence can no longer grow vegetatively. The onset of flowering thus prevents future vegetative growth at the level of individual meristems. Limiting the number of meristems available for differentiation and reproduction can thus produce tradeoffs: a plant with that allocates most of its meristems to reproduction now will not be able to allocate those meristems to reproduction later [Geber \(1990\)](#); [Watson \(1984\)](#).

In plants where reproduction is fatal (monocarpic plants), plants must balance their investment in and the timing of growth and reproduction because both processes draw on a shared set of resources. Theoretical models of life history evolution typically represent this as a trade-off in energetic investment. However, plant development is modular and can constrain future energetic allocation to growth or reproduction.

Fox 1990 (Components of flowering time variation) discusses experiments with *Eriogonum* demonstrating that patterns of reproduction are the product of growth and development.

## 1.1 Dynamic optimization

Overview of model types that address connection of life history and timing or reproduction. Specific benefits of optimal control. Original models have been extended and enriched. I think this should be reduced to 1-2 concise paragraphs that also address other modeling approaches that have been used to study this kind of problem (e.g. Ackerly and Wong?) and why we chose to use optimal control theory

A shared assumption of reproductive allocation models, dynamic optimization models, and evolutionary demographic theory is that demographic parameters are themselves parts of organisms (Fox 1990, p 1420).

Modifications to original models include varying functions for productivity and reproduction (e.g. seasonal pattern, overlap or not), tissue loss and maintenance costs, multiple organs, allocation to storage, different types of survivorship curves, allometric relationships of reproductive to vegetative mass, and environmental stochasticity. The value in these models comes from an ability to explore how allocation decisions respond to different assumptions about variables such as resource use or variability in season length.

A key assumption of the classic models is that plants are making allocation decisions about carbon, which is assumed to be the limiting resource. Although this assumption has been extended to include other nutrients, plant development complicates the picture. Because plants have modular structures, vegetative and reproductive growth are coupled insofar as plant architecture limits the total potential number of flowers or inflorescences. More generally, whether a plant is in a vegetative or reproductive phase is the product of decisions about the fate of primary or axillary meristems. This perspective aligns with a source-sink perspective on plant growth that suggests potential photosynthesis is not the sole determinant of plant growth but that plant growth is instead a balance of source (photosynthate) and sinks (maintenance, organ production, etc.) Körner (2015); ?.

Some of the models have also been empirically tested, and have helped inform intuition about things like seasonal variation in photosynthesis or storage. Yet many models continue to predict a bang-bang allocation strategy which is not observed in many natural systems. However, no such models have been written.

Here, we apply these ideas to develop a system of ordinary differential equations that describes the dynamics of plant development and constrains growth by the availability of photosynthate. This approach places the allocation decisions at the level of meristems (decisions about meristem fate) and leaves flexibility about much these decisions are limited by photosynthate. In classic models, any quantity of vegetative biomass can support unlimited primary meristem divisions which can in turn contribute to unlimited number of floral meristems.

## 1.2 Questions

Life history theory typically assumes that trajectories of growth and reproduction are shaped by resource allocation decisions. Descriptions of development (Figure 3 and 5) highlight how growth and fecundity depend on meristem production. Models that do not explicitly represent resource and development can not distinguish between the origin of tradeoffs. See White et al. (2016) for a complementary perspective on sources and sinks in plant growth and Körner (2015) for a review on how sinks might often limit plant growth. Fox (1992) suggests allometric models are not sufficient and models that incorporate development will be necessary.

Resource limitation generates negative correlations between growth and fecundity within a life stage because both compete for resources. In a situation where resources are limited, we might expect to see trade-offs that are the result of resource allocation decisions (we wouldn't see these decisions when resources are not limited).

Meristem limitation generates positive correlations between growth and fecundity within a life stage because both depend on meristem production. In a situation where meristems are limited, we might expect to see trade-offs that are the result of meristem allocation decisions (we wouldn't see these decisions when meristems are not limited).

I will address the following questions. **First**, I will use the models to determine whether including differentiation and growth of meristems reduces the likelihood of obtaining a strategy with an instantaneous switch [Cohen \(1971\)](#). Put another way, are graded allocation strategies optimal when vegetative and reproductive growth are coupled [Fox \(1992\)](#)? **Second**, I will look at the control strategies of decisions (e.g. meristem division) and the cumulative impact on control of resource budget. Do the control strategies of meristem decisions (e.g. bang-bang) translate to resource budgets (also being bang-bang?) [Fox \(1992\)](#)? **Third**, I will ask when plants are more likely to be resource versus meristem limited. Specifically, I will focus on how the optimal strategy changes with increasing levels of environmental variation; are plants likely to be meristem limited in scenarios with high levels of uncertainty about season length in order to maintain the ability to capitalize on those longer seasons? Wyatt, Schemske, Stebbins, Salomonson 1994

- When does flowering start? This asks when plants start allocating meristems to reproduction, or when plants start producing inflorescence meristems. In the model for determinate inflorescences, this would be when  $p(t) < 1$ . In the model for indeterminate inflorescences, this would be when  $p(t) - q(t) < 1$  or  $q(t) > 0$ .
- How quickly do plants commit resources to flowering? This asks whether there is an instantaneous or graded allocation to reproduction.
- How do allocation strategies respond to different levels of interannual variation? How does the optimal control shift with increasing variance in season length?

- How do optimal strategies respond to different rates of division in primary and inflorescence meristems,  $\beta_1$  and  $\beta_2$ ? For example, what is the optimal control for different levels  $\beta_1 < \beta_2$  (primary meristems divide more slowly than inflorescence meristems),  $\beta_1 = \beta_2$  (primary and inflorescence meristems divide at equal rates), or  $\beta_1 > \beta_2$  (primary meristems divide more quickly than inflorescence meristems)?
- What is resource limitation in these models? What is meristem limitation in these models?
- Which developmental mode favors meristem limitation? MAG suggest that determinate development should favor meristem limitation because the meristem can be consumed by a floral meristem while indeterminate development can always keep growing.
- When are resource allocation models appropriate for understanding the developmental decisions that plants make? When are resource allocation models insufficient for understanding the developmental decisions that plants make?

Parker and Maynard-Smith (1990) describe how comparative studies and quantitative genetics can be used in conjunction with optimization to understand phenotypes. Specifically, they suggest that quantitative genetics can be used to identify constraints that are relevant for optimization models. Comparative methods can then be used to test the predictions of those models. Here's a quote: "discovery of a genetic covariance can indicate presence of a developmental constraint that must be taken into account when formulating an optimization model". Experiments and interspecies comparisons can also help discover these constraints.

Various lines of evidence exist that point to constraints. First, there are experiments that show genetic covariance/correlation of flowering time and meristem number/tiller number. We have data from plants from different habitats (e.g. Geber 1990, Schmitt et al. 1993), from RILs (e.g. Haselhorst et al. 2011), from the result of selection experiments (e.g. Mitchell-

Olds 199x?). Also Duffy et al. 1999, Kudoh et al. 2002, Watson 1984, Diggle 1993, Gardner and Latta 2008, Latta and Gardner 2009, Austen et al. 2014, Friedman et al. 2015, Rubin et al. 2018, van Tienderen 1996. Second, we have studies of development with mutants/knock-outs in Arabidopsis: Bradley et al. 1997, Karami et al. 2020, Melzer et al. 2008, Baumann et al. 2015. These experiments show that modifying flowering time genes (e.g. *tfl*) has an effect on the number of meristems, establishing that there is pleiotropy. Third, we have studies focusing on developmental stages (e.g. Baker and Diggle 2011). Crop selection (

Here are some expectations: early flowering reduces meristem number. Late flowering increases meristem number. Environmental risk (e.g. dry habitats) promote the evolution of annuals and early flowering. This could be an interspecific comparison (within genera) or intraspecific (populations in riskier habitats flower earlier). Annuals derive from perennial ancestors (phylogenetic).

