Reconstructing Dynamics of Unmodeled Variables

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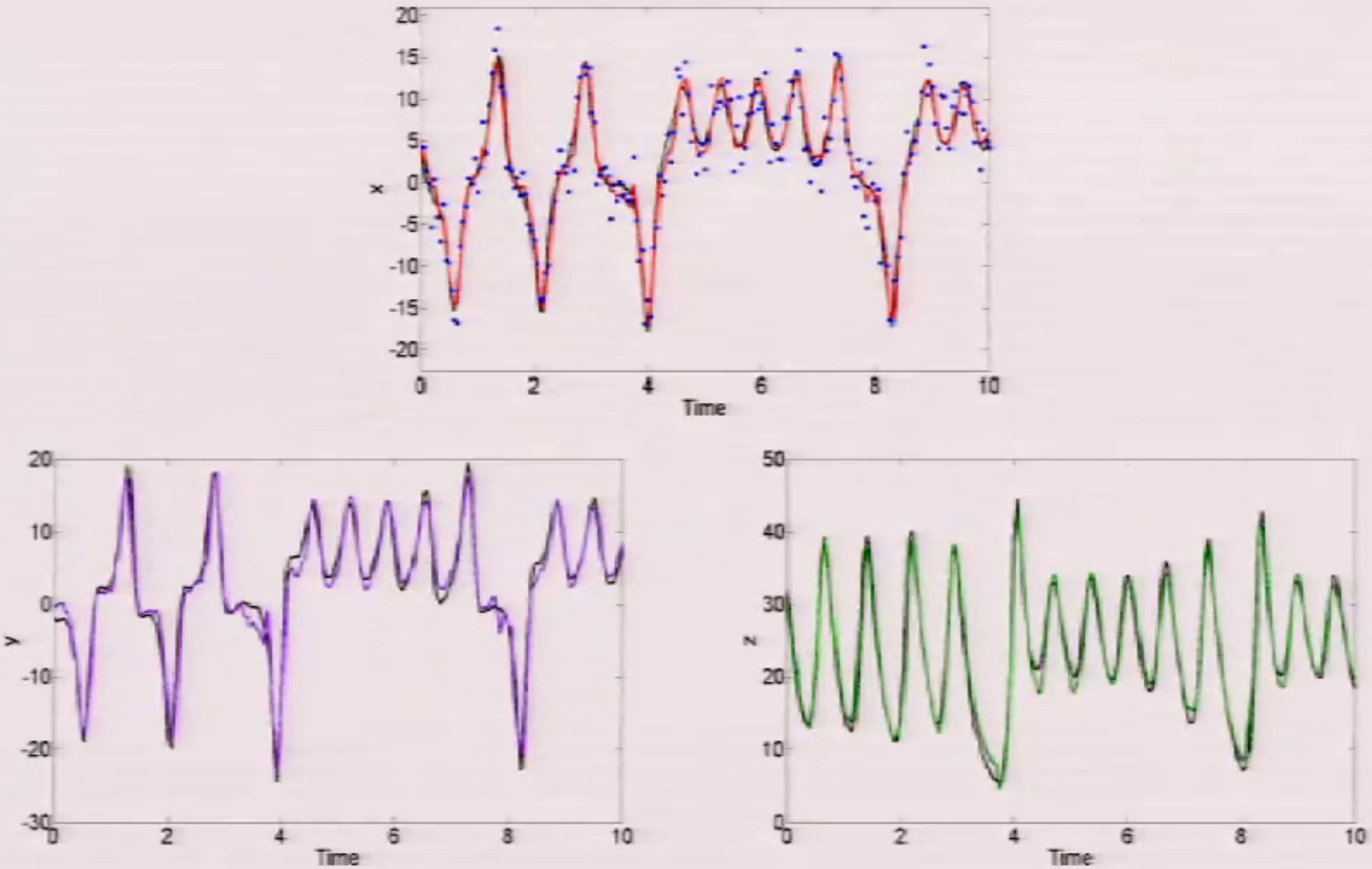
May 17, 2015

- Collect noisy measurements from the physical system
- Select an appropriate assimilation model
- Fuse data with model- estimate unmeasured system variables and parameters (e.g. ensemble Kalman filtering)

