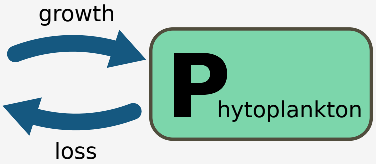
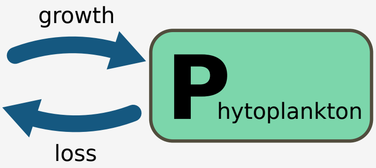
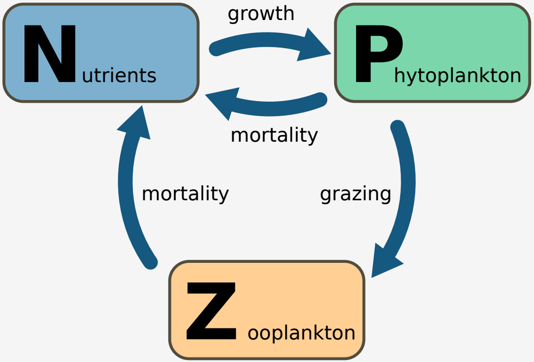
from `Pgrowth` to NPZ

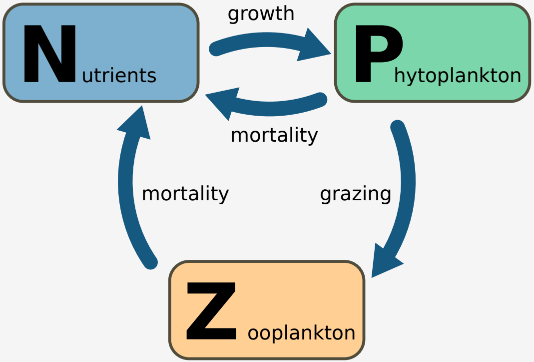


from `Pgrowth` to NPZ





from `Pgrowth` to NPZ



$$\text{growth:} \quad \theta_{\mathtt{vmax}} \frac{N}{N + \theta_{\mathtt{nuthalfsat}}} P$$

$$\text{grazing:} \quad \theta_{\mathtt{graz}} PZ$$

$$P \text{ mortality:} \quad \theta_{\mathtt{mort\_p}} P$$

$$Z \text{ mortality:} \quad \theta_{\mathtt{mort\_z}} Z^2$$

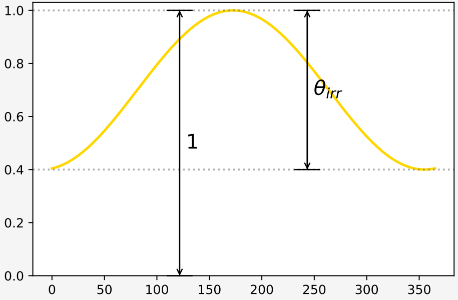
$$\frac{\partial N}{\partial t} = -\theta_{\mathtt{vmax}} \frac{N}{N + \theta_{\mathtt{nuthalfsat}}} P + \theta_{\mathtt{mort\_p}} P + \theta_{\mathtt{mort\_z}} Z^2$$

$$\frac{\partial P}{\partial t} = \theta_{\mathtt{vmax}} \frac{N}{N + \theta_{\mathtt{nuthalfsat}}} P - \theta_{\mathtt{graz}} PZ - \theta_{\mathtt{mort\_p}} P$$

$$\frac{\partial Z}{\partial t} = \theta_{\mathtt{graz}} PZ - \theta_{\mathtt{mort\_z}} Z^2$$

- Modulate phytoplankton growth by annual light cycle (modeled to roughly represent day length in the northern hemisphere, with a minimum on Dec 21).

$$1 + 0.5 \cdot \left(\theta_{\mathtt{irr}} \cdot \sin\left(\frac{2\pi}{365}(t - 81.25)\right) - \theta_{\mathtt{irr}}\right) \qquad \text{with } \theta_{\mathtt{irr}} \in [0, 1]$$



- growth: $\theta_{\mathtt{vmax}} \left(1 + 0.5 \cdot \left(\theta_{\mathtt{irr}} \cdot \sin\left(\frac{2\pi}{365}(t - 81.25)\right) - \theta_{\mathtt{irr}}\right)\right) \frac{N}{N + \theta_{\mathtt{nuthalfsat}}} P$
- 6 parameters in total: $\theta_{\mathtt{vmax}}, \theta_{\mathtt{nuthalfsat}}, \theta_{\mathtt{graz}}, \theta_{\mathtt{mort\_p}}, \theta_{\mathtt{mort\_z}}$ and $\theta_{\mathtt{irr}}$ which we will all estimate in Stan

