Assimilation *in silico* and in practice: Open source computational tools for simulating CO_2 assimilation and fitting models to data

Christopher D. Muir

University of Hawai'i Mānoa

MOTIVATION

- Mathematical models make sense of data and generate testable predictions
- Statistics should connect theory with data
- Quantitative methods in plant physiology are often complex and opaque

SOFTWARE OBJECTIVES

- Open source methods that are transparent and available online
- Easy for beginners
- Customizable for experts
- Modular to combine in new ways
- Connected with other tools

GETTING STARTED

Find updated instructions on my website

- Install R (www.cran.r-project.org)
- Install RStudio (optional, www.rstudio.com)
- Install maturing packages from CRAN. Open the R application and install packages using the following code:

```
install.packages("gunit")
install.packages("photosynthesis")
install.packages("tealeaves")
```

- Install experimental packages from GitHub. Open the R application and install packages using the following code:

```
install.packages("remotes")
library(remotes)
install_github("leafoptimizer")
```

PHYTECLUB: R ECOSYSTEM FOR PLANT PHYSIOLOGY

Community Input | User Feedback | Refinement

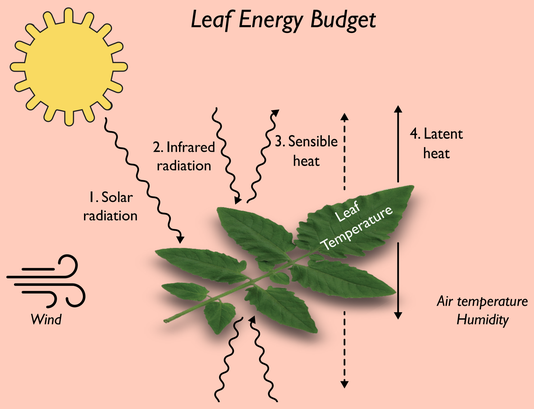
Concept	*Experimental*	*Maturing*	*Stable*
{bayCi}	{leafoptimizer}	{gunit} {tealeaves} {photosynthesis}	

MATURING PACKAGES

{tealeaves} models leaf temperature using energy balance

Environmental parameters:
Air temperature, sunlight, humidity, wind speed, air pressure

Leaf parameters:
Stomatal conductance, stomatal ratio, leaf size, absorbtivity



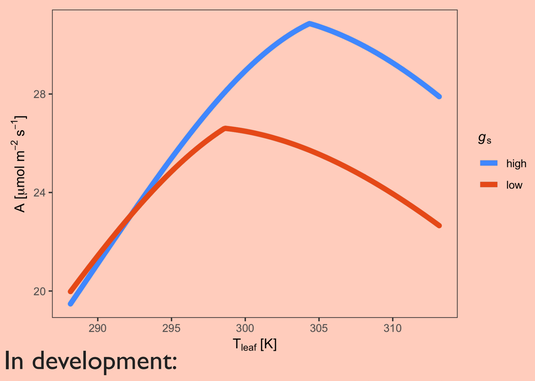
In development:
Sun angle, leaf angle, non-equilibrium, spatially explicit. What else? Your input welcome!

{photosynthesis} models C_3 photosynthesis with temperature dependence

Farquhar-von Caemmerer-Berry (1980) biochemical model of photosynthesis

Customizable leaf temperature responses for biochemical and diffusional parameters.

Integrates with {tealeaves} to optionally model leaf temperature simultaneously



In development:
Limtations calculations, customizable conductance models. What else? Your input welcome!

EXPERIMENTAL

{leafoptimizer} models optimal leaf traits for a given environment

Classic Cowan & Farquhar (1977) optimization

Find traits (e.g. stomata, leaf size) that optimize carbon gain minus costs

Potential applications:
Stomatal ratio and conductance (Muir 2019)
Leaf size, orientation
Nutrient allocation

CONCEPT

{bayCi} analyzes *A*-C_i response curves using Bayesian multilevel models in RStan

Fits Farquhar-von Caemmerer-Berry (1980) model to gas exchange data

Benefits:
- Partition photosynthetic variance among individuals, populations, species, etc.
- Uses informative parameter priors rather than fixing unknown values
- Accurate estimation and uncertainty

Leaf a note!

Comments, criticisms, and contributions welcome

```
library(photosynthesis)

bake_par <- make_bakepar()
constants <-
 make_constants(use_tealeaves = TRUE)

enviro_par <- make_enviropar(
 replace = list(
  T_air = set_units(seq(288:313, K)
   ), use_tealeaves = TRUE
 )

leaf_par <- make_leafpar(
 replace = list(
  g_sc = set_units(c(2, 4), umol/m^2/s/Pa)
   ), use_tealeaves = TRUE
 )

ph <- photosynthesis(leaf_par,
 enviro_par, bake_par, constants,
 use_tealeaves = TRUE)
```

CONTACT

cdmuir@hawaii.edu
cdmuir.netlify.com
github.com/cdmuir
@thegoodphyte

REFERENCES

Cowan IR, Farquhar GD. 1977. Stomatal function in relation to leaf metabolism and environment. *Symposia of the Society for Experimental Biology*, 31: 471–505.

Farquhar GD, von Caemmerer S, Berry J. 1980. A biochemical model of photosynthetic CO_2 assimilation in leaves of C_3 species. *Planta*, 149: 78–90.

Muir CD. 2019. Is amphistomy an adaptation to high light? Optimality models of stomatal traits along light gradients. *Integrative & Comparative Biology*, https://doi.org/10.1093/icb/icz085