Generating Data

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Suppose we want to define an example GRN inference problem. In general, we approach this problem from the perspective of differential equations. We hope that there is a system of differential equations for a given regulatory network that is able to determine the time-based progression of expression. Specifically for a given gene g the expression of g, denoted by x_g is governed by

$$\partial x_g = F(x, \theta, t)$$

for a given F and parameters θ. In our case, we only consider $\{x_h \mid h \in N(g)\}$, or the expression profiles of neighboring genes in a proposed regulatory network.

We can do this is in julia with the `NeuralGRN.jl` package. To start load the nessary packages and define a few constants like initial conditions and the function F.

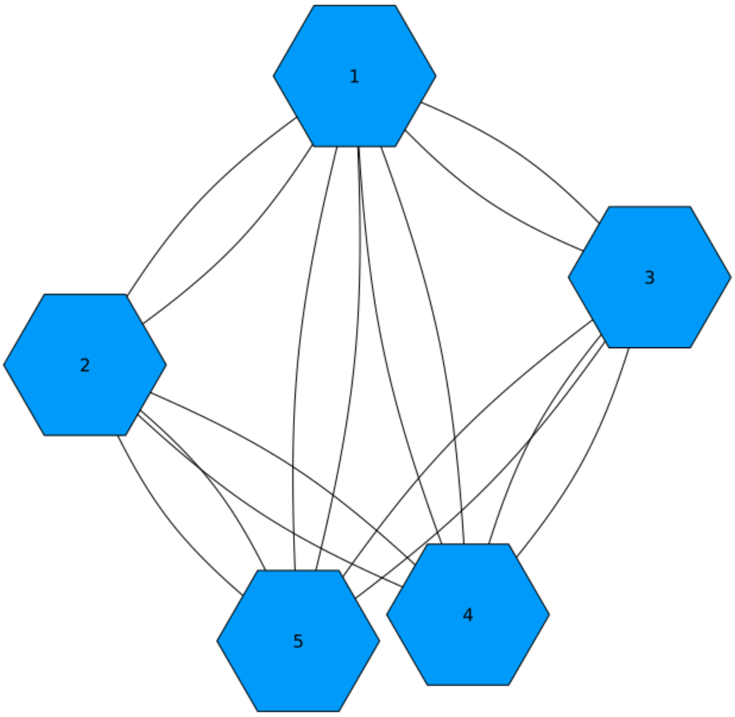
```
using NeuralGRN, LightGraphs, Plots, StatsPlots, LinearAlgebra, Distributions,
GraphRecipes
n = 5;
x_0 = rand(Normal(0, 0.2), n);
p = rand(Normal(), n, n);
propogate(u, p, t) = 10 * (u ⋅ p) * cos(5 * t) * exp(-0.5*t);
τ = 0:0.01:3 |> Array;
```

The F we chose for this example is

$$\partial x_g = 10(x_h \cdot \theta_g)\cos(5t)e^{-\frac{t}{2}}$$

More importantly, though, we need a computational graph that defines the relationships between different genes in our sample GRN. The following is a random graph, but any `SimpleGraph` would do.

```
g = erdos_renyi(n, 0.7);
plot(g, names=string.(1:n), nodesize = 0.4, fontsize = 10, fmt = :svg)
```

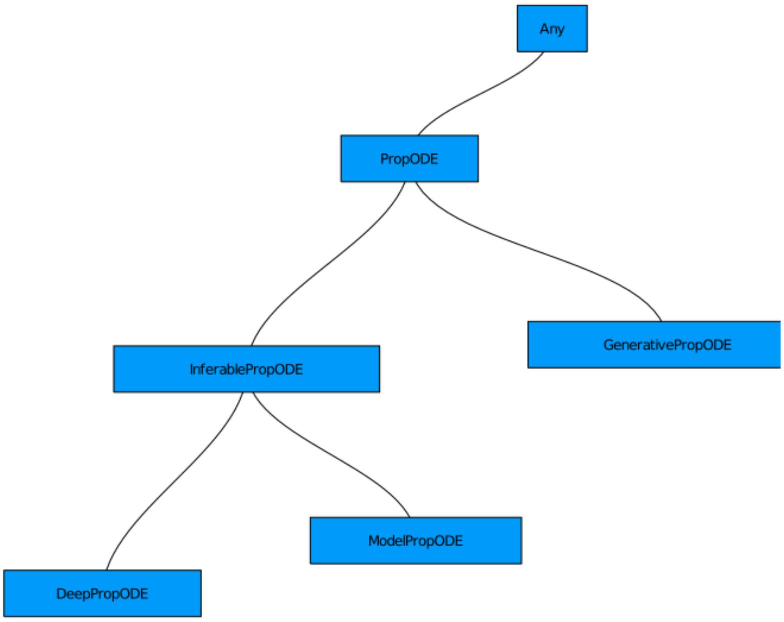


We now define a generative model using the inputs from above.

```
gen = GenerativePropODE(x_0, fill(propogate, n), p, g, τ);
```