Stan functions block

```
functions {
   real[] npz(real t,        // time
              real[] x,      // state
              real[] theta,  // parameters
              real[] x_r,    // fixed real data (empty)
              int[] x_i) {   // fixed integer data (empty)

    /*
    guide to theta:
    theta[1]:  vmax          maximum growth rate in Michaelis Menten formulation
    theta[2]:  nuthalfsat    nutrient half saturation in Michaelis Menten formulation
    theta[3]:  graz          zooplankton grazing rate
    theta[4]:  mort_p        phytoplankton mortality rate
    theta[5]:  mort_z        zooplankton mortality rate
    theta[6]:  irr           light amplitude
    */

    real n = fmax(0.0, x[1]);
    real p = fmax(0.0, x[2]);
    real z = fmax(0.0, x[3]);

    real light = 1.0 - 0.5*(theta[6]*sin(pi()*((t-81.25)/182.5)) - theta[6]);
    real growth = theta[1]*n/(theta[2]+n) * light * p;
    real grazing = theta[3]*p*z;
    real ploss = theta[4]*p;
    real zloss = theta[5]*z*z;

    return {-growth+ploss+zloss,growth-grazing-ploss,grazing-zloss};
    }
}
```

goal: estimate

- parameters
- initial conditions
- observation error for each observed variable

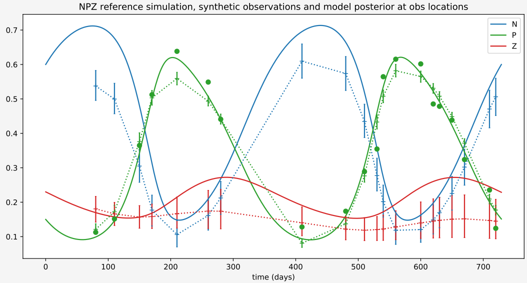
```
parameters {
    real<lower=0> vmax;
    real<lower=0> nuthalfsat;
    real<lower=0> graz;
    real<lower=0> mort_p;
    real<lower=0> mort_z;
    real<lower=0,upper=1> irr;
    real<lower=0> x0[3];            // initial conditions
    real<lower=0> sigma[nobsvar];   // obs error
}
transformed parameters {
    real theta[6] = {vmax,nuthalfsat,graz,mort_p,mort_z,irr};
    real x[nobs, 3] = integrate_ode_rk45(npz, x0, 0, tobs, theta,
                                         rep_array(0.0, 0), rep_array(0, 0),
                                         1e-5, 1e-4, 1e4);
}
model {
    vmax        ~ normal(0.1, 0.1);
    nuthalfsat ~ uniform(0.0, 1.0);
    graz        ~ normal(0.01, 0.01);
    mort_p      ~ normal(0.01, 0.01);
    mort_z      ~ normal(0.01, 0.01);
    irr         ~ uniform(0.0, 1.0);
    x0[1:3]     ~ normal(0.1, 0.1);
    for (iobs in 1:nobs){
        obs[iobs,] ~ normal(x[iobs,iobsvar], sigma);
    }
}
```

exercise

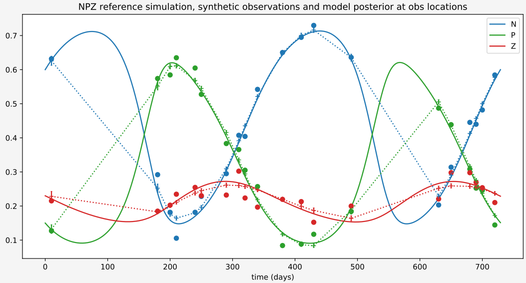
- choose: Turn all 3 variables into observed variables OR select only one observed variable.
- Examine the effect on the output.

