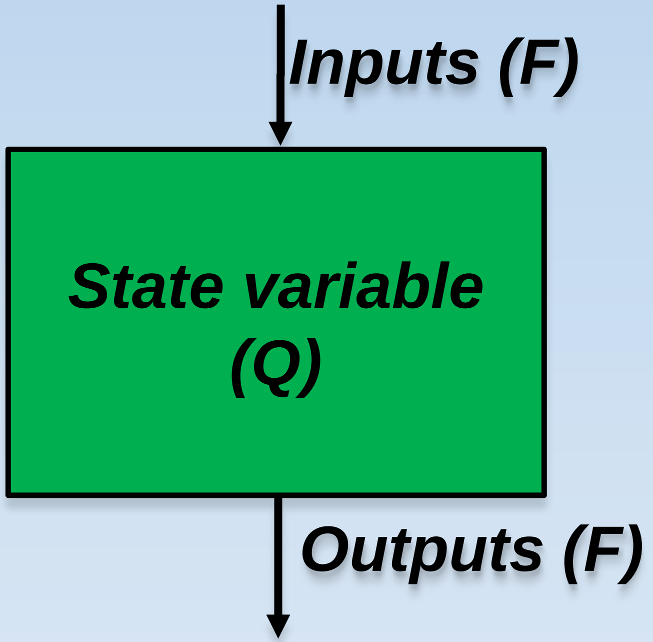
Introduction and model construction



Timothy J. Hackmann[1], Mark D. Hanigan[2], Veridiana L. Daley[3]
[1]University of Florida
[2]Virginia Tech
[3]University of Kentucky

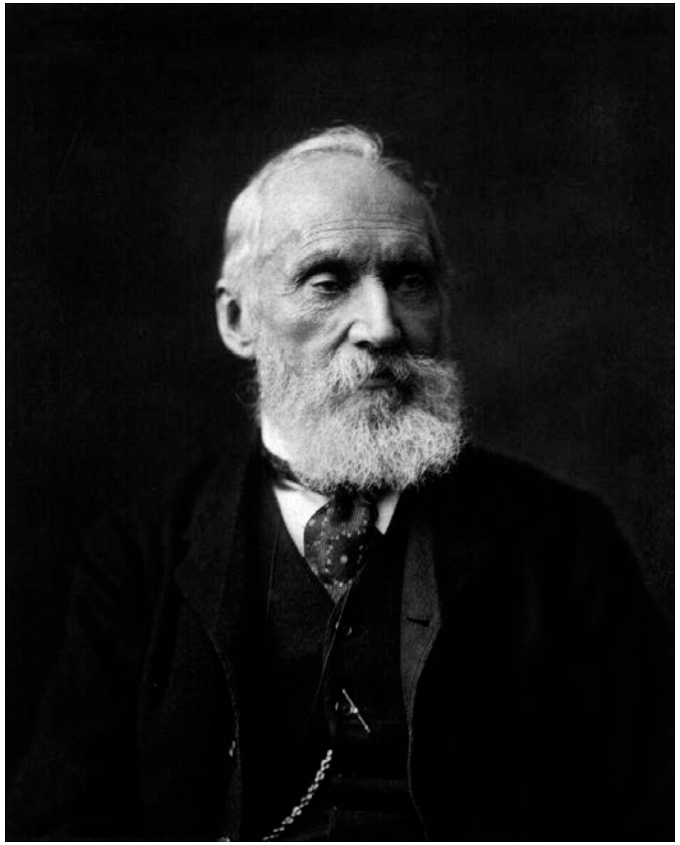
Learning objectives

- Explain the motivation for modeling
- Compare and contrast different types of models
- Outline the steps of constructing and evaluating a model

Why modeling?

"When you cannot express [something] in numbers, your knowledge is of a meager and unsatisfactory kind . . . you have scarcely, in your thoughts, progressed the level of science."

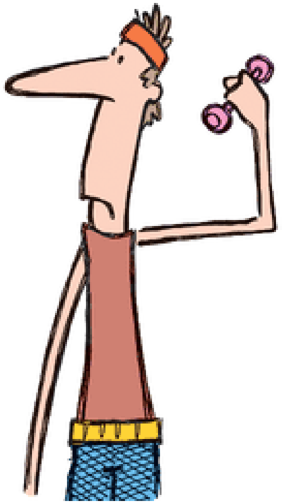
Lord Kelvin



Why modeling?

<u>WEAK HYPOTHESIS</u>

"NDF is a major factor determining the level of feed intake by cattle."



<u>STRONG HYPOTHESIS</u>

Intake = 1.2 × BW / % NDF

Equation: Mertens. 1985. In Georgia Nutr Conf. pp. 1-18.
Images: app.hedgeye.com/insights/37422-cartoon-of-the-day-muscle-vs-russell?type=video

Goal of modeling

- Take a hypothesis
- Convert it a system of equations
- Determine how well the equations describe reality

