Open and reproducible science: From theory to equations, algorithms, and plots

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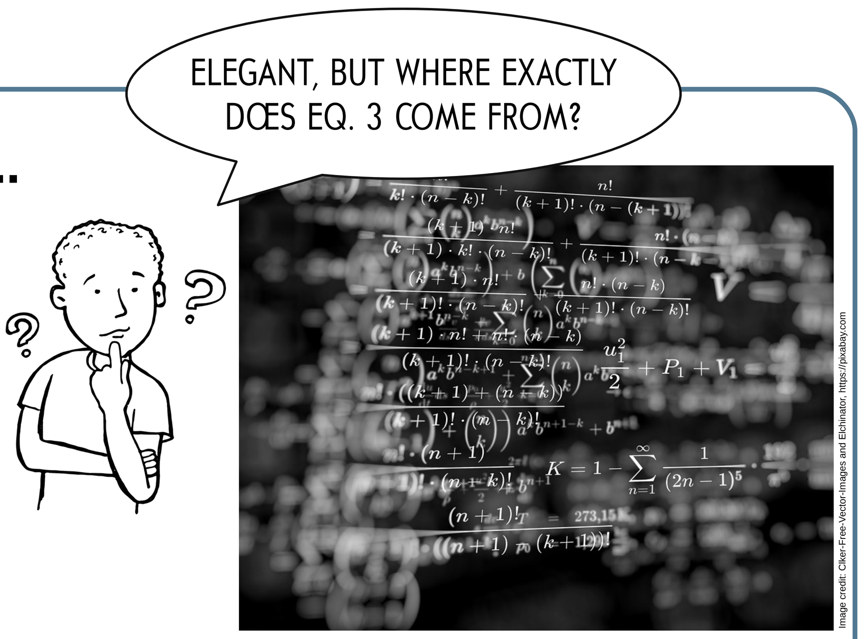
Motivation



Mathematical expressions are...

- the result of scientific theory
- the starting point of new theory
- carriers of explicit and implicit assumptions
- often of unclear origin
- sometimes void of meaning
- at the base of quantitative computations and predictions

→ **Need an open computational framework to transparently link data to algorithms, equations and their underlying theory and assumptions.**

Open-source: python, SymPy, ESSM and jupyter

python.org

"Python is a programming language that lets you work more quickly and integrate your systems more effectively."
- Transparent, free and open source
- Well documented and easy to learn
- Interactive, inclusive
- Community-developed, extendable

sympy.org

"SymPy is a Python library for symbolic mathematics."
- Transparent, free and open source
- Solve systems of equations and inequalities symbolically
- Step-by-step manipulations of expressions
- Plethora of mathematical solvers and operations (differentials, integrals, summations, factorials, ...)

github.com/environmentalscience/essm

"Environmental Science using Symbolic Math (ESSM) contains helpers to deal with physical variables and units."
- Transparent, free and open source
- Record dimensions, units and standard values with variable definitions
- Record dependencies between expressions
- Automatically check for dimensional consistency

jupyter.org

"The Jupyter Notebook is an open-source web application that allows you to create and share documents that contain live code, equations, visualizations and narrative text."
- Transparent, free and open source
- Interactive
- Easy to share and collaborate

Example: Unit mystery in PT equation

The Priestley-Taylor (PT) equation (Priestley & Taylor, 1972) for large scale evaporation is widely used, yet its derivation is not entirely clear.

A key step in the derivation is Equation 3:

> for all time. It had been earlier concluded by one of the authors (Priestley 1959) that the solution would then be $\psi=0$ for all t and z and thus
>
> $$\frac{LE}{H}=\frac{L}{c_p}\left(\frac{\partial q_s}{\partial T}\right)_{T=\overline{T}}=\frac{s}{\gamma}, \qquad (3)$$
>
> c_p is the specific heat of air at constant pressure, s is defined as $\partial q_s/\partial T$ at the appropriate temperature, and γ is c_p/L.

Since the units of the variables were not specified in the paper, we make **informed guesses** based on the description in the text and **widespread literature conventions**. The resulting variables in a Jupyter Notebook:

In [7]:
```python
generate_metadata_table([E_w, H_w, L_E, c_pa, q_s, s_PT, gamma_PT])
```

Out[7]:

Symbol	Name	Description	Definition	Default value	Units
γ	gamma_PT	Priestley-Taylor gamma = c_p/L	$\frac{c_{pa}}{L}$	-	K^{-1}
c_{pa}	c_pa	Specific heat of dry air.		1010.0	$J K^{-1} kg^{-1}$
E	E_w	Wet surface evaporation (E in Priestley and Taylor, 1972))		-	$kg s^{-1} m^{-2}$
H	H_w	Wet surface sensible heat flux (positive outwards)		-	$W m^{-2}$
L	L_E	Latent heat		2450000.0	$J kg^{-1}$
q_s	q_s	Specific humidity at saturation		-	$kg m^{-3}$
s	s_PT	Priestley-Taylor $\partial q_s/\partial T$	$\frac{d}{dT} q_s$	-	$kg K^{-1} m^{-3}$

Entering Eq. 3 as a physical equation in essm returns error:

In [8]:
```python
eq3 = Eq(L_E*E_w/H_w, L_E/c_pa*s_PT)
display(eq3)
try:
    class eq_3(Equation):
        """Equation 3 in Priestley and Taylor (1972)"""
        expr = eq3
except Exception as error:
    print(error)
```

$$\frac{EL}{H} = \frac{Ls}{c_{pa}}$$

```
Dimension of "L_E*s_PT/c_pa" is Dimension(mass/length**3), but it should be the
same as E_w*L_E/H_w, i.e. Dimension(1)
```

Indeed, the left-hand-side of Eq. 3 is dimensionless, while the right-hand side is not:

In [9]:
```python
derive_baseunit(eq3.rhs)
```

Out[9]: $\frac{kg}{m^3}$

No amount of guessing led to dimensional consistency of Eq. 3 and the problem carries through the whole paper, as *γ* and *s* must, but do not have the same units, e.g. Eq. 5:

In [29]:
```python
alpha = Symbol('alpha')
eq5 = Eq(LE / (LE + H_w), alpha * s_PT/(s_PT + gamma_PT))
display(eq5)
try: derive_baseunit(eq5.rhs)
except Exception as e1: print(e1)
```

$$\frac{LE}{H + LE} = \frac{s\alpha}{\gamma + s}$$

```
Dimension of "s_PT" is Dimension(mass/(length**3*temperature)), but it should be
the same as gamma_PT, i.e. Dimension(1/temperature)
```

Example: PT vs. Penman equation

The PT equation is based on a derivation by Penman (1948), who used different variable definitions:

In [31]:
```python
generate_metadata_table([Delta_eTa, gamma_P])
```

Out[31]:

Symbol	Name	Description	Definition	Default value	Units
Δ	Delta_eTa	Slope of saturation vapour pressure at air temperature		-	$Pa K^{-1}$
γ_P	gamma_P	Penman gamma, gamma = beta(e_s - e_d)/(T_s - T_a)	$\frac{\beta(-e_d+e_s)}{-T_a+T_s}$	-	$Pa K^{-1}$

We can easily **substitute** Penman's variables and the energy balance into the original PT Eq. 5, **solve** for LE, and **plot** the resulting PT equation against the original Penman equation:

In [32]:
```python
eq5P = eq5.subs({s_PT: Delta_eTa, gamma_PT: gamma_P}); display(eq5P)
derive_unit(eq5P.rhs)
```

$$\frac{LE}{H + LE} = \frac{\Delta\alpha}{\Delta + \gamma_P}$$

Out[32]: 1

Finally consistent units!

In [34]:
```python
class eq_enbalance(Equation):
    """Surface energy balance."""
    expr = Eq(R - G, LE + H_w)
eq_enbalance
```

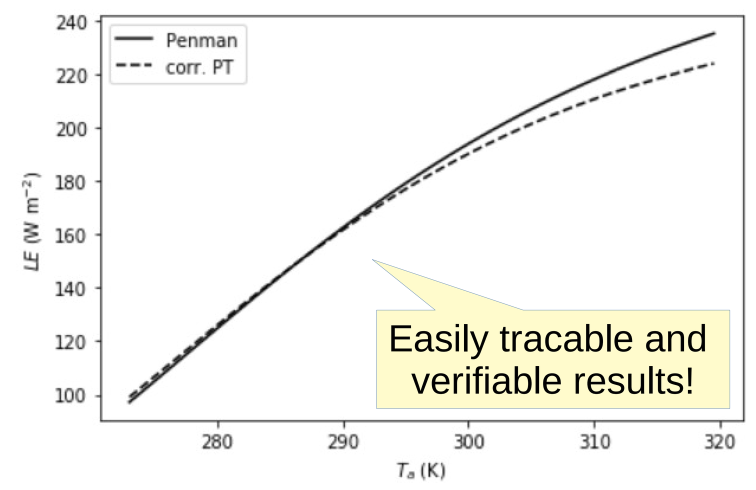
Out[34]: $-G + R = H + LE$

In [35]:
```python
class eq_8P(eq_enbalance.definition, eq_5P.definition):
    """Eq. 8 in Priestley & Taylor (1972) using Penman's variable definitions
    soln = solve([eq_5P, eq_enbalance], LE, H_w)
    expr = Eq(LE, soln[LE])
eq_8P
```

Out[35]: $LE = -\frac{\Delta\alpha(G - R)}{\Delta + \gamma_P}$

```python
vdict[e_a] = eq_ea.rhs.subs(vdict)
vdict[e_d] = 0.5 * vdict[e_a]
vdict[f_u] = 0.1
expr1 = eq_16.rhs.subs(vdict)
expr2 = eq_8P.rhs.subs(vdict)
xvar = T_a
ylvar = LE
xmin = 273.
xmax = 320.
lefty = [(expr1, 'Penman'), (expr2, 'corr. PT'
plot_expr2(xvar, ylvar, xmin, xmax, lefty)
```

Create dictionary with forcing and computed data and progressively substitute into previously defined equations



Easily tracable and verifiable results!

Share entire notebook

renkulab.io/projects/stanislaus.schymanski/essm_egu_2020

No more guess-work!

Acknowledgements and Literature

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Priestley, C. H. B. and Taylor, R. J.: On the Assessment of Surface Heat Flux and Evaporation Using Large-Scale Parameters, Month. Weath. Rev., 100(2), 81–92, 1972.

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