- At each measurement form an ensemble of state vectors
- Model f is applied to this ensemble and observed with function h. Form the *prior* state estimate x_k^- and the predicted observation y_k^-
- Construct the resulting covariance matrices
- Update the state and covariance estimates with the observation y_k

$$\begin{aligned}
K_k &= P_k^{xy}(P_k^{y})^{-1} \\
P_k^{+} &= P_k^{-} - P_k^{xy}(P_k^{y})^{-1}P_k^{yx} \\
x_k^{+} &= x_k^{-} + K_k\left(y_k - y_k^{-}\right).
\end{aligned}$$

Assume: We know all equations and estimate with Kalman filter



$$\dot{x} = \sigma(y - x) \qquad \dot{y} = x(\rho - z) - y \qquad \dot{z} = xy - \beta z$$

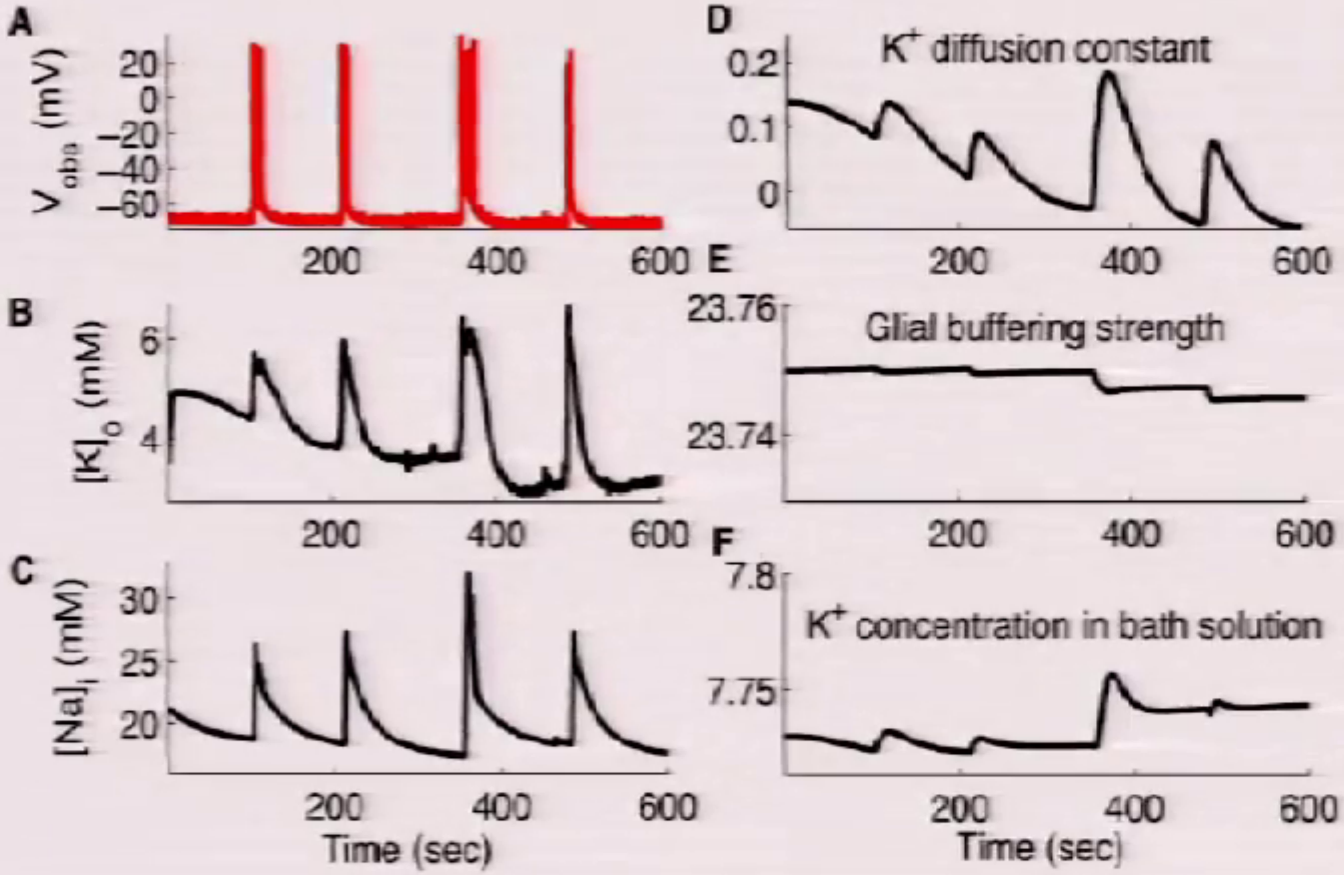


Figure 4. Assimilating spontaneous seizure data by whole cell recording from CA1 hippocampal pyramidal neurons. (A) Measured V (red) from single PCs during spontaneous seizures. Estimated (black) $[K]_o$ (B), $[Na]_i$ (C), K^+ diffusion constant (D), glial buffering strength (E), and K^+ concentration in bath solution (F). Data provided by Jokubas Ziburkus. Panel (A) modified from [23] with permission American Physiological Society.
doi:10.1371/journal.pcbi.1000776.g004