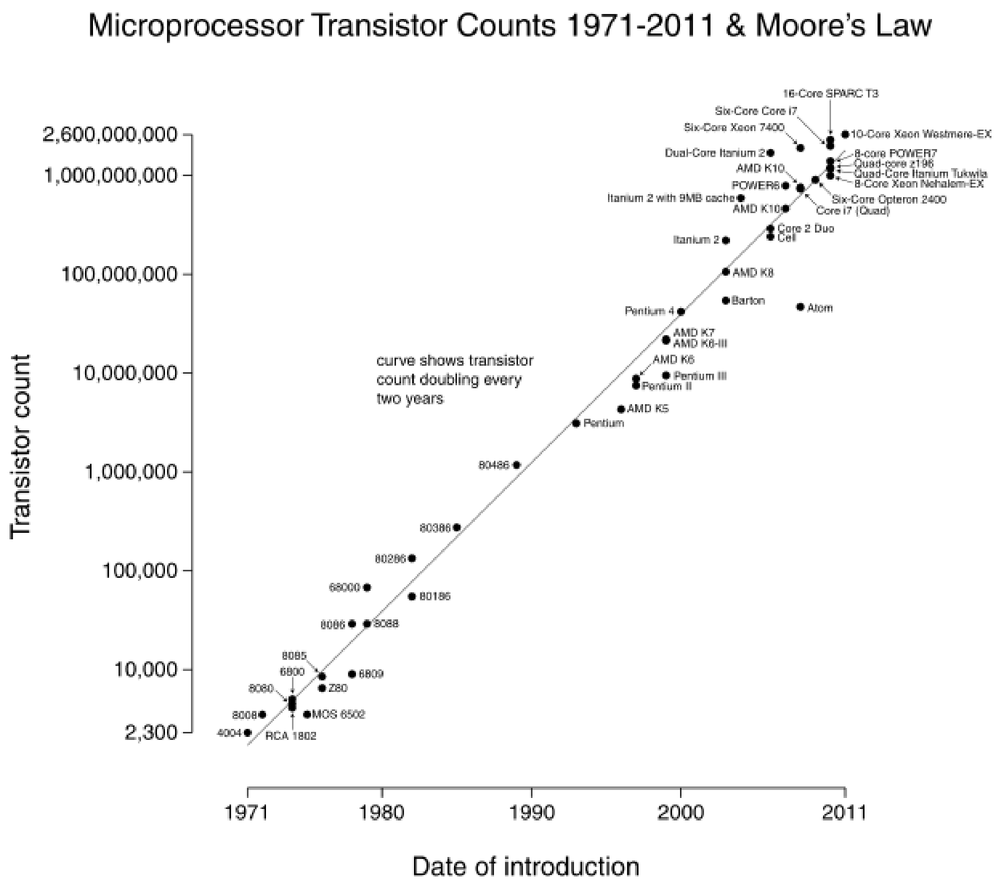
Types of models

- Empirical vs. mechanistic
- Deterministic vs. stochastic
- Static vs. dynamic

Empirical vs. mechanistic

- Empirical
  - Represents relationship between two or more variables
    - Usually regression equation
  - Ignores underlying biological or physical causes
  - Example: Moore's Law

Moore's law

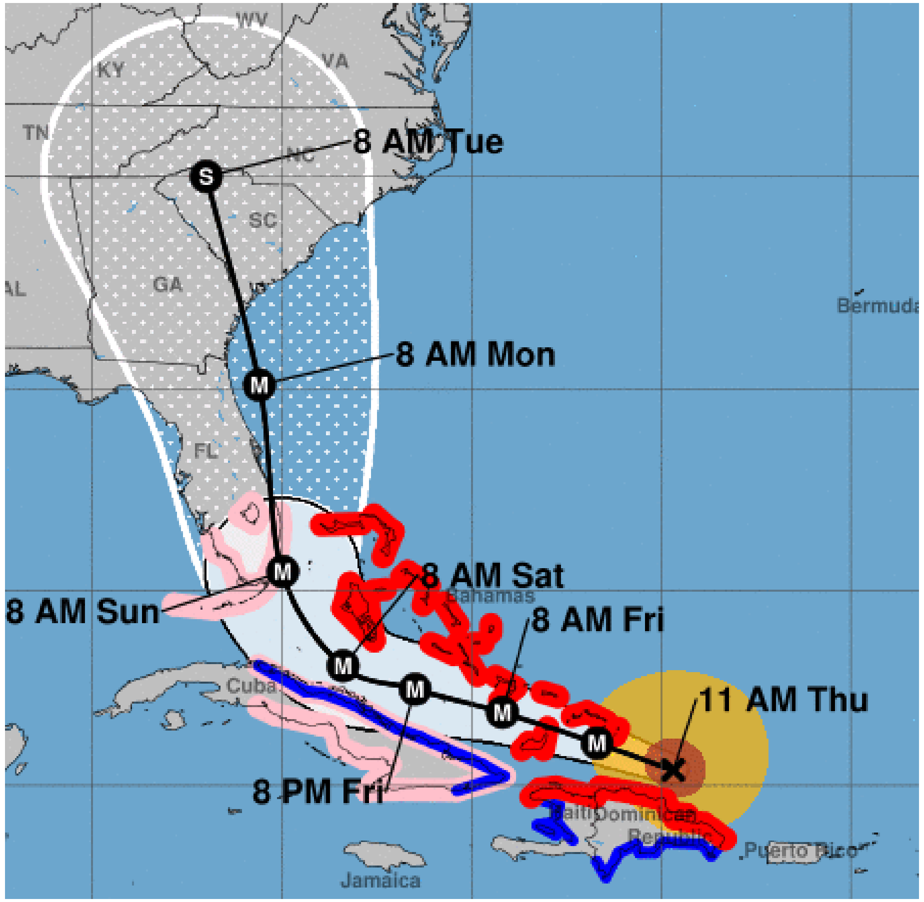


https://en.wikipedia.org/wiki/Moore%27s_law#/media/File:Transistor_Count_and_Moore%27s_Law_-_2011.svg

Empirical vs. mechanistic

- Mechanistic
  - Represents underlying biological or physical causes
  - Example: weather models