Goals: connect vegetative branching, inflorescence development, trade-offs, and flowering time. Distinguish meristem versus resource limitation as the trade-off shaping life history evolution. Explore the effect of environmental variation on flowering time via development. Does including development lead to bang-bang control or graded allocation, and how does this depend on development mode.

- Distinguish meristem versus resource allocation as the trade-off shaping life history evolution.

- Geber, Fox, Lehtila and Larsson

- Define conditions for meristem vs. resource limitation.

- Set up boundary conditions or test cases that demonstrate meristem vs. resource limitation.

- Does including development lead to bang-bang control or graded allocation, and how

150 does this depend on development mode.

151 – Hypotheses: Cohen, King and Roughgarden, Fox, Iwasa

152 – Recover optimal controls.

153 – Compare results to the strategies from the Cohen or King and Roughgarden  
154 00models.

155 • Explore the effect of environmental variation on flowering time via development.

156 – Hypotheses: Stebbins 1974, Wyatt 1982, Prusienkiewicz et al. 2007,

## 157 2 General approach

158 We took the following approach to solving the problem outlined above. First, we sought  
159 to develop differential equations that capture the basic processes of plant development that  
160 are relevant to our questions. To accomplish this goal, we reviewed existing literature on  
161 plant development, models of plant development. Second, we specified the optimal control  
162 problem and goals. This step included defining Hamiltonian for cases with and without  
163 state variable constraints. Third, we solved the optimal control for the case without state  
164 variable constraints. We took this step in order to develop intuition about the system and to  
165 determine initial conditions for the numerical solution. Finally, we implemented a numerical  
166 algorithm to obtain solutions to the optimal control problem.

## 167 3 Models of plant development

168 The description of plant development that I give here should be directly connected to a  
169 figure demonstrating the different types of divisions that I base the model on. The file ba-  
170 sic-inflorescence in the notes folder should be helpful for this. I think I need to make the



case that the interplay between meristem and resource allocation are well-represented by two basic developmental decisions: whether or not the plant branches, and whether the inflorescence is determinate or indeterminate. I will try to marshal: (1) a brief overview of research on genetics of development, (2) role of these processes in shaping plant morphology, (3) life history arguments.

Development in flowering plants can be characterized as a series of decisions at the meristems Kellogg (2000). The primary shoot divides at the shoot apical meristem (SAM) and produces additional primary shoot meristems (main branch) and axillary meristems (AM), each of which is subtended by a leaf. The axillary meristems can develop into an axillary branch or remain quiescent. Each axillary branch has similar dynamics as the primary shoot meristem (though potentially at different rates). The shoot apical meristem is converted to an inflorescence meristem (IM) through internal or external signals. In turn, inflorescence meristems give rise to floral meristems (FM).

In plants with determinate inflorescences, the inflorescence meristem is eventually converted to a terminal flower, which consumes the meristem. Tomato is an example of a plant with a determinate inflorescence and sympodial growth Park et al. (2012). In plants with indeterminate inflorescences, the inflorescence meristem only produces flowers at axillary positions. *Arabidopsis* is an example of a plant with an indeterminate inflorescence and monopodial growth Bradley (1997).

The ‘rules’ characterizing plant development have been used to model the evolution of inflorescence architecture Prusinkiewicz et al. (2007). The meristem dynamics that underly inflorescence architecture are also likely involved in organizing branching architecture Park et al. (2012). Lindenmayer systems (L-systems) are a grammar that is capable of reconstructing the branching architecture of various organisms (e.g. algae, bacteria, plants). L-system statements highlight the overlap in decision rules that determine branching in vegetative and reproductive growth.

Cohen (1971) identified development as a factor that could help explain why an instant switch in allocation from vegetative to reproductive growth is rarely observed. Development connects growth and reproduction, and constrains how plants can shift allocation to reproduction ?. Life history models for plants have not included developmental processes, which may limit their applicability and interpretation ?. For example, it may be easier to test the predictions from models that separate meristems and biomass. Also, models that do not represent development can not determine whether allocation patterns are the result of selection on developmental decisions or resource allocation directly. The broader issue here is whether resource-based models can adequately represent plant life histories, or whether it is necessary to include development to describe the biological processes underlying life histories ?. **need to work on this paragraph**

I first describe resource allocation models Cohen (1971); King and Roughgarden (1982). I then describe how I represent meristem and resource allocation in models for plant life histories. These models are developed from ideas in Itzkovitz et al. (2012); Kellogg (2000); Prusinkiewicz et al. (2007); ?. First, I write models for plants with determinate inflorescences. Next, I write models for plants with indeterminate inflorescences.

### 3.1 Resource allocation models

The plant growth model developed by Cohen (1971) and later elaborated by King and Roughgarden (1982) represents resources allocated to vegetative and reproductive pools. I summarize the model in equations 1 and 2 and state diagram 1. In the model,  $x_1$  and  $x_2$  are the weights of the vegetative and reproductive parts of the plant, respectively. Photosynthesis is assumed to be linearly related to the weight of the vegetative part of the plant. The control function  $u(t)$  is the proportion of photosynthate that is allocated to the vegetative pool.

King and Roughgarden (1982) propose that the long-term, optimal reproductive strategy will maximize the geometric mean of reproductive success. They propose that the function that should be optimized is the expectation of the log of fitness,  $J = (1/T) \int_0^T \log(x_2) dt$ . They used the following system of equations:

$$\begin{aligned}\dot{x}_1 &= u(t)x_1 \\ \dot{x}_2 &= (1 - u(t))x_1\end{aligned}\tag{1}$$

subject to

$$\begin{aligned}0 &\leq u(t) \leq 1 \\ 0 &< x_1, 0 \leq x_2\end{aligned}\tag{2}$$

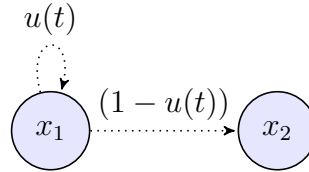


Figure 1: State diagram describing the photosynthate allocation model.

## 4 Determinate inflorescences

In plants with determinate inflorescences, the shoot apical meristem forms a terminal flower and an axillary bud (Bartlett and Thompson (2014)). In tomato, the primary shoot meristem converts to a floral meristem and a sympodial inflorescence meristem; this pattern is iterated to form the inflorescence (Park et al. (2012)).

I describe the developmental decisions in a plant with determinate inflorescences using three types of divisions (Figure 3) (Itzkovitz et al. (2012)). First, a primary meristem can

227 divide at the shoot apical meristem to give rise to two primary meristems: the main branch  
 228 and an axillary bud. These divisions generate a vegetative, branching architecture. Second,  
 229 a primary meristem can divide at the shoot apical meristem to give rise to an inflorescence  
 230 meristem and a floral meristem. These divisions end vegetative growth and mark the transi-  
 231 tion from vegetative to reproductive growth along an axis. Third, an inflorescence meristem  
 232 can divide into an inflorescence meristem and a floral meristem. These divisions are the only  
 233 possible fate for inflorescence meristems. Using these categories assumes that there is no  
 234 terminal division into two floral meristems. The end of season terminates flowering. This  
 235 assumption is somewhat unrealistic because some plants do stop flowering.