G. Ullah and S. Schiff, PLoS Computational Biology **6**, e1000776 (2010).

1. Data from a physical system

2. **Model** representing the system

3. Filter
   - For linear models, can use Kalman filter
   - For nonlinear models, can approximate nonlinearity using extended or ensemble Kalman filter

"Essentially, all models are wrong, but some are useful." (George P. Box)

"Everything should be made as simple as possible, but not simpler." (Albert Einstein)

- Models are poorly known or equations are noisy
  - Kalman filter is equipped to handle this

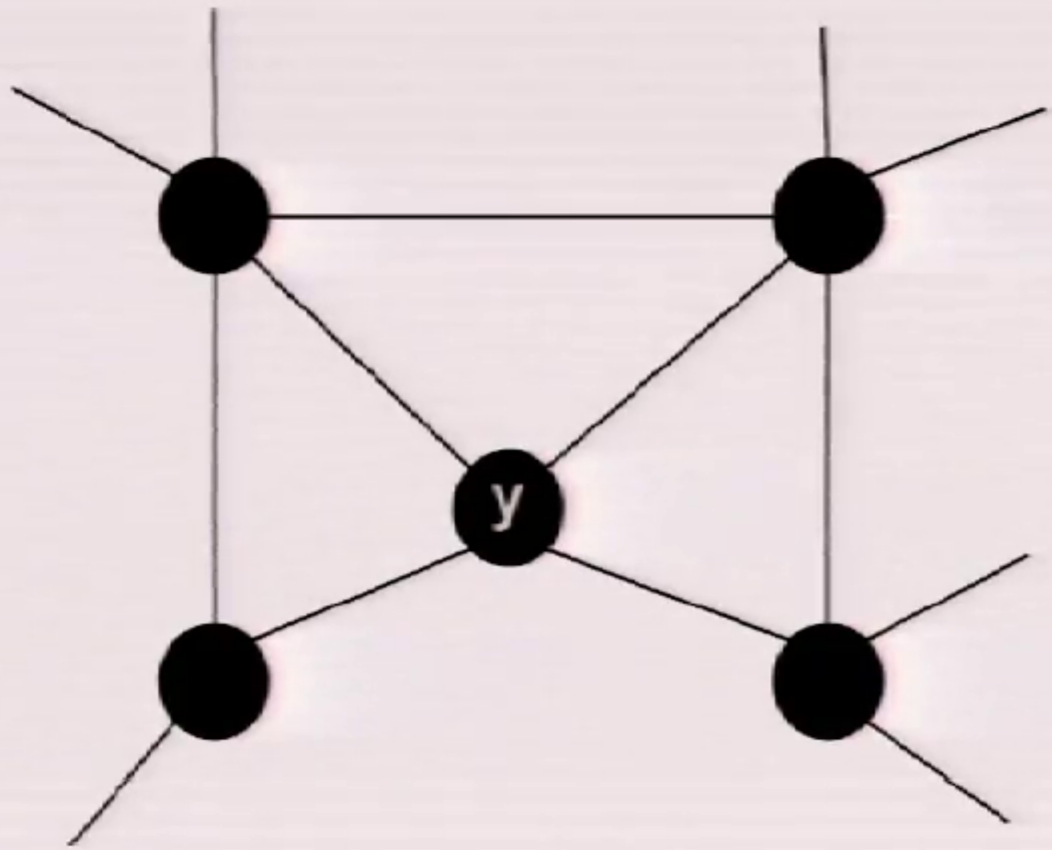
- Missing equations, i.e., variables of system not present in the model
  - Traditional filtering/data assimilation methodology can't handle this

- **Situation: Unmodeled Variables**

- Variable in question has no explicit dynamical equation
  - Knowledge of how variable interacts with other dynamics
  - Limited time series of variable available