Hurricane trajectory simulation

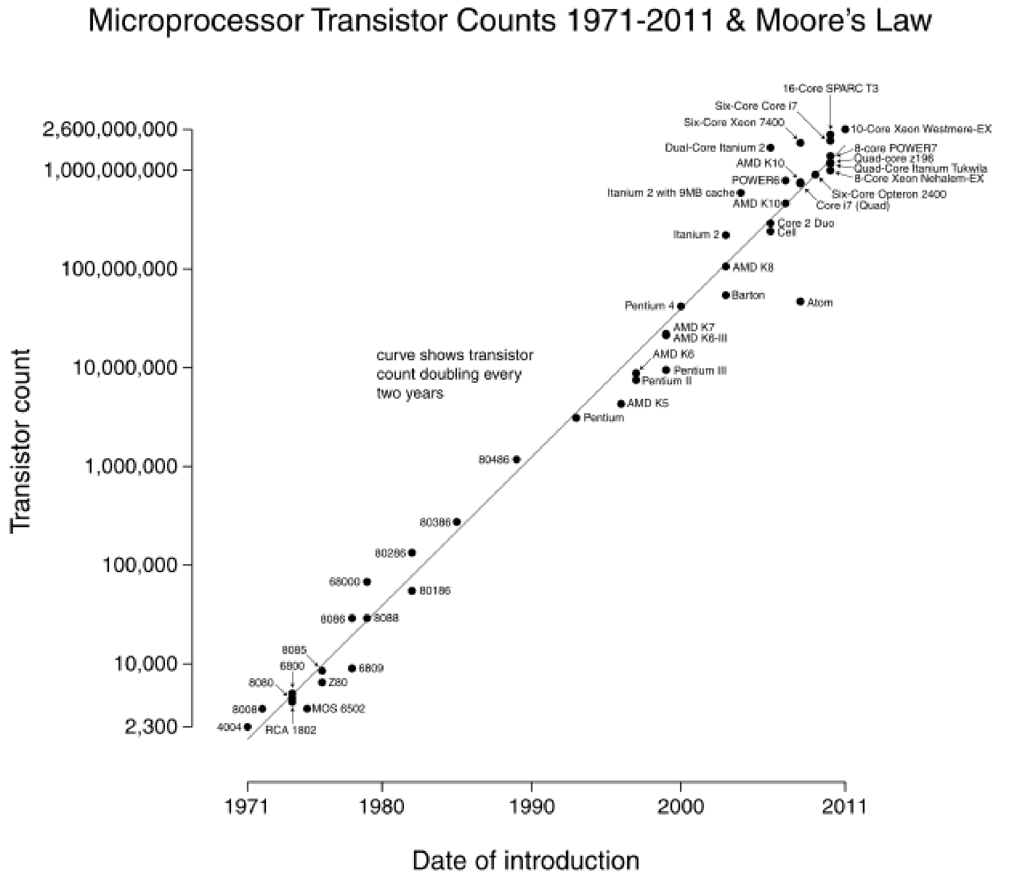


https://www.nhc.noaa.gov/archive/2017/IRMA_graphics.php?product=5day_cone_with_line_and_wind

Deterministic vs. stochastic

- Deterministic
  - Assumes that neither variables nor predictions have uncertainty
  - Example: Moore's law

Moore's law

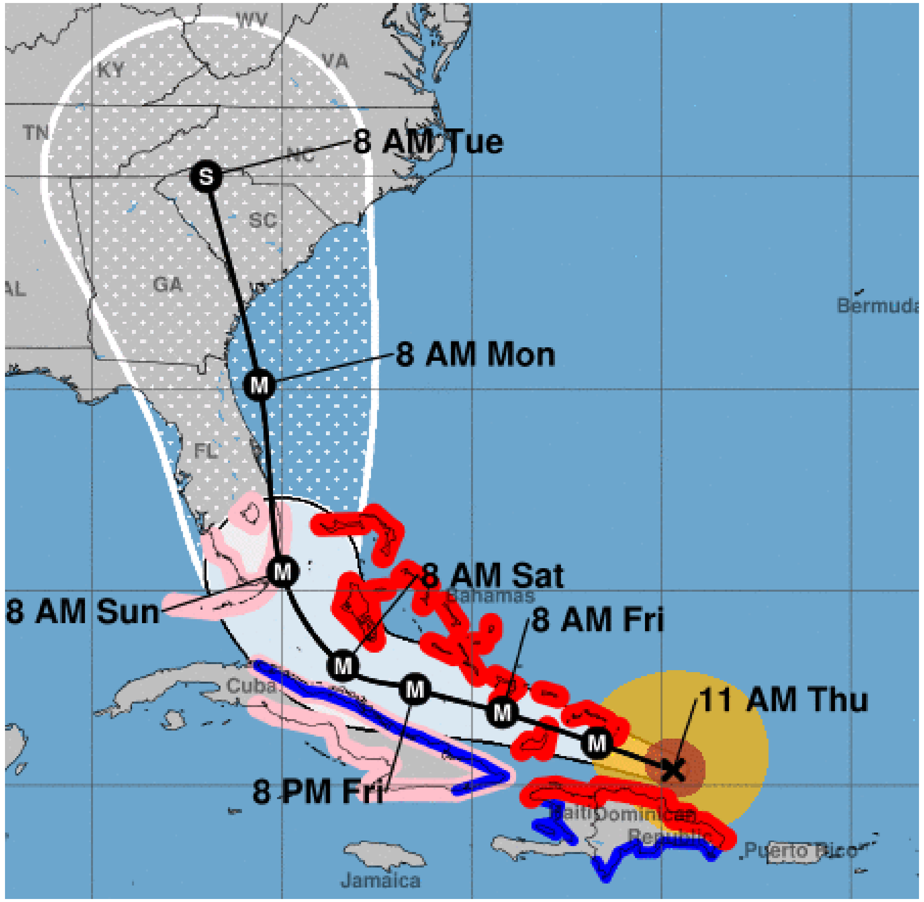


https://en.wikipedia.org/wiki/Moore%27s_law#/media/File:Transistor_Count_and_Moore%27s_Law_-_2011.svg

Deterministic vs. stochastic

- Stochastic
  - Assumes variables and thus predictions have uncertainty
  - Example: weather models