exercise

```
iobsvar = np.array([i_p])
sigma = np.array([0.03])
```

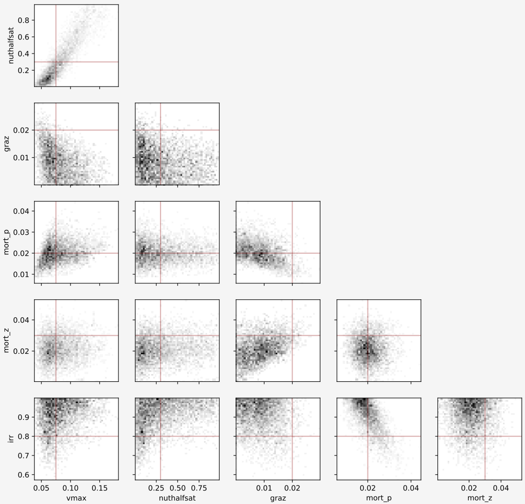



```
iobsvar = np.array([i_n,i_p,i_z])
sigma = np.array([0.03,0.03,0.03])
```

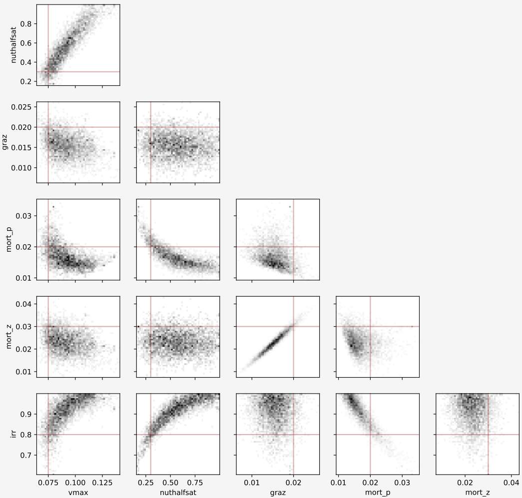


exercise

```
iobsvar = np.array([i_p])
sigma = np.array([0.03])
```



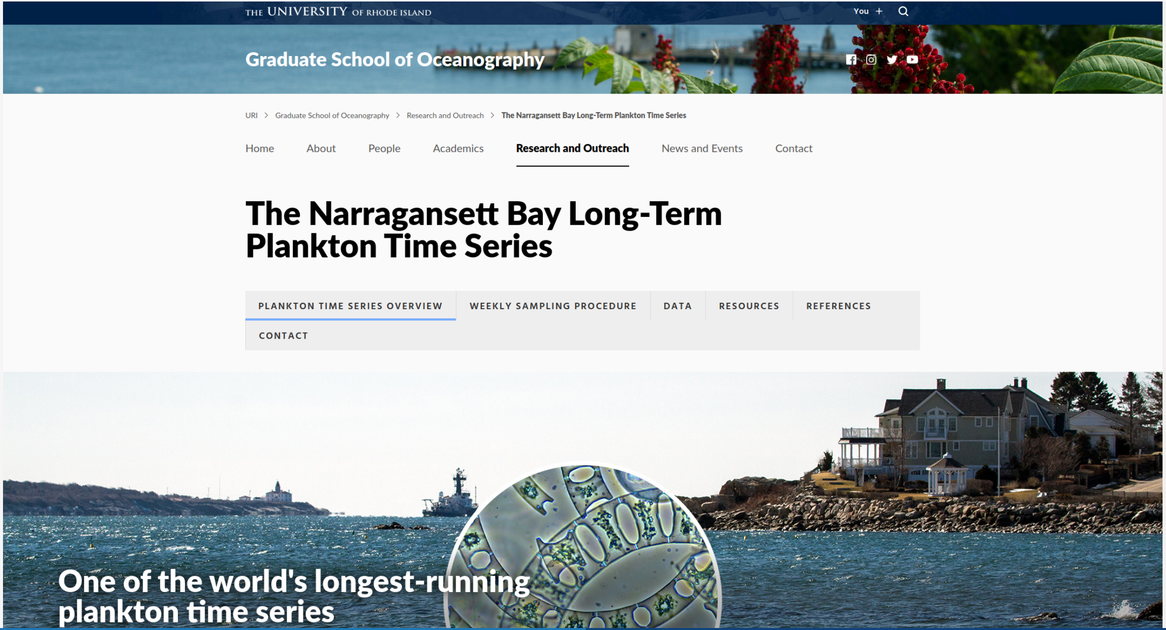

```
iobsvar = np.array([i_n,i_p,i_z])
sigma = np.array([0.03,0.03,0.03])
```