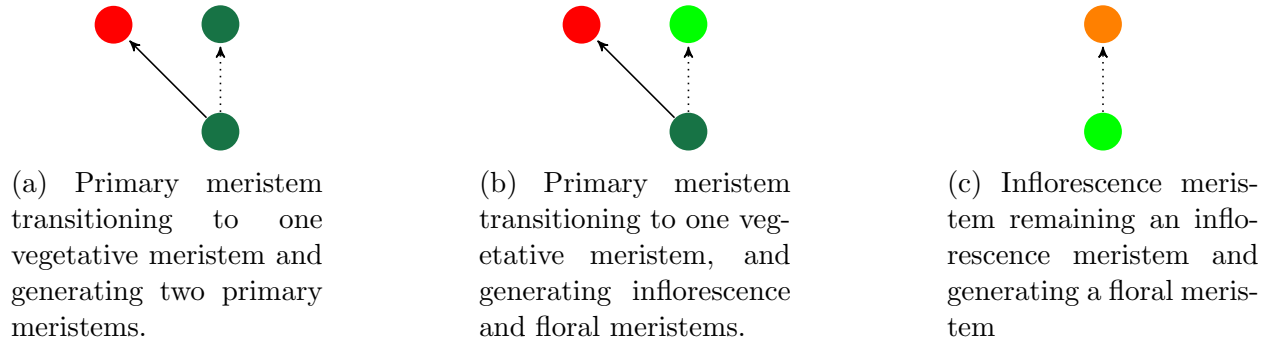


Figure 2: Meristem transitions in plants with determinate inflorescences.

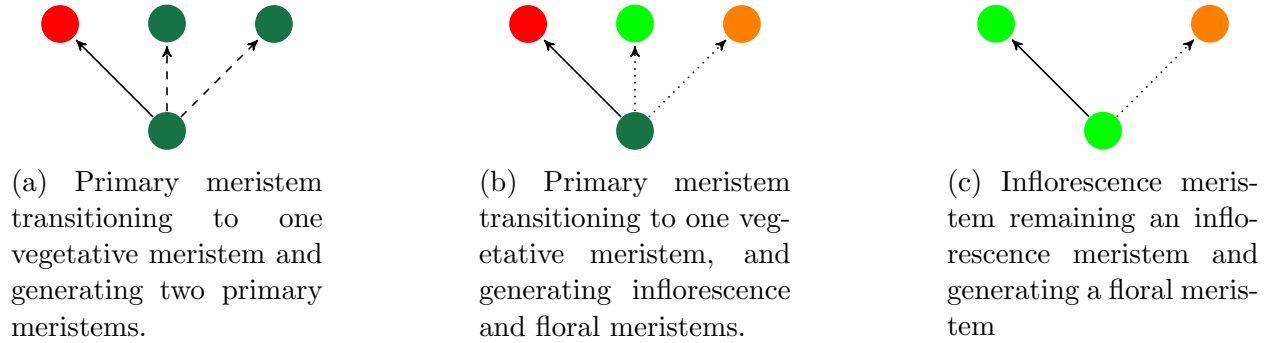


Figure 3: Meristem transitions in plants with determinate inflorescences.

236 I use these types of divisions/transitions to summarize the meristem dynamics for plants  
 237 with determinate inflorescences in a system of equations with constraints (Equation 3 and 4)

238 and a state diagram (Figure 4). In this model,  $P$ ,  $V$ ,  $I$ , and  $F$  are the populations of primary,  
 239 vegetative, inflorescence, and floral meristems, respectively. Primary meristems divide at a  
 240 rate  $\beta_1$ . Inflorescence meristems divide at a rate  $\beta_2$ , and are thus converted to floral meristems  
 241 at a rate  $\beta_2$ . Each division by an inflorescence meristem produces one inflorescence meristem  
 242 and one floral meristem. The probability that a primary meristem divides into two primary  
 243 meristems (branch and axillary meristem) and a vegetative meristem is given by the control  
 244 function,  $p(t)$ . The probability that a primary meristem divides into a vegetative meristem,  
 245 inflorescence meristem, and a floral meristem is given by  $1 - p(t)$ .

246 To summarize Figure 4, panel (A) occurs proportional to the number of primary meris-  
 247 tems at a rate  $\beta_1 p(t)$ . Panel (B) occurs proportional to the number of primary meristems at  
 248 a rate  $\beta_1(1 - p(t))$ . Panel (C) occurs proportional to the number of inflorescence meristems  
 249 at a rate  $\beta_2$ .

The goal of this optimization problem is to maximize  $F$ . The variable in the model is  
 $T$ , the length of the season. The model is described by the following system of differential  
 equations:

$$\begin{aligned}
 \dot{P} &= 2\beta_1 p(t)P - \beta_1 p(t)P - (1 - p(t))\beta_1 P \\
 \dot{V} &= \beta_1 p(t)P + (1 - p(t))\beta_1 P \\
 \dot{I} &= \beta_1(1 - p(t))P \\
 \dot{F} &= \beta_1(1 - p(t))P + \beta_2 I
 \end{aligned} \tag{3}$$

subject to

$$\begin{aligned}
0 &\leq p(t) \leq 1 \\
0 &< P \\
0 &\leq I \\
0 &\leq F
\end{aligned} \tag{4}$$

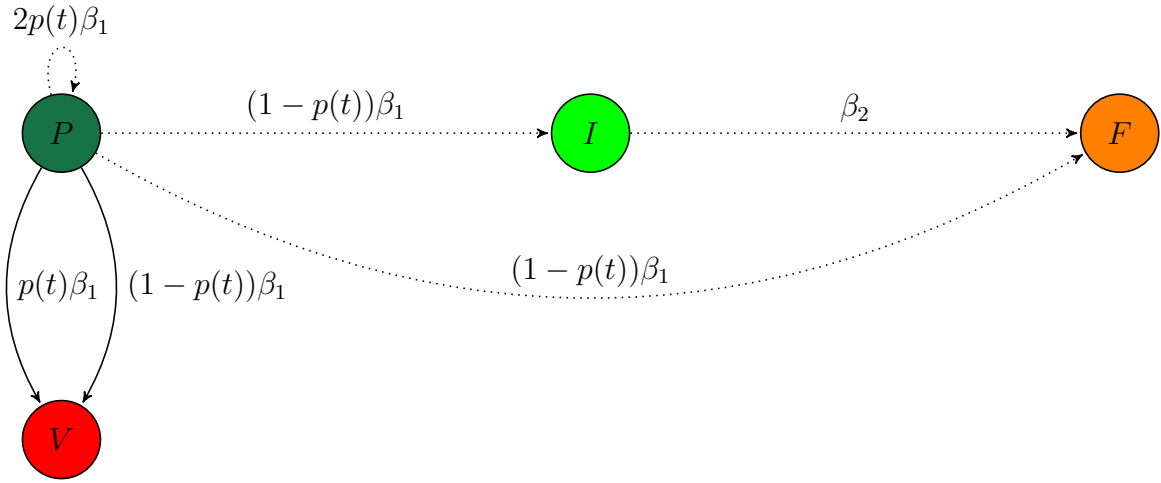


Figure 4: State diagram describing the dynamics for plants with determinate inflorescences.