Hurricane trajectory simulation

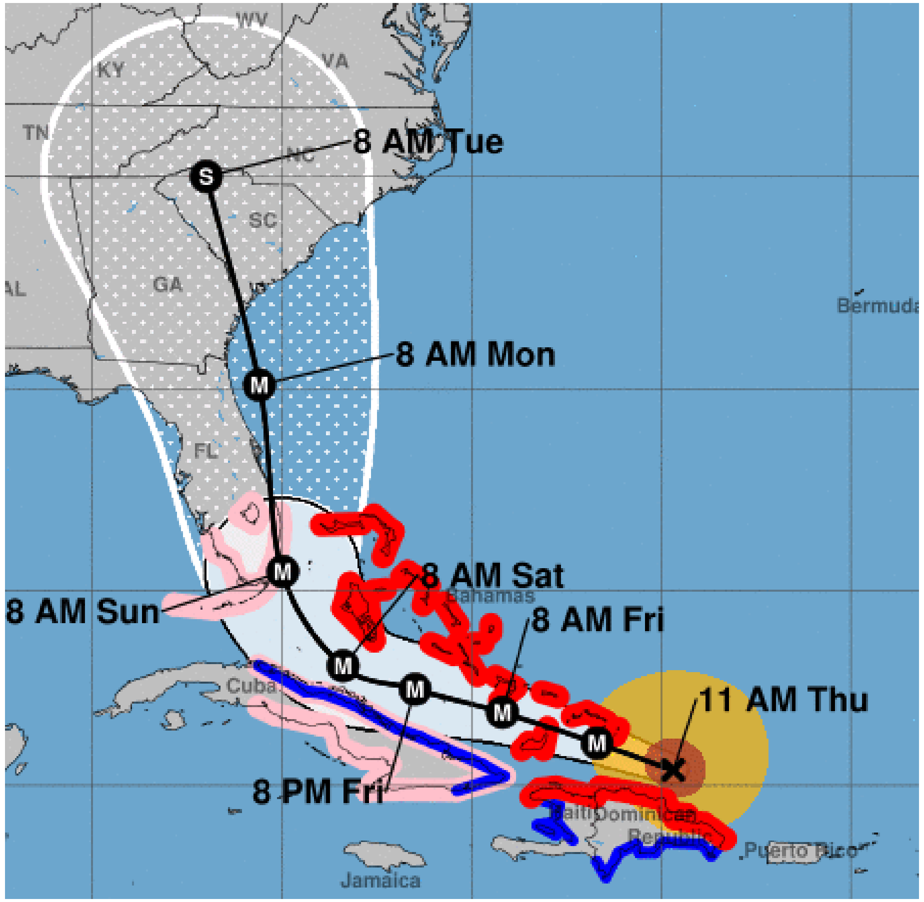


https://www.nhc.noaa.gov/archive/2017/IRMA_graphics.php?product=5day_cone_with_line_and_wind

Static vs. dynamic

- Dynamic
  - Variables are
    - a function of time
    - represented in differential equations (Baldwin, 1995)
  - Model has a “runtime”
    - States change over time
    - State at *t* is starting point for predicting state at *t* + 1
  - Example: weather models

Hurricane trajectory simulation

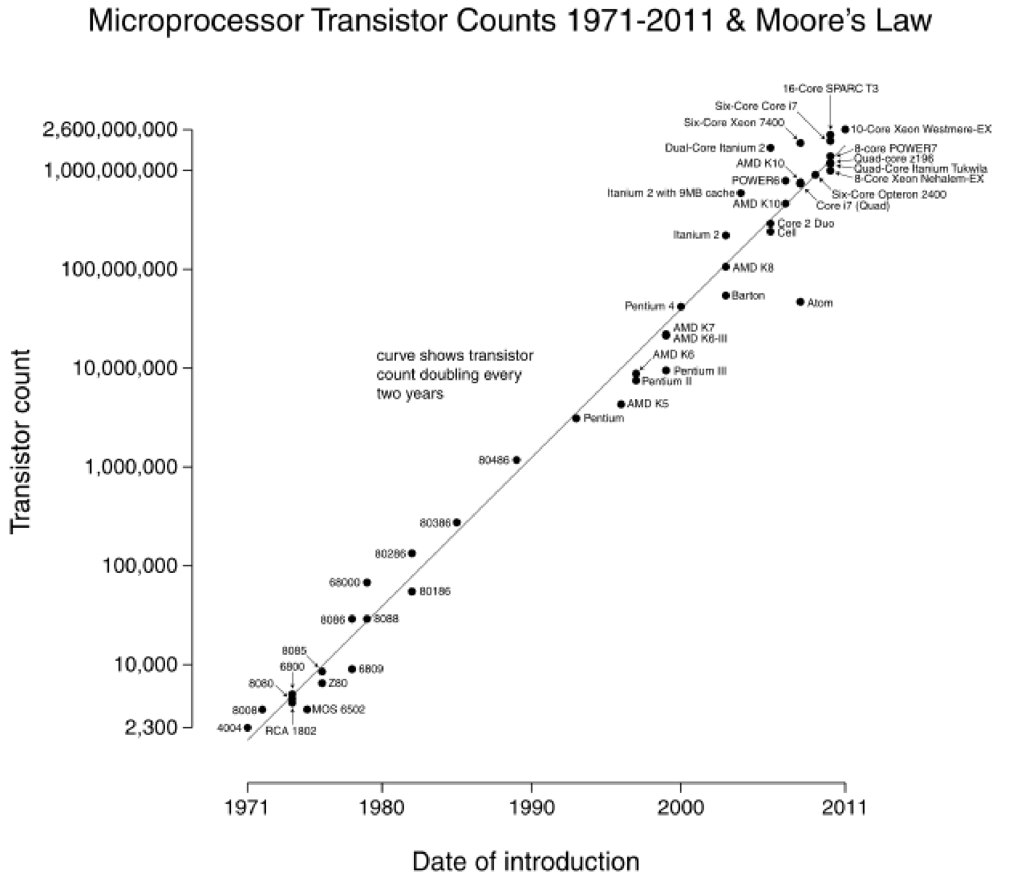


Reference: Baldwin. 1995. Modeling ruminant digestion and metabolism. Chapman & Hall.
Image: https://www.nhc.noaa.gov/archive/2017/IRMA_graphics.php?product=5day_cone_with_line_and_wind

Static vs. dynamic

- Static
  - Variables are not
    - Represented in differential equations
  - Regression equations are static
    - Even if time is a variable
    - This distinction has confused even modelers
  - Example: Moore's law

Moore's law



https://en.wikipedia.org/wiki/Moore%27s_law#/media/File:Transistor_Count_and_Moore%27s_Law_-_2011.svg

Examples

- Dairy NRC
  - Empirical, deterministic, static
- CNCPS (v. 6.5)
  - Semi-mechanistic, deterministic, static
- Molly
  - Mechanistic, deterministic, dynamic

NRC. 2001. Nutrient requirements of dairy cattle. 7th rev ed.
Van Amburgh. 2015. J Dairy Sci. 98:6361
Baldwin. 1995. Modeling ruminant digestion and metabolism

Organizational levels

Description	Level
Herd	$i + 1$
Animal	i
Organ	$i - 1$
Tissue	$i - 2$
Cell	$i - 3$

Data for empirical model (Animal, i)

Data for mechanistic model (Organ, Tissue, Cell: $i - 1$ to $i - 3$)

Steps

Identify objective

↓

Draw block diagram

↓

Write equations

↓

Define parameters values

↓

Solve model and generate predictions

↓

Evaluate predictions

Objective

- Defines
  - Goal
  - Model type
  - Organizational levels

Objective

- *Defines*
  - *Goal*
  - *Model type*
  - *Organizational levels*
- Example
  - *"Develop a mechanistic, dynamic, deterministic model to predict digestion of feed carbohydrate in the rumen"*