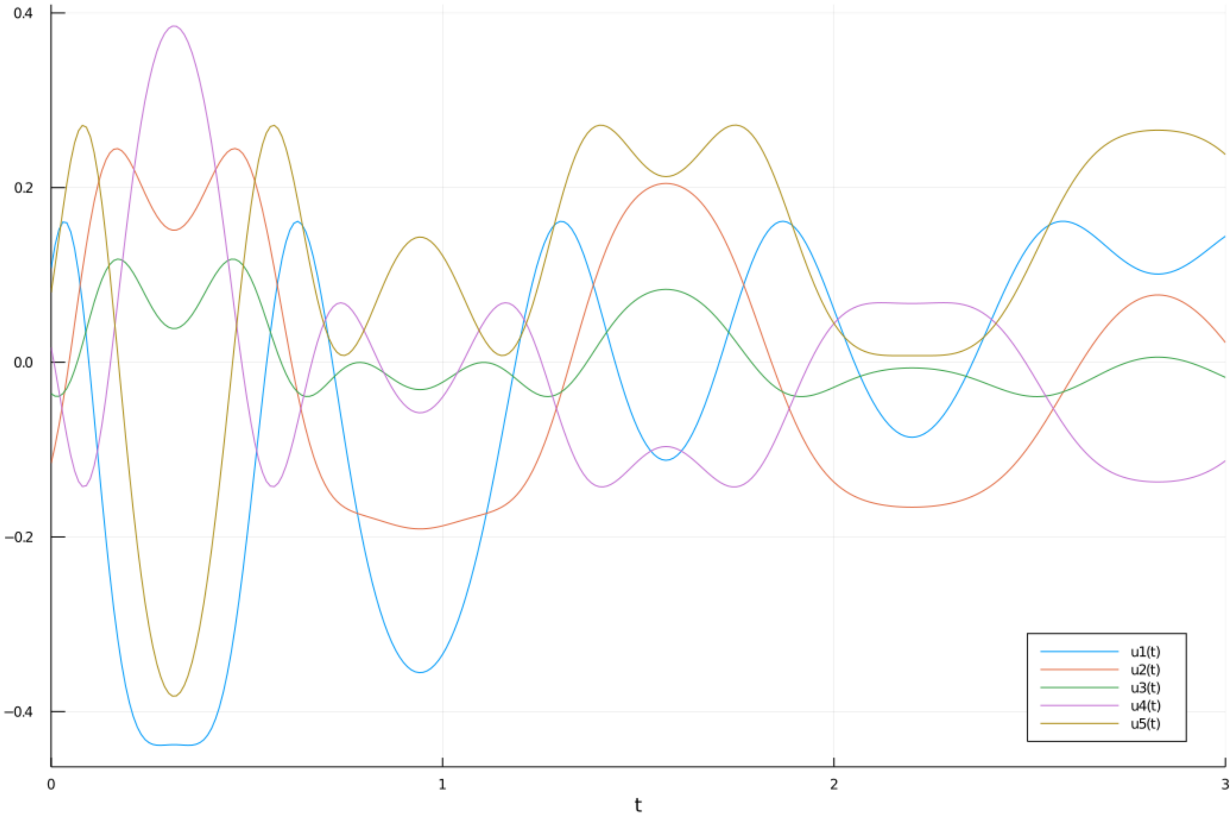
Using the `generate` function we can solve this system with the given parameters. This is all done courtesy of `DifferentialEquations.jl`. Note here that any subtype of `PropODE` can use the generate method which give inferred models based on real data the ability to project expression into the future. The following is a type diagram for the `PropODE` so you can see the different models in the works.

```
plot(NeuralGRN.PropODE, method = :tree, fontsize = 8, nodeshape = :rect, fmt = :svg)
```



We can run the inference and then plot the resulting data.

```
results = generate(gen);
plot(results, legend = :bottomright, fmt = :svg)
```


0.4
0.2
0.0
−0.2
−0.4
0
1
2
3
t
u1(t)
u2(t)
u3(t)
u4(t)
u5(t)