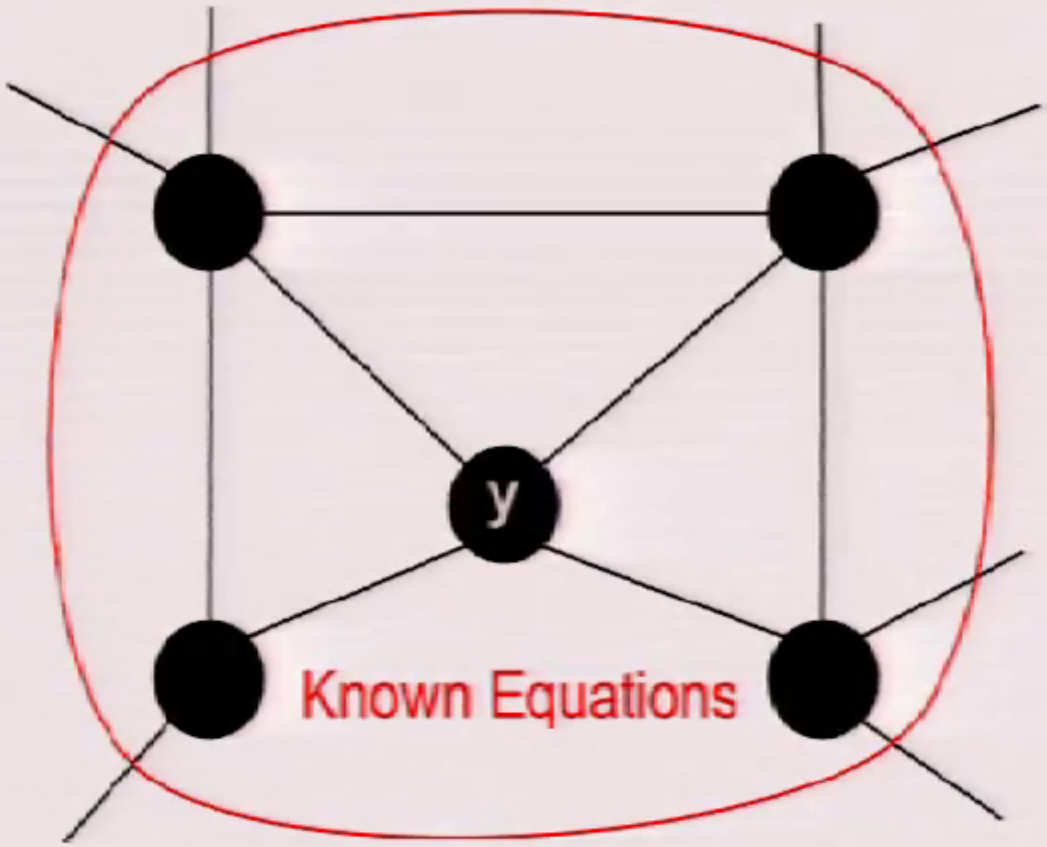
- How can we reconstruct and use these unmodeled variables?