Steps

Identify objective

↓

Draw block diagram

↓

Write equations

↓

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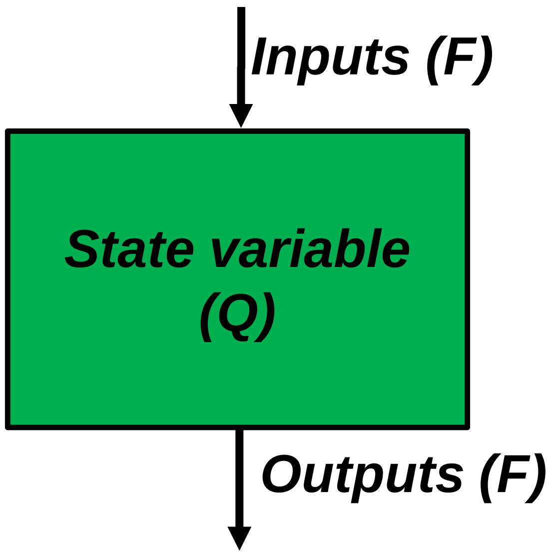
↓

Evaluate predictions

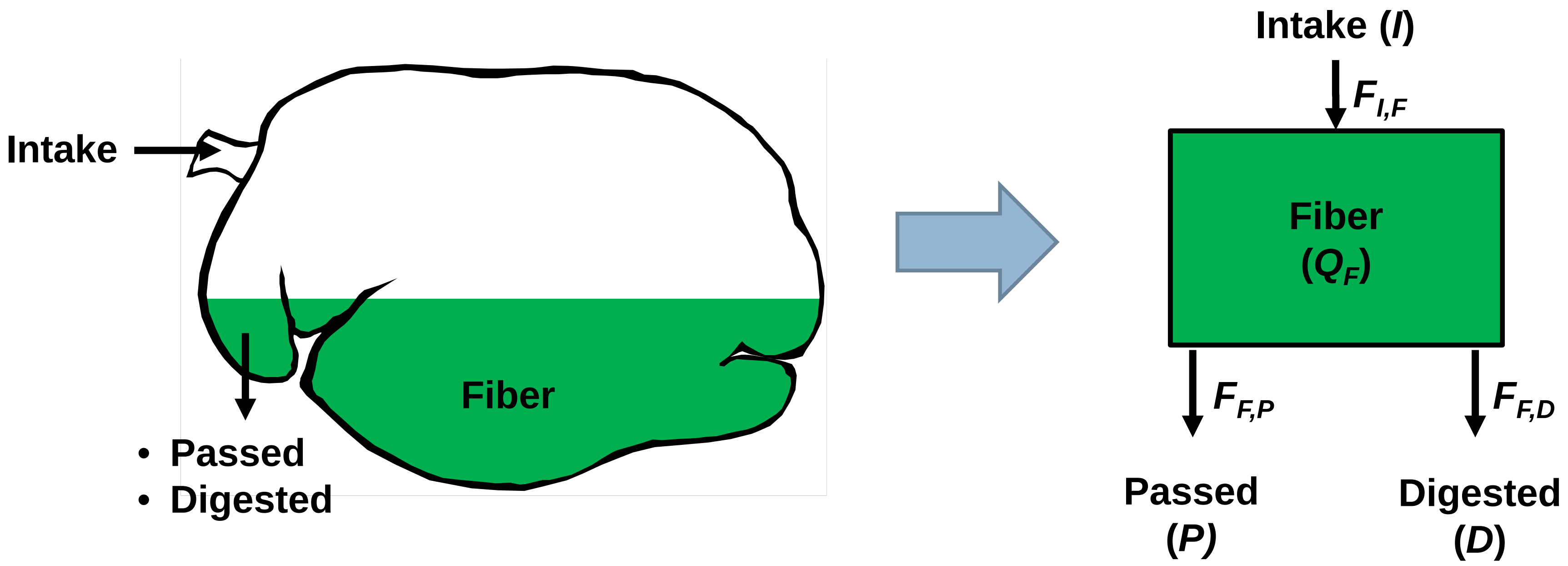
Block diagram

- Organizes model conceptually
  - Rectangle = state variable (pool)
  - Arrows = inputs and outputs (fluxes)