250 The equation  $\dot{P} = 2\beta_1 p(t)P - \beta_1 p(t)P - (1-p(t))\beta_1 P$  describes how primary meristems  
251 that divide into two primary meristems add to the pool  $P$  in proportion to size of the pool  
252 of primary meristems. These divisions also add to the vegetative meristem pool  $V$ . The  
253 process here is that a primary meristem unit becomes a vegetative meristem, and gives rise  
254 to two new primary meristems. Primary meristems are lost from the primary meristem pool  
255 when divisions give rise to inflorescence and floral meristems.

256 The equation  $\beta_1 p(t)P + (1-p(t))\beta_1 P$  describes the dynamics of the vegetative meristems.  
257 Primary meristems contribute to the vegetative pool when primary meristems propagate.  
258 The transition from primary to vegetative meristems is a proper flow. Primary meristems

also contribute to the vegetative pool when primary meristems divide into inflorescence and floral meristems. This is also a flow.

The equation  $\dot{I} = \beta_1(1 - p(t))P$  describes the dynamics of the inflorescence meristems. Primary meristems contribute to inflorescence meristems when they; this happens with probability  $1 - p(t)$  and proportional to the primary meristem pool  $P$ .

The equation  $\dot{F} = \beta_1(1 - p(t))P + \beta_2 I$  describes the dynamics of the floral meristems. Primary meristems contribute to floral meristems with probability  $1 - p(t)$  and proportional to the primary meristem pool  $P$ . Inflorescence divisions also contribute to floral meristems and occur proportional to the size of the inflorescence meristem pool.

## 4.1 Model description

Qualitatively, this model describes the accumulation of primary meristems through division at the shoot apical meristem (SAM). Without further modification to the model, all primary meristems have active SAMs (can produce further primary meristems through division). Primary meristems that are converted to inflorescence meristems or floral meristems can not revert to primary meristems. Inflorescence meristems divide and produce inflorescence and floral meristems, but can not produce more vegetative axillary meristems. For values of  $p(t) = 0$ , plants produce vegetative, inflorescence, and floral meristems in proportion to the available primary meristem pool.

There are two rates in the model: the rate of primary meristem division and the rate of inflorescence meristem division. High rates of primary meristem division ( $\beta_1$ ) correspond to morphologies with short internodes (e.g. rosettes) or high levels of branching. Low rates of primary meristem division correspond to morphologies with long internodes and low levels of branching. High rates of inflorescence meristem division ( $\beta_2$ ) correspond to tightly packed inflorescences. Low rates of inflorescence meristem division correspond to spaced

283 floral meristems.

284 In this model, committing a primary meristem to flowering consumes the branch. The  
 285 process produces a terminal flower and inflorescence meristem; this structure can be iterated  
 286 but can't revert to producing primary meristems. This should show up in the model because  
 287 the decision for total asymmetric branching ( $p(t) = 0$ ) will convert primary meristems to  
 288 inflorescence and floral meristems. This means that once all meristems are committed to  
 289 flowering, the only way in which reproductive biomass (i.e. floral meristems) will get added  
 290 is by division of the inflorescence meristems.

## 291 4.2 Equations

The optimal control problem we are interested in is

$$\begin{aligned}
 & \max_u \int_0^T \log(F(t)) dt \\
 & \text{subject to } \dot{P} = 2\beta_1 p(t)P - \beta_1 p(t)P - (1 - p(t))\beta_1 P \\
 & \quad \dot{V} = \beta_1 p(t)P + (1 - p(t))\beta_1 P \\
 & \quad \dot{I} = \beta_1 (1 - p(t))P \\
 & \quad \dot{F} = \beta_1 (1 - p(t))P + \beta_2 I \\
 & \quad 0 < P, \ 0 \leq V, \ 0 \leq I, \ 0 \leq F, \\
 & \quad 0 \leq p(t) \leq 1, \ 0 \leq q(t) \leq 1.
 \end{aligned}$$



If we set  $\beta_1, \beta_2$  to be functions of vegetative biomass, we write the system of equations:

$$\begin{aligned}
\dot{P} &= 2[q(t)V]p(t)P - [q(t)V]p(t)P - (1 - p(t))[q(t)V]P \\
\dot{V} &= [q(t)V]p(t)P + (1 - p(t))[q(t)V]P \\
\dot{I} &= [q(t)V](1 - p(t))P \\
\dot{F} &= [q(t)V](1 - p(t))P + [1 - q(t)]VI
\end{aligned} \tag{5}$$

The Hamiltonian here is:

$$H = \log(F) + \boldsymbol{\lambda}^T [P \ V \ I \ F] \tag{6}$$

$$= \log(F) + (PV(2\lambda_1 - \lambda_3 - \lambda_4)p + (P - I)V\lambda_4 + PV(\lambda_3 + \lambda_2 - \lambda_1))q + IV\lambda_4 \tag{7}$$

If season length is uniformly distributed over, season length factors out of the objective function. The objective function is independent of the control . For this problem, the optimality condition is

$$\begin{aligned}
\frac{\partial H}{\partial p} &= PV(2\lambda_1 - \lambda_3 - \lambda_4)q = 0 \text{ at } u^* \\
\frac{\partial H}{\partial q} &= PV(2\lambda_1 - \lambda_3 - \lambda_4)p + (P - I)V\lambda_4 + PV(\lambda_3 + \lambda_2 - \lambda_1) = 0 \text{ at } u^*.
\end{aligned} \tag{8}$$

The transversality condition is

$$\lambda_1(T) = \lambda_2(T) = \lambda_3(T) = \lambda_4(T) = 0. \tag{9}$$

The adjoint equations are

$$\begin{aligned}
-\frac{\partial H}{\partial P} &= \dot{\lambda}_1 = -(V(2\lambda_1 - \lambda_3 - \lambda_4)p + V(\lambda_4 + \lambda_3 + \lambda_2 - \lambda_1))q \\
-\frac{\partial H}{\partial V} &= \dot{\lambda}_2 = -(P(2\lambda_1 - \lambda_3 - \lambda_4)p + (P - I)\lambda_4 + P(\lambda_3 + \lambda_2 - \lambda_1))q - I\lambda_4 \\
-\frac{\partial H}{\partial I} &= \dot{\lambda}_3 = V\lambda_4q - V\lambda_4 \\
-\frac{\partial H}{\partial F} &= \dot{\lambda}_4 = -\frac{1}{F}
\end{aligned} \tag{10}$$

## 5 Indeterminate inflorescences

In plants with indeterminate inflorescences, the inflorescence meristem only produces flowers at axillary positions. For example, in *Arabidopsis* the primary shoot meristem converts to an inflorescence meristem that bears floral meristems in axillary positions [Bradley \(1997\)](#).

I describe the developmental decisions in a plant with indeterminate inflorescences using four types of divisions ((Figure 5). First, a primary meristem can divide at the shoot apical meristem to give rise to two primary meristems: the main branch and an axillary bud. These divisions lead to a vegetative, branching architecture. Second, a primary meristem can divide at the shoot apical meristem to give rise to a primary meristem and an inflorescence meristem: a branch and an inflorescence. These divisions produce either (1) an axillary inflorescence or (2) an inflorescence along the main branch and a vegetative, primary meristem that can continue branching. Third, a primary meristem can divide at the shoot apical meristem to give rise to two inflorescence meristems. Fourth, an inflorescence meristem can divide to give rise to an inflorescence meristem and a floral meristem. Inflorescence meristems have a single fate: they produce a branch with floral meristems in axillary positions.