We like to think of dynamical systems as networks



Goal: Predict y

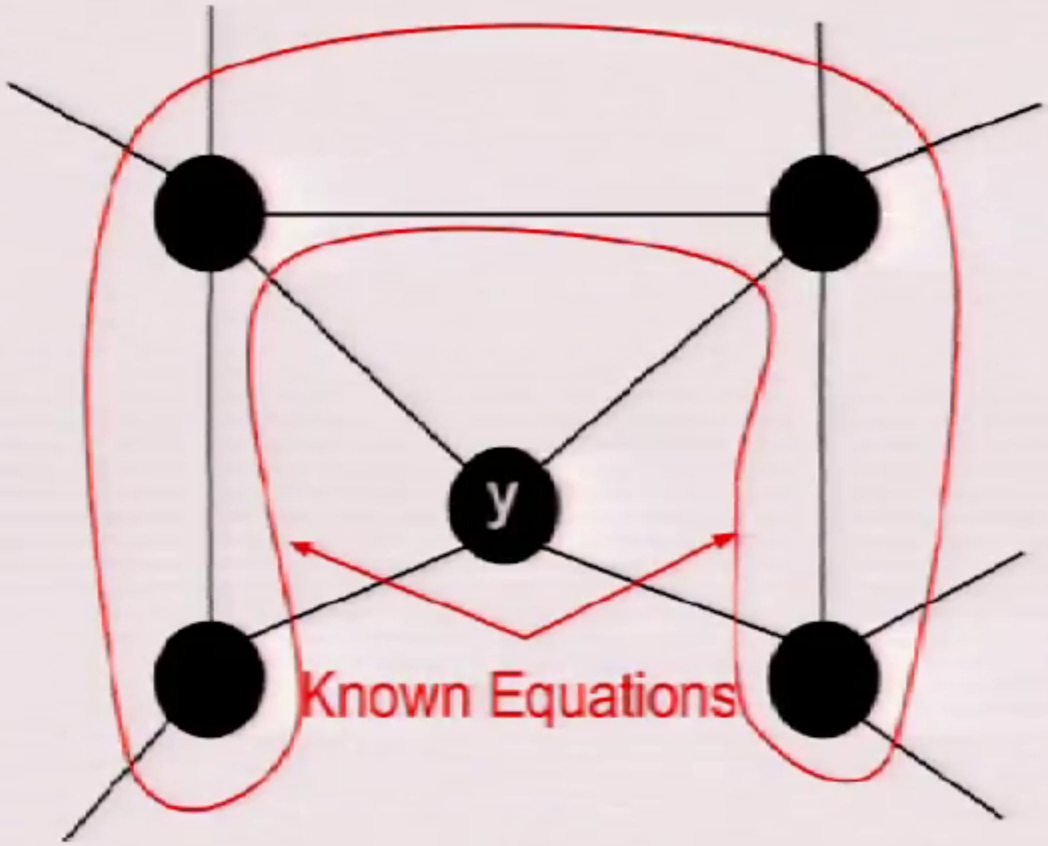
Traditional Data Assimilation



Goal: Predict y

Assume: All variables modeled, observe some variables and reconstruct others

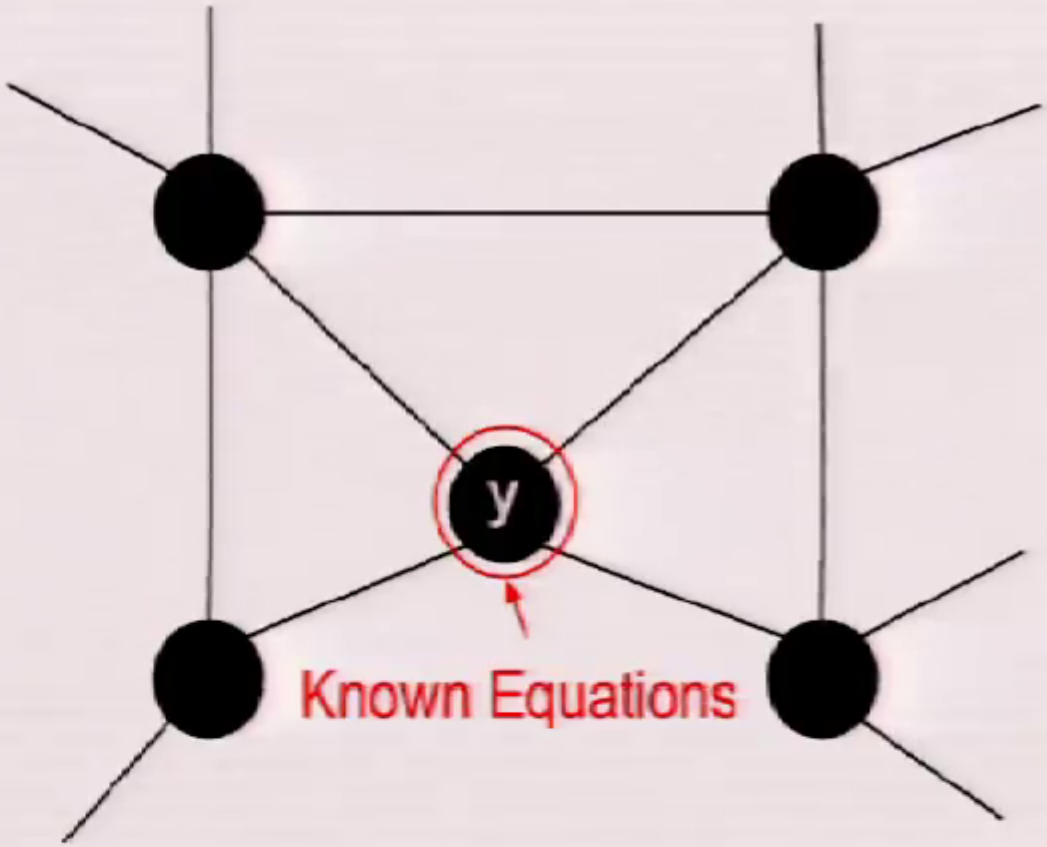
Problem 1



Goal: Predict y

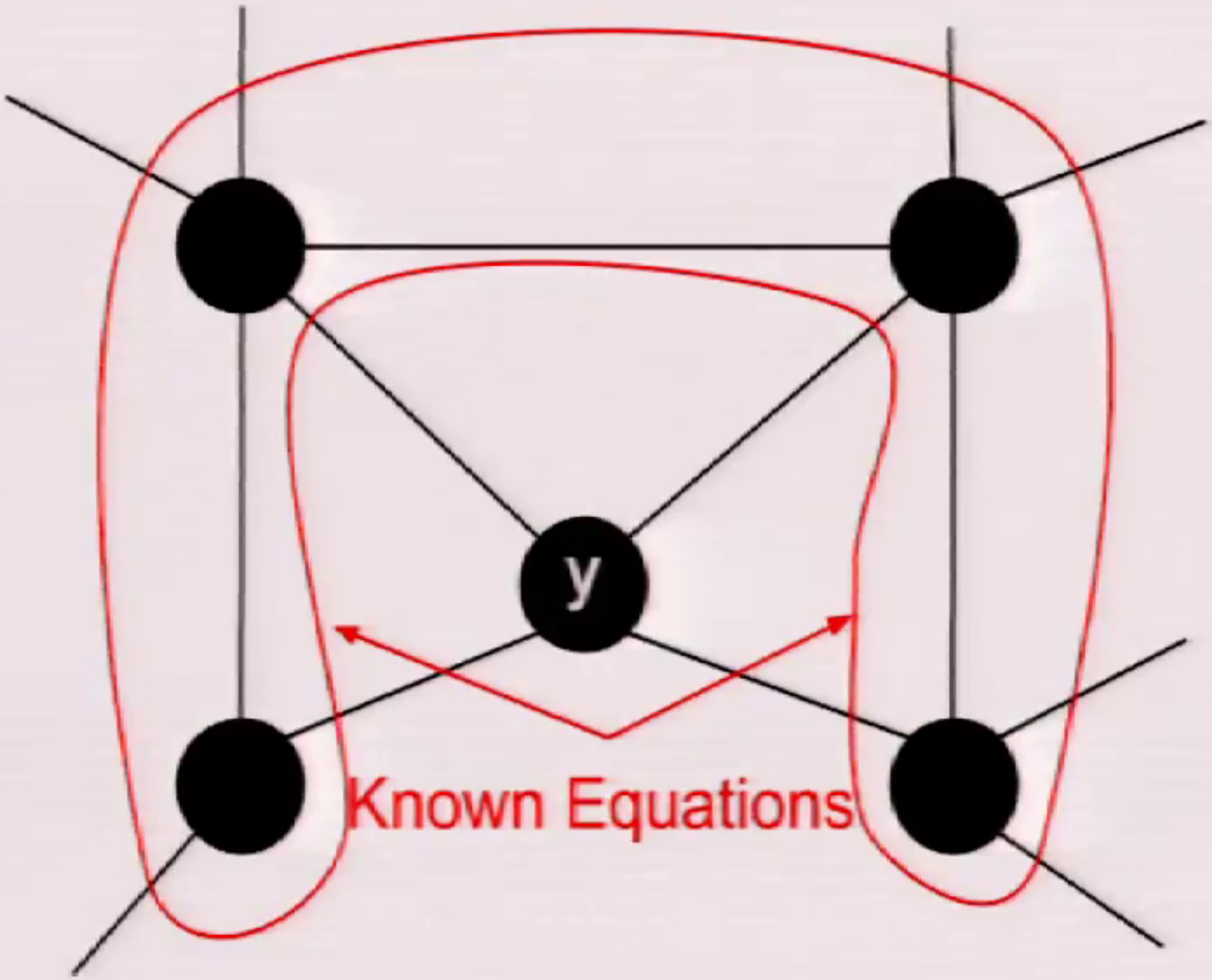
Assume: y unmodeled, other variables modeled. Observe some variables and reconstruct others; training data of y available

Problem 2



Goal: Predict y

Assume: y modeled, all other variables unmodeled. Observe all variables


y
Known Equations

- **Goal:** Estimate a variable not explicitly represented in model (i.e. an **unmodeled variable**)
- **Idea:** Take the dynamics of several different models and reconstruct unmodeled quantity

Platypus approach to data assimilation (or multiple model data assimilation)

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Platypus approach to data assimilation (or multiple model data assimilation)

Using Multiple Models