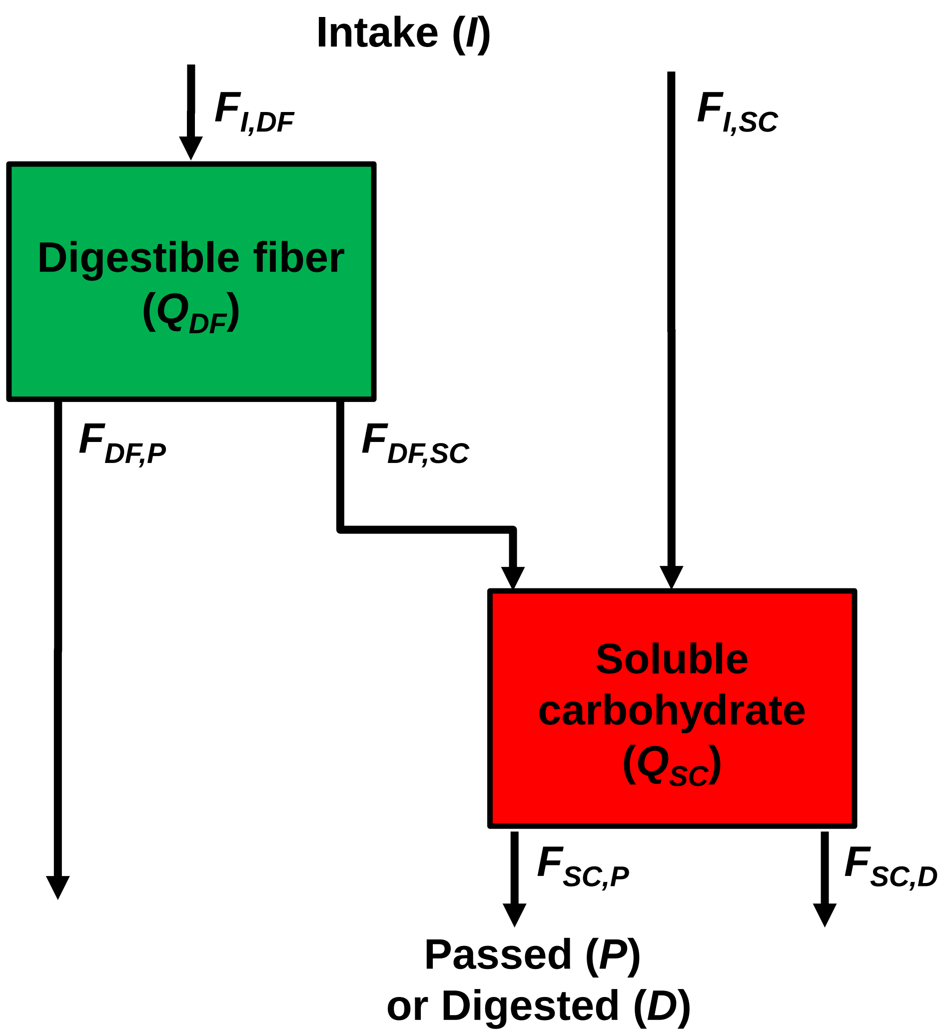
Block diagram

- Example
  - Fiber digestion in rumen



Block diagram

- Multiple pools connected (usually)



Steps

Identify objective

↓

Draw block diagram

↓

➡ Write equations

↓

Define parameters values

↓

Solve model and generate predictions

↓

Evaluate predictions

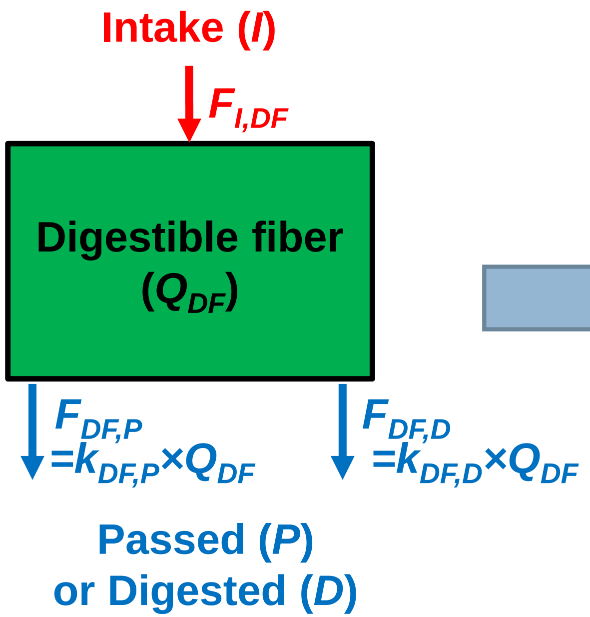
Differential equations

- Written from block diagram
- Dynamic models
  - Define change in state variables (pools) over time

$$\frac{d(State\ variable)}{dt} = Inputs - Outputs$$

Differential equations

- Example



$$\frac{d(Fiber)}{dt} = Intake - (Passed + Digested)$$

$$\frac{d(Q_{DF})}{dt} = F_{I,DF} - (F_{FD,P} + F_{DF,D})$$

$$= F_{I,DF} - (k_{DF,P} + k_{DF,D}) \times Q_{DF}$$

Steps

Identify objective

↓

Draw block diagram

↓

Write equations

↓

➡ Define parameters values

↓

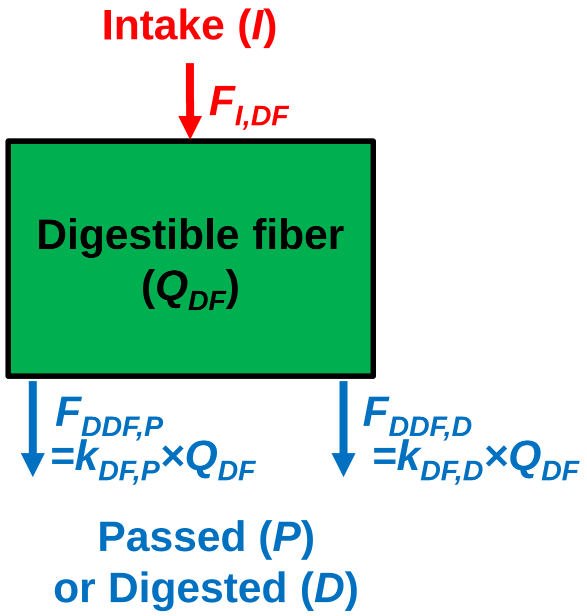
Solve model and generate predictions

↓

Evaluate predictions

Define parameter values

- Measure using experiments
- Typical values
  - $F_{I,DF} = 0.30 \text{ kg h}^{-1}$
  - $k_{DF,P} = 0.05 \text{ h}^{-1}$
  - $k_{DF,D} = 0.05 \text{ h}^{-1}$