I use these types of divisions/transitions to summarize the meristem dynamics for plants with indeterminate inflorescences in a system of equations with constraints (Equation 15

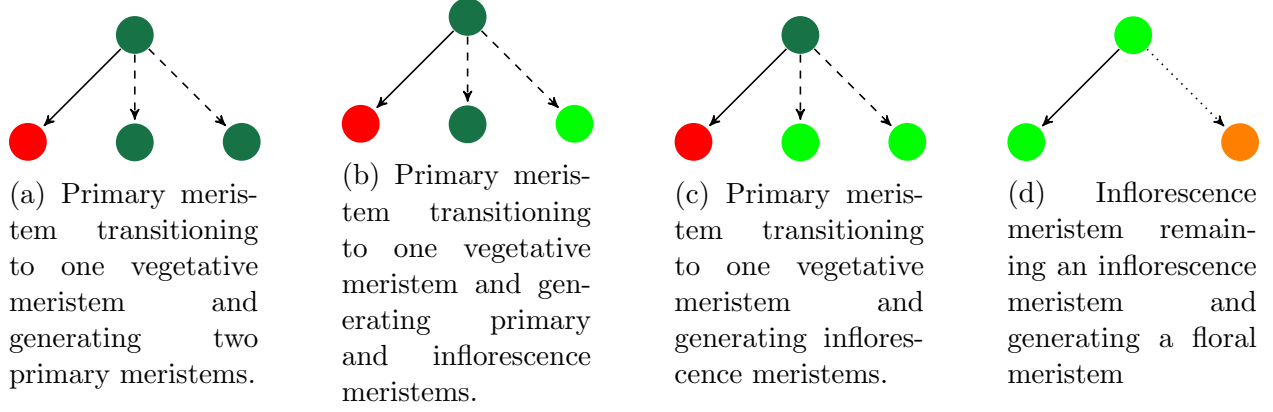


Figure 5: Meristem transitions in plants with indeterminate inflorescences.

and 17) and a state diagram (Figure 6). In this model,  $P$ ,  $V$ ,  $I$ , and  $F$  are the populations of primary, vegetative, inflorescence, and floral meristems, respectively.

## 5.1 Description of diagram

The division shown in Figure 5A occurs at rate  $\beta_1 p(t)$ . The rate is the product of  $\beta_1$ , the ..., and  $p(t)$ , the probability with which the division shown in Figure 5A occurs. It results in the net gain of one primary meristem and gain of one vegetative meristem. The differential equations corresponding to this are:

$$\begin{aligned}
 \dot{P} &= 2\beta_1 p(t)P - \beta_1 p(t)P = \beta_1 p(t)P \\
 \dot{V} &= \beta_1 p(t)P \\
 \dot{I} &= 0 \\
 \dot{F} &= 0
 \end{aligned} \tag{11}$$

The division shown in Figure 5B occurs at a rate  $\beta_1 q(t)$ . The rate is the product of  $\beta_1$ , the ..., and  $q(t)$ , the probability with which the division shown in Figure 5B occurs. It results in the gain of one vegetative meristem and the gain of one inflorescence meristem. The differential

equations corresponding to this are:

$$\begin{aligned}
\dot{P} &= 0 \\
\dot{V} &= \beta_1 q(t) P \\
\dot{I} &= \beta_1 q(t) P \\
\dot{F} &= 0
\end{aligned} \tag{12}$$

The division shown in Figure 5C occurs at a rate  $\beta_1 r(t)$ . The rate is the product of  $\beta_1$ , the ..., and  $r(t)$ , the probability with which the division shown in Figure 5C occurs. It results in the net gain of two inflorescence meristems, gain of one vegetative meristem, and the loss of one primary meristem. The differential equations corresponding to this are:

$$\begin{aligned}
\dot{P} &= -\beta_1 r(t) P \\
\dot{V} &= \beta_1 r(t) P \\
\dot{I} &= 2\beta_1 r(t) P \\
\dot{F} &= 0
\end{aligned} \tag{13}$$

The division shown in Figure 5D occurs at a rate  $\beta_2$ . It results in the net gain of one floral meristem. The differential equations corresponding to this are:

$$\begin{aligned}
\dot{P} &= 0 \\
\dot{V} &= 0 \\
\dot{I} &= 0 \\
\dot{F} &= \beta_2 I
\end{aligned} \tag{14}$$

The full system of differential equations for the system thus becomes:

$$\begin{aligned}
\dot{P} &= \beta_1(p(t) - r(t))P \\
\dot{V} &= \beta_1(p(t) + q(t) + r(t))P \\
\dot{I} &= \beta_1(q(t) + 2r(t)) \\
\dot{F} &= \beta_2 I
\end{aligned} \tag{15}$$

I assume that

$$p(t) + q(t) + r(t) \leq 1 \tag{16}$$

Because they are probabilities, the controls  $p(t)$ ,  $q(t)$ , and  $r(t)$  are constrained on  $[0, 1]$ . The difference between controls (e.g.  $p(t) - r(t)$ ) is not constrained and can be negative. For example, when the probability of division into two inflorescence meristems is greater than the probability of division into two primary meristems, the value of  $\dot{P} < 0$  and corresponds to a decrease in the size of the primary meristem pool. If all primary meristem divisions are like in Panel A,  $\dot{I} = 0$ . If  $p + q + r < 1$  at any point, than it's beneficial to increase  $p$ .

The goal of this optimization problem is to maximize  $F$ . The variable in the model is  $T$ , the length of the season. The model is described by the system of differential equations above 15 and subject to

$$\begin{aligned}
0 \leq p(t) \leq 1, \quad 0 \leq q(t) \leq 1, \quad 0 \leq r(t) \leq 1, \\
0 < P, \quad 0 \leq V, \quad 0 \leq I, \quad 0 \leq F
\end{aligned} \tag{17}$$

I also tried to summarize the dynamics in a state diagram:

The equation  $\dot{P} = \beta_1(p(t) - q(t))P$  describes how primary meristems that divide into