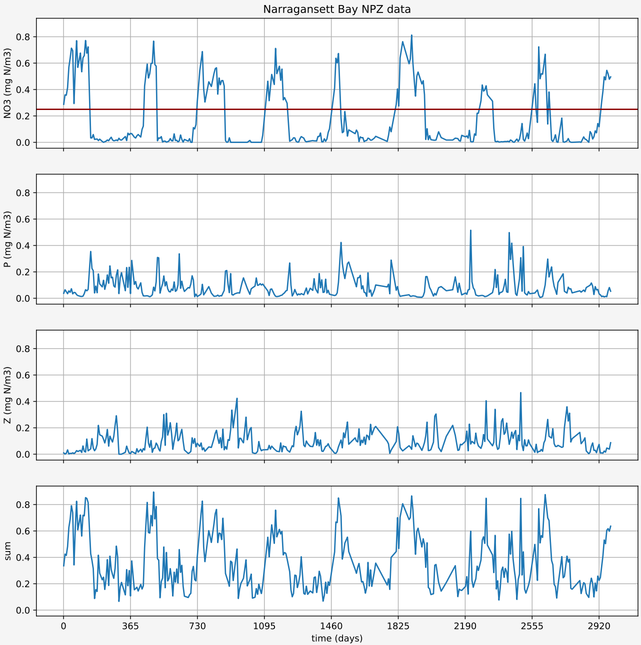
adding real data: Narragansett Bay data set

adding real data: Narragansett Bay data set

https://web.uri.edu/gso/research/plankton/



adding real data: Narragansett Bay data set



- introduce a background concentration for each variable and allow mixing with that background concentration
- have a winter period for each year with stronger mixing and different background concentrations
- estimate start and duration of winter period for each year (initial guess is based on data)
- estimate background concentrations for winter and regular period (same for each year)

add supply (nudging/relaxation) term:

$$\frac{\partial N}{\partial t} = \ldots + \theta_{\mathtt{mix}} \cdot (\theta_{\mathtt{bgconc\_n}} - N)$$

exercise

- The prior distributions for the parameter are all quite "tight", because the model and Stan can be quite sensitive to the parameter choice.
- Modify one of the priors and examine the effects on the prior model solution. Be sure to modify the prior in the first part of the notebook before the data is being fit.
- If you feel adventurous, modify the prior in the second piece of Stan code as well and run it with fitting data.

```
// priors for parameters
    vmax        ~ normal(0.15, 0.03);
    nuthalfsat  ~ normal(0.17, 0.04);
    graz        ~ normal(0.15, 0.04);
    mort_p      ~ normal(0.02, 0.01);
    mort_z      ~ normal(0.02, 0.005);
    bgconc_n1   ~ normal(0.01, 0.001); // (regular)
    bgconc_n2   ~ normal(0.66, 0.08);  // (winter)
    bgconc_p1   ~ normal(0.11, 0.01);  // (regular)
    bgconc_p2   ~ normal(0.05, 0.005); // (winter)
    bgconc_z1   ~ normal(0.09, 0.01);  // (regular)
    bgconc_z2   ~ normal(0.05, 0.03);  // (winter)
    mix1        ~ normal(0.01, 0.03);  // (regular)
    mix2        ~ normal(0.19, 0.02);  // (winter)
```

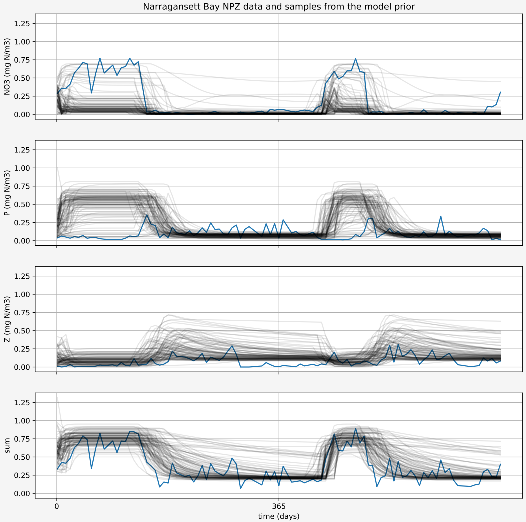
going from

```
vmax          ~ normal(0.15, 0.03);
```