Steps

Identify objective

↓

Draw block diagram

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Write equations

↓

Define parameters values

↓

Solve model and generate predictions

↓

Evaluate predictions

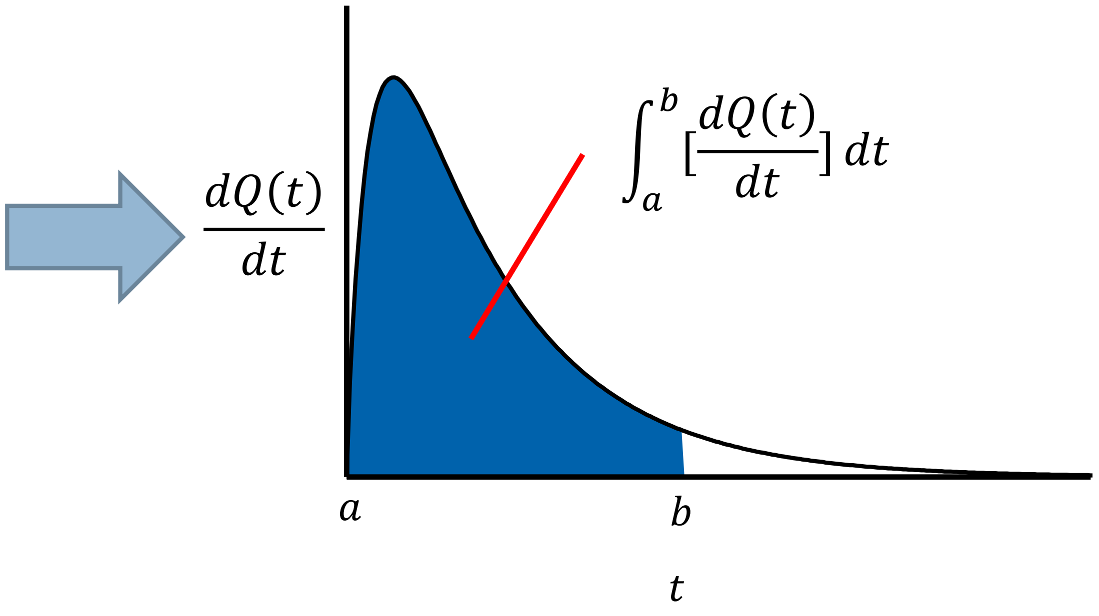
Solution

- Equations need to be solved to generate predictions
- Simple models have **analytical solutions**
- Complex models have **numerical solutions** only

Solution

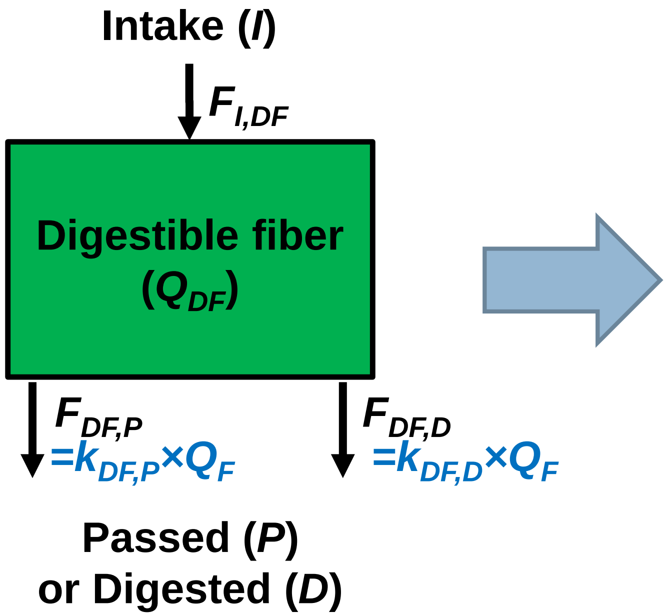
- Analytical solution
  - Integrate using rules taught in calculus courses

$$Q(t) = \int [\frac{dQ(t)}{dt}]\, dt$$



Solution

- Analytical solution
  - Example



$$Q_{DF}(t) = \int [\frac{dQ_{DF}(t)}{dt}]\, dt$$

$$= \frac{F_{I,DF}}{k_{DF,P} + k_{F,D}} + [Q_{DF}(0) - \frac{F_{I,DF}}{k_{DF,P} + k_{DF,D}}] \times \exp[-(k_{DF,P} + k_{DF,D}) \times t]$$

Make predictions by evaluating this expression at any time **t**

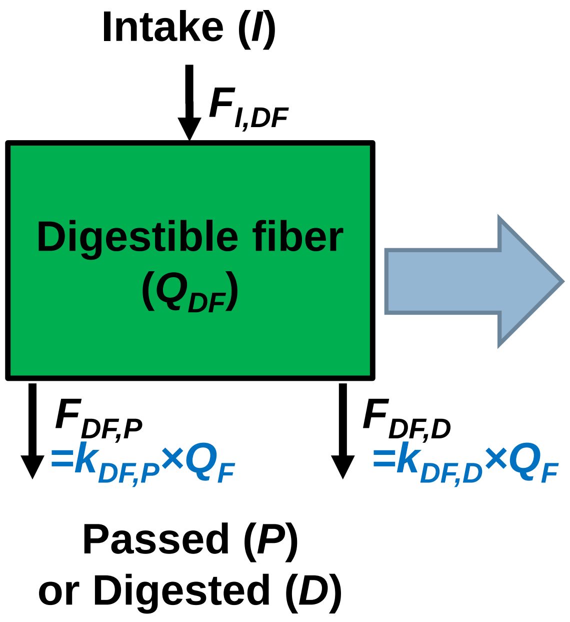
Solution

- Numerical solution
  - Integrate by calculating value numerically over short time intervals (Δt)
  - Done with **difference equations**