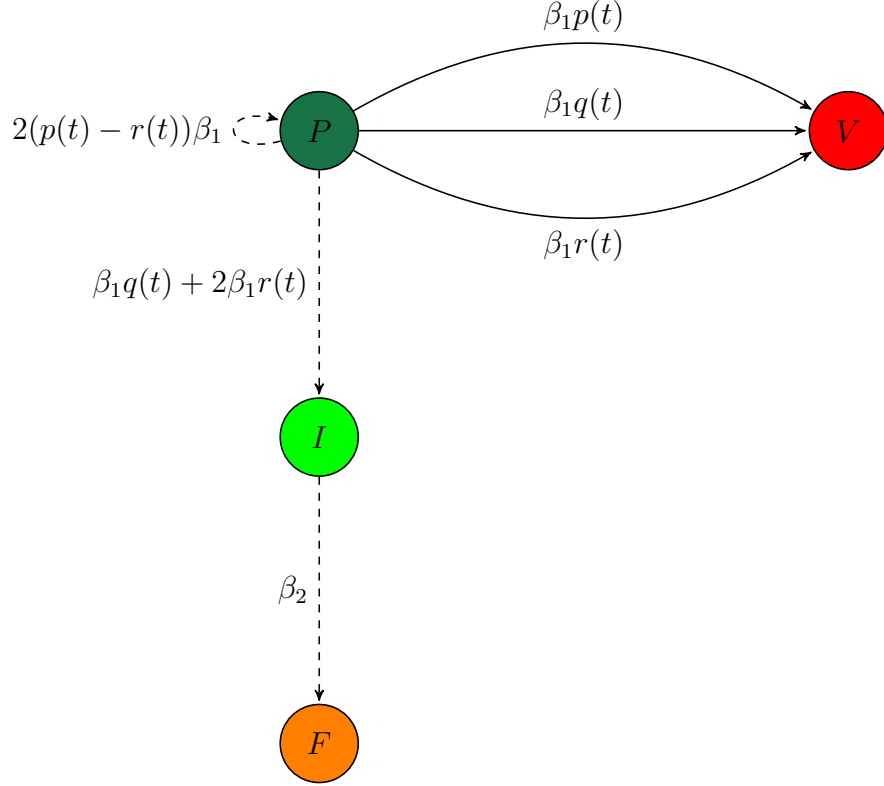


Figure 6: State diagram describing the dynamics for plants with indeterminate inflorescences.

two primary meristems add to the pool  $P$ , and primary meristems that divide into two inflorescence meristems subtract from the pool  $P$ .

The equation  $\dot{I} = \beta_1(1 - p(t) - q(t))P + 2\beta_1 q(t)P + \beta_2 I$  describes how primary meristems contribute to inflorescence meristems when they divide asymmetrically (i.e. do not divide into two primary meristems or into two inflorescence meristems); this happens with probability  $1 - p(t) - q(t)$  and when they divide into two inflorescence meristems with probability  $q(t)$ . Because the primary meristem divides into two inflorescence meristems, the value is doubled in the equation. Finally, inflorescence divisions occur proportional to the size of the inflorescence meristem pool.

The equation  $\dot{F} = \beta_2 I$  describes how inflorescence meristems divide proportional to the size of the inflorescence meristem pool. Each division produces a floral meristem.

## 5.2 Model description - NEED TO UPDATE

Qualitatively, this model describes the accumulation of primary meristems through division at the shoot apical meristem. Without further modification to the model, all primary meristems have active SAMs (can produce further primary meristems through division). Primary meristems that are converted to inflorescence meristems can not be reverted to primary meristems. These inflorescence meristems can divide and produce floral meristems but can not produce more axillary meristems with the potential to produce more inflorescence meristems. For values of  $p(t) = q(t) = 0$ , plants produce both primary and inflorescence meristems.

There are two rates in the model: the rate of primary meristem division and the rate of inflorescence meristem division. High rates of primary meristem division ( $\beta_1$ ) correspond to morphologies with short internodes (e.g. rosettes) or high levels of branching. Low rates of primary meristem division correspond to morphologies with long internodes and low levels of branching. High rates of inflorescence meristem division ( $\beta_2$ ) correspond to tightly packed inflorescences. Low rates of inflorescence meristem division correspond to spaced inflorescences.

Another point that I need to elaborate on is how vegetative pools and meristem pools are related. See Korner 2015 for one opinion, as well as Fatichi for a complementary view. Some way of modeling this as source/sink dynamics (cf. Neubert?)

### 5.3 Optimal control problem and goals

### 5.4 Analysis of optimal control problem

### 5.5 Numerical algorithm

## Numerical Approach

The canonical methods used to solve optimal control problems are the Pontryagin maximum principle and the Hamilton-Jacobi-Bellman equations. Despite the power of these analytic approaches, it remains challenging to apply them to problems with more than a handful of states or multiple types of constraints. Numerical methods to solve optimal control problems include forward-backward sweep method (Lenhart and Workman), and discretize-then-optimize. Here, we use a form of the latter, the **control parameterization** method.

We attempted to solve the optimal control using a forward-backward sweep method (Lenhart and Workman 20XX) but were unable to define the appropriate adjoint equations for the constrained problem. We then applied a form of the ‘control parameterization method’ described by Lin et al. (2014).

We wrote the function ‘control’, which computes values of derivatives for state variables in the ODE system, the accumulated penalty for violating constraints, and the accumulated objective function. We solved our ordinary differential equations using the R package **deSolve** (sotaert 2014). Our equations exhibited stiffness so we applied the Adams methods (Sotaert). Although **deSolve**’s default integration method (lsoda) detects stiffness properties, we followed the suggestion in Sotaert et al. and selected the Adams method. We penalized values of the control that violated constraints by raising the absolute value of the difference of control values that lie outside the supported region to the power of 1.25. Orig-



inally, we squared this difference but this penalty is shallow for small errors and thus not differentiable. The code snippet below outlines the general structure of the control function.

---

```
376 derivs = numeric(3);
377
378 control <- function(t,y,parms,f1,f2,f3) {
379
380   ## entries in y (system of ODEs)
381   X = y[1];
382
383   ## Control intervals
384   u <- f(t);
385
386   ## Apply positivity constraints, penalize if violated
387   ut = max(u,0); bad = abs(u-ut)^1.25; u = ut;
388
389   ## Apply upper bound constraint, penalize if violated
390   ut = min(u,1); bad = bad + abs(u-ut)^1.25;
391
392   ## Derivative of state variable
393   derivs[1] = u * X;
394
395   ## Cumulative penalty
396   derivs[2] = bad;
397
398   ## Cumulative objective function
399   derivs[3] = log(X);
400
```

```
401   return(list(derivs));
```

```
402 }  
403
```

---

404 [Lin et al. \(2014\)](#) provide an overview of the control parameterization method. In this  
405 approach, the control is approximated by a "linear combination of basis functions" which  
406 are often "piecewise-constant basis functions." In practice, this means that we divide our  
407 time horizon into an evenly spaced grid with  $n$  points that has  $n - 1$  intervals. The control  
408 function is approximated by  $n - 1$  control intervals. The value on these intervals is optimized.  
409 The grid points remain fixed during optimization. In practice, we divide up our time horizon  
410 with grid points and generate a function that performs constant interpolation on the interval  
411 between the grid points. The code below demonstrates this procedure in R:

---

```
413 ## Generate grid points
```

```
414 topt=seq(0,5,length=11);
```

```
415
```

```
416 ## Generate random set of control values
```

```
417 par = runif(length(topt),0.01,0.05);
```

```
418
```

```
419 ## Generate function for interpolation
```

```
420 f = approxfun(topt,par,rule=2);  
421
```