to

```
vmax          ~ normal(0.5, 0.5);
```

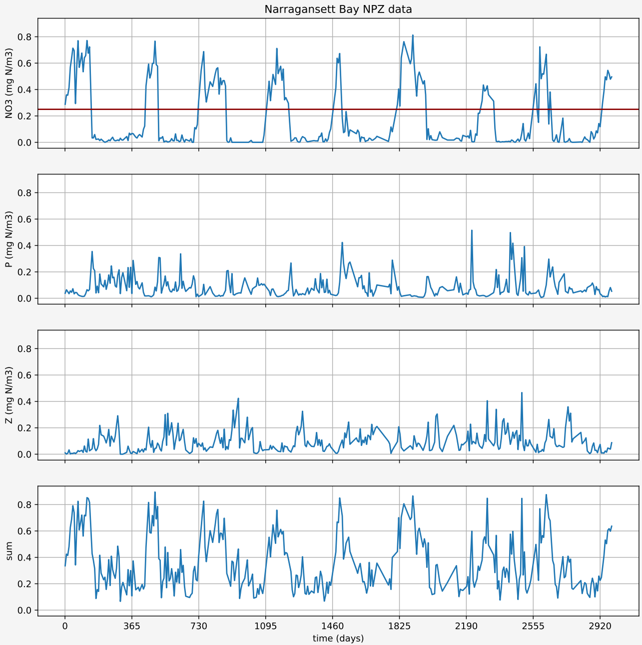
results in



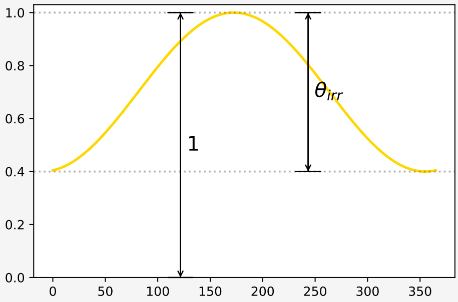
hackathon ideas

1. develop a different model for supply and loss of N
2. add in light limitation
3. come up with priors for the winter period start and duration without an informed guess
4. modify the NPZ model formulation (unobserved N contained in a detritus variable, light limitation in winter?)
5. add new observations (there are more in the Narragansett Bay dataset)

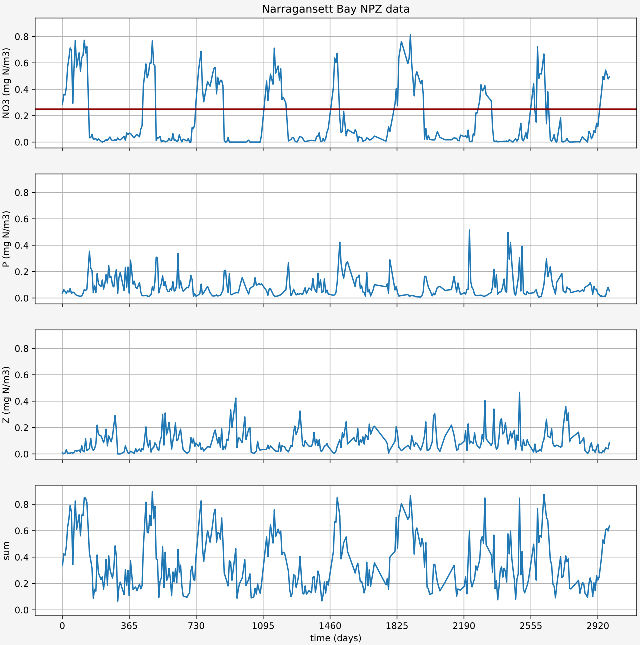
idea: develop a different model for supply and loss of N



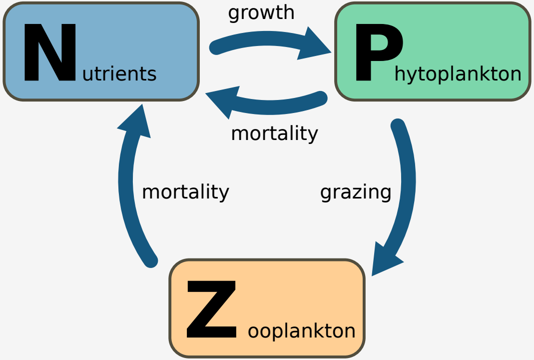
idea: add in light limitation



idea: come up with priors for the winter period start and duration without an informed guess



idea: modify the NPZ model formulation (unobserved N contained in a detritus variable, light limitation in winter?)



add new observations (there are more in the Narragansett Bay dataset)

candidates:

- other nutrients like phosphorous
- ...