$$Q(t+\Delta t) \approx Q(t) + \frac{dQ(t)}{dt} \times \Delta t$$

Solution

- Numerical solution
  - Example



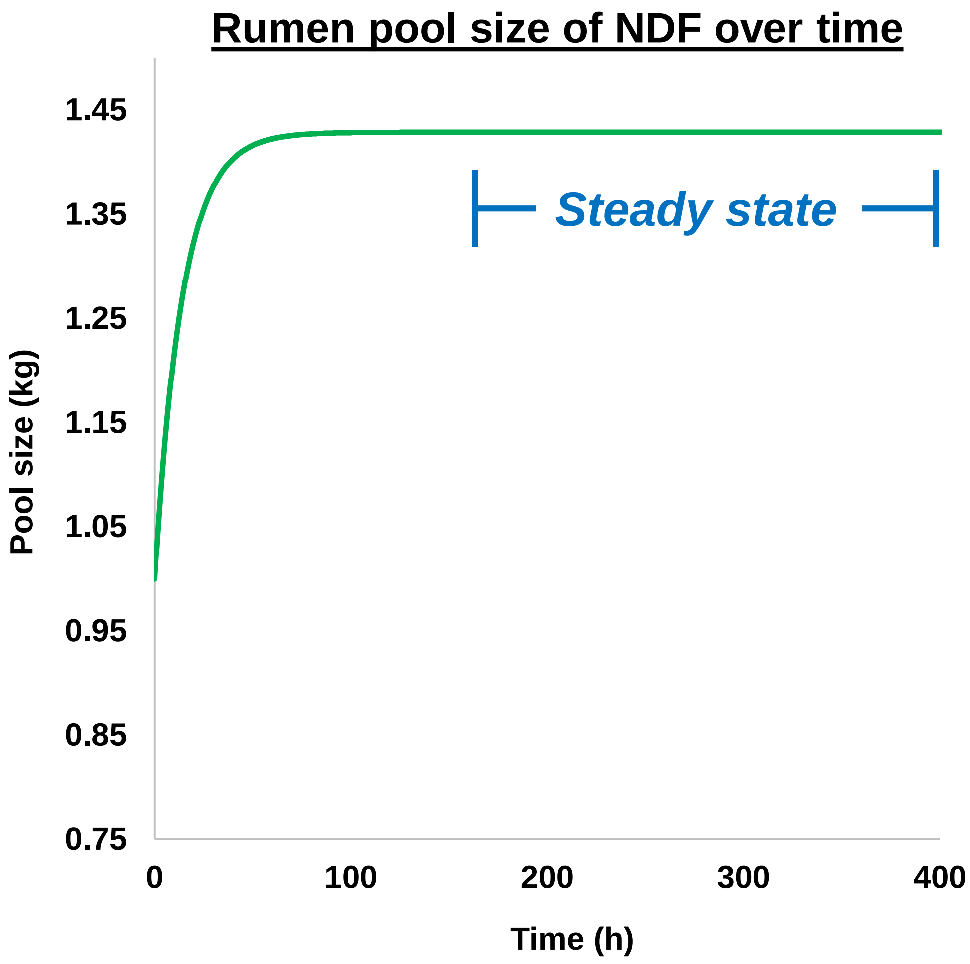
$$Q_{DF}(t+\Delta t) \approx Q_{DF}(t) + \frac{dQ_{DF}(t)}{dt} \times \Delta t$$

$$\approx Q_{DF}(t) + \left[F_{I,DF} - k_{DF,P} \times Q_{DF}(t) - k_{DF,D} \times Q_{DF}(t)\right] \times \Delta t$$

Make predictions by evaluating this expression iteratively (over time)

Solution

- Steady state
  - Reached when value of state variables no longer change
  - Predictions reported for many models are at steady state



Steps

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Write equations

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Define parameters values

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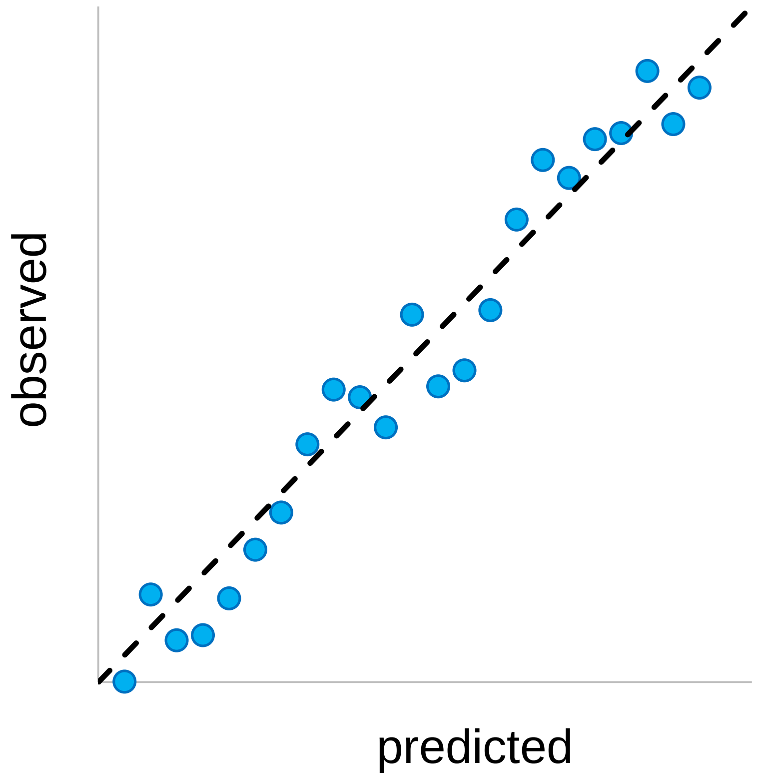
Solve model and generate predictions

↓

➡ Evaluate predictions

Evaluation

- Compare how well predictions match reality
  - Topic of Lesson 2 (Ermias Kebreab)
- Revise model as needed



Steps

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Write equations

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Define parameters values

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Solve model and generate predictions

↓

Evaluate predictions

Revision

Revision

Other things being equal, simpler explanations are generally better than more complex ones.

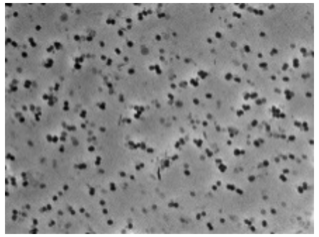
William of Ockham

Revision

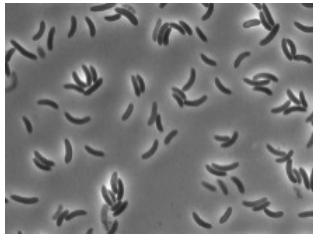
Baldwin et al. (1970)

Rumen model with three microbial groups

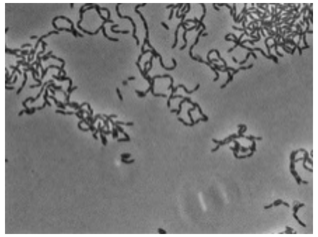
Cellulolytics (Group A)



Amylolytics (Group B)



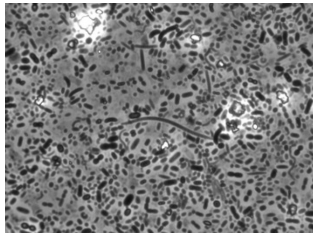
Generalists (Group C)



Baldwin et al. (1977)

Revision using “one bug” approach

Mixed microbes



Baldwin et al. 1970. In Physiology of digestion and metabolism of the ruminant
Baldwin et al. 1977. Agric Sys. 2:255
Baldwin. 1995. Modeling ruminant digestion and metabolism

Take home messages

- Modeling is more than just skill with numbers!
- Modeling starts with an objective
- There are many different types of models, but all are constructed using same steps
- Modeling is a cyclical process, and evaluation of predictions directs revision and further experimentation