---

422 We use the control intervals in our optimization routine. We write a function to be  
423 optimized. This function (optimfun) takes values for the control  $\theta$  as its only argument. The  
424 control is used to generate the control intervals. The control intervals are used in combination  
425 with the initial conditions and model parameters to solve the differential equation that  
426 governs the evolution of the state variables (control). The function containing the differential  
427 equation also calculates an integrated constraint violation penalty, which sums across all

```

428 violations of the state and parameter constraints. The function containing the differential
429 equation also calculates the value of the objective function. The final value maximizes the
430 objective function, and introduces a penalty for constraint violations and solutions with
431 instability (oscillation).
432 

---


433 optim_fun = function(theta){
434
435     ## Generate function for interpolation
436     f = approxfun(topt, theta, rule=2);
437
438     ## Vectorize initial conditions and parameters
439     y0 = c(inits,other)
440
441     ## Solve ODE
442     out = ode(y=y0, times=seq(0,5,by=0.1), control, method=odemethod,
443             parms=mParms, f=f);
444
445     ## Get final value of constraint penalty
446     pen = out[nrow(out),"pen"]; # integrated constraint violation penalty
447
448     ## Get final value of objective function
449     obj = out[nrow(out),"obj"];
450
451     ## Calculate penalty for instability
452     wiggly = diff(diff(tMat[,1])) + diff(diff(tMat[,2])) + diff(diff(tMat[,3]));
453
454     ## Sum up the value function
455     val = obj - pwt*pen - lambda*sum(wiggly^2) ## SPE: sum instead of mean on

```

```

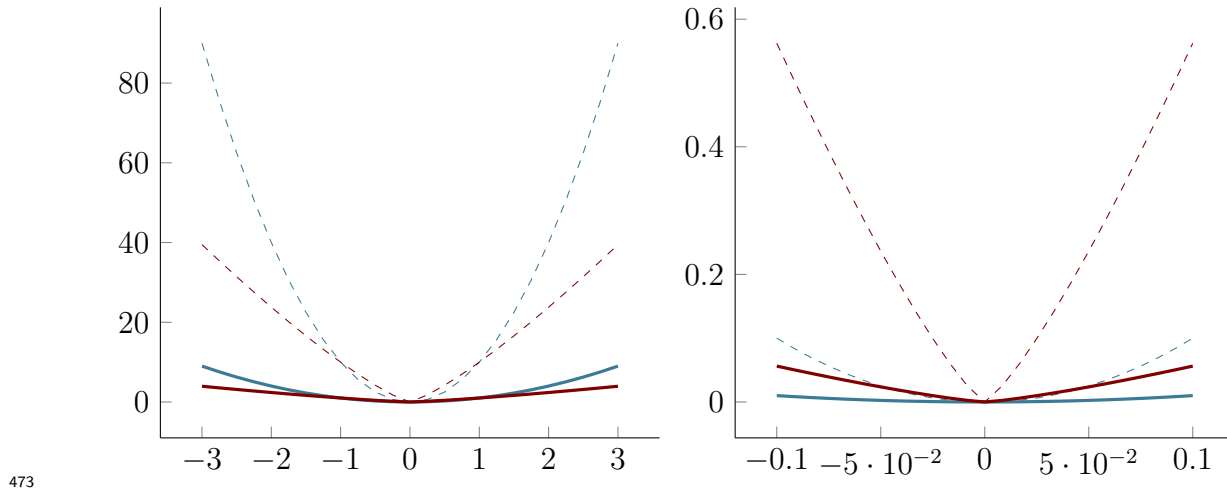
456     wiggleness
457     return(-val)
458 }
459

```

---

We initially considered a quadratic loss function to impose penalties for constraint violations. The quadratic loss function is added on to the objective function for optimization. We weight the penalty to deal with sharp changes in slope of the value function. The quadratic loss function is relatively shallow at small values, so we turned to a modified loss function,  $\text{abs}(f(x) - x)^{1.25}$ . The function has a greater slope at small values but is smooth. The figure below shows the quadratic and modified loss function over large constraint violations,  $(-3, 3)$ , and small constraint violations,  $(-0.1, 0.1)$ . The solid lines are the unweighted loss functions (weight=1; quadratic is blue, modified is red). The dashed lines are the loss functions weighted by a constant of 10.

We started optimization with a smaller penalty for constraint violations (penalty = 1), which is similar to a penalty weight of 10 for a quadratic loss function at small values. After a first round of optimization, we imposed a larger penalty for constraint violation (penalty = 10).



Finally, we initialize our optimization routine. In general, we use a combination of strate-

gies to initialize the optimization routine. For some parameters, we randomly generate values on the support of the control functions (e.g.  $0 \leq u(t) \leq 1$ ). In other cases, we initialize our optimization with values from the analysis of unconstrained versions of our optimal control problem. We then set weights for the penalty we apply for constraint violations and instability. We choose to start with large penalties that decrease with each iteration of optimization; this has the effect of penalizing constraint violations early in the routine when the control is likely to be further from the optimum and reducing the weight of subsequent, smaller violations to the constraints.

---

```
## Randomly generate initial values for control
par0 = runif(2*length(topt),0.01,0.05);

## Generate initial values for control from analysis of unconstrained problem
# beta2 is maxed-out at the end in the unconstrained problem (from analysis of
  adjoint equations)
# so start with the max first
par0 = c(par0, mParms[2]*seq(0,1,length=length(topt))^2)

## optimize: start with a large lambda, and decrease it with each iteration.
# pwt=1; lambda=0.2; fvals = numeric(5);
# SPE: large penalty weight, and large lambda at first
pwt=10; lambda=1; fvals = numeric(40);
```

---

Once all of this machinery is in place, we proceed to iteratively solve our control problem. We take the following approach:

- Use the Runge-Kutta-4 method (rk4) for ODEs and Nelder-Mead for optimization (1

iteration).

- Reset the controls to lie within their constraints.
- Use the implicit Adams method (impAdams or impAdamsd) for ODEs and BFGS for optimization (1 iteration).
- Reset the controls to lie within their constraints. - do I do this here as well?
- Enter an optimization loop. Within the loop:
  - Use the implicit Adams method (impAdams or impAdamsd) for ODEs and Nelder-Mead for optimization.
  - Reset the controls to lie within their constraints.
  - Use the implicit Adams method (impAdams or impAdamsd) for ODEs and BFGS for optimization (1 iteration).
  - Reduce the weight for lambda by half.
  - Reduce the weight for constraint violation by half. (?)
  - What's the particular logic of this procedure - need to write a bit about this.

---

```

fit = optim(par0, fn=optim_fun, method="Nelder-Mead", control =
list(maxit=5000, trace=4, REPORT=1));

```

---

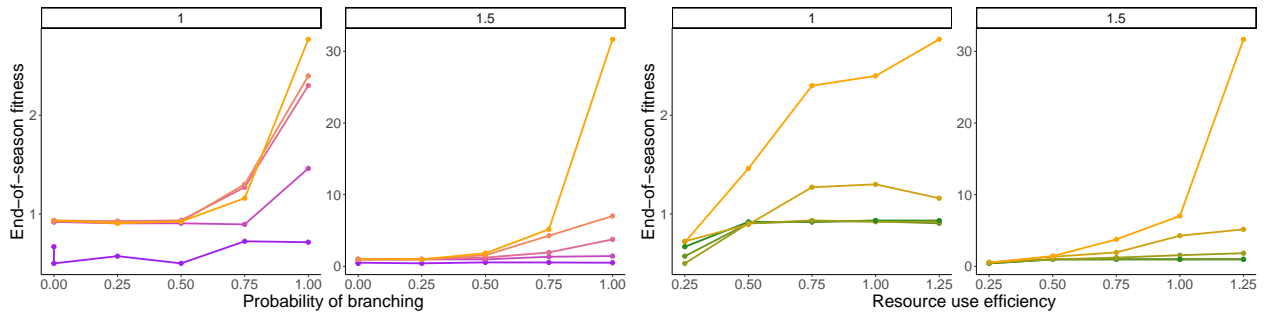
## 6 Results

### 6.1 Optimal strategies

I will use the models to determine whether including differentiation and growth of meristems reduces the likelihood of obtaining a strategy with an instantaneous switch ?. Put another way, are graded allocation strategies optimal when vegetative and reproductive growth are coupled Fox (1992)?

### 6.2 Development patterns

I will ask when plants are more likely to be resource versus meristem limited depending on their relative propensity for branching and resource use efficiencies. Specifically, I will focus on how the optimal strategy changes as the probability of branching and resource use efficiency varies jointly.

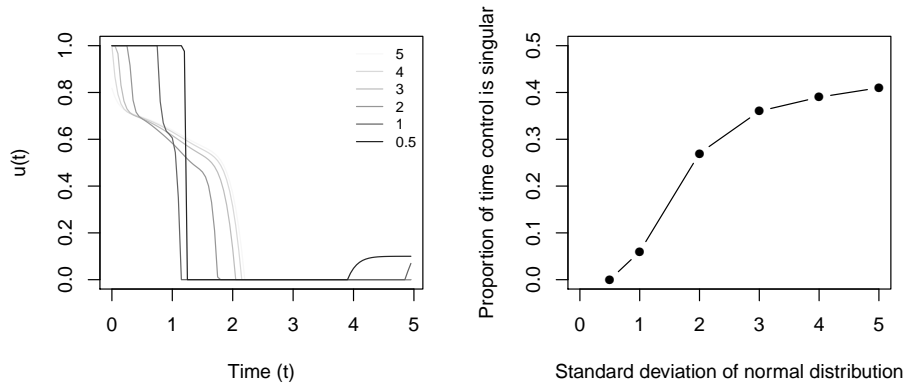


Steve and I have discussed that the degree of resource or meristem limitation would be best analyzed in terms of sensitivities, rather than the end-of-season fitnesses I have presented above.

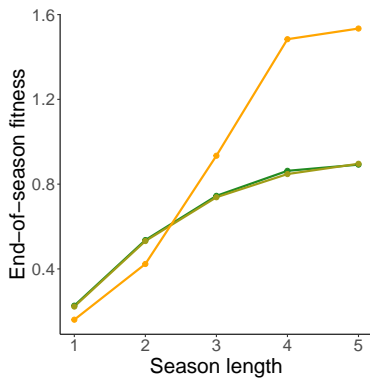
## 6.3 Environmental variation

I will ask when plants are more likely to be resource versus meristem limited. Specifically, I will focus on how the optimal strategy changes with environmental variation; are plants likely to be meristem limited in scenarios with high levels of uncertainty about season length as a result of selection for the ability to capitalize on longer, if infrequent, seasons?

In resource-only models (e.g. King and Roughgarden 1982), increasing variation in season length increases the proportion of the season in which the singular, graded control is optimal.



Below, I've included a plot of how end of-season fitness changes as a function of season length under a uniform distribution of season lengths for varying probabilities of branching.





## References

- Bartlett, M. E. and B. Thompson. 2014. Meristem identity and phyllotaxis in inflorescence development. *Frontiers in Plant Science*, **5**.
- Bradley, D. 1997. Inflorescence Commitment and Architecture in *Arabidopsis*. *Science*, **275**:80–83.
- Cohen, D. 1971. Maximizing final yield when growth is limited by time or by limiting resources. *Journal of Theoretical Biology*, **33**:299–307. Tex.isbn: 0022-5193 tex.mendeley-tags: optimal control.
- Cole, L. C. 1954. The population consequences of life history phenomena. *The Quarterly review of biology*, **29**:103–137. Tex.isbn: 00335770.
- Fox, G. A. 1992. Annual plant life histories and the paradigm of resource allocation. *Evolutionary Ecology*, **6**:482–499. Tex.mendeley-tags: optimal control.
- Geber, M. A. 1990. The cost of meristem limitation in *Polygonum arenastrum*: Negative genetic correlations between fecundity and growth. *Evolution*, **44**:799–819. Tex.mendeley-tags: empirical.
- Itzkovitz, S., I. Blat, T. Jacks, H. Clevers, and A. van Oudenaarden. 2012. Optimality in the Development of Intestinal Crypts. *Cell*, **148**:608–619.
- Kellogg, E. A. 2000. A model of inflorescence development. In K. L. Wilson and D. A. Morrison, editors, *Monocots: Systematics and Evolution*, pages 84–88. CSIRO Publishing, Collingwood, VIC, Australia.
- King, D. and J. Roughgarden. 1982. Graded allocation between vegetative and reproductive

growth for annual plants in growing seasons of random length. Theoretical Population Biology, **22**:1–16. Tex.isbn: Alphabetical tex.mendeley-tags: optimal control.

Körner, C. 2015. Paradigm shift in plant growth control. Current Opinion in Plant Biology, **25**:107–114.

Lande, R. and S. J. Arnold. 1983. The measurement of selection on correlated characters. Evolution, **37**:1210–1226.

Lin, Q., R. Loxton, K. Lay Teo, ,Department of Mathematics and Statistics, Curtin University, GPO Box U1987 Perth, Western Australia 6845, and ,Department of Mathematics and Statistics, Curtin University of Technology, GPO Box U 1987, Perth, W.A. 6845. 2014. The control parameterization method for nonlinear optimal control: A survey. Journal of Industrial & Management Optimization, **10**:275–309.

McSteen, P. and O. Leyser. 2005. SHOOT BRANCHING. Annual Review of Plant Biology, **56**:353–374. Tex.isbn: 1543-5008 (Print)\r1543-5008 (Linking) tex.mendeley-tags: empirical.

Park, S. J., K. Jiang, M. C. Schatz, and Z. B. Lippman. 2012. Rate of meristem maturation determines inflorescence architecture in tomato. Proceedings of the National Academy of Sciences, **109**:639–644. Tex.isbn: 1091-6490 (Electronic)\r0027-8424 (Linking).

Prusinkiewicz, P., Y. Erasmus, B. Lane, L. D. Harder, and E. Coen. 2007. Evolution and development of inflorescence architectures. Science, **316**:1452–1456.

Wang, B., S. M. Smith, and J. Li. 2018. Genetic regulation of shoot architecture. Annual Review of Plant Biology, **69**:437–468. Tex.isbn: 1545-2123 (Electronic) 1543-5008 (Linking) tex.mendeley-tags: empirical.

587 Watson, M. A. 1984. Developmental constraints: Effect on population growth and pat-  
588 terns of resource allocation in a clonal plant. *The American Naturalist*, **123**:411–426.  
589 Tex.mendeley-tags: empirical.

590 White, A. C., A. Rogers, M. Rees, and C. P. Osborne. 2016. How can we make plants  
591 grow faster? A source–sink perspective on growth rate. *Journal of Experimental Botany*,  
592 **67**:31–45.

## **Supplementary material**

### **Background for hypotheses.**

Explanation of key papers that motivate the hypotheses in this manuscript. The document describes results from these papers that are relevant to understanding and interpreting the data in this manuscript. Link to document: ...

### **Numerical methods.**

Description of numerical methods used to solve the optimal control problems. Includes outline of algorithm and code for a generic version of the optimal control problem. Link to document: ...

### **Resource allocation model.**

Explanation of models representing plant life history as a resource allocation problem, and analysis of how these models connect to the ones presented in this manuscript. Link to document: ...

### **Analysis of optimal control problem.**

Presents an analysis of the optimal control problem. Link to document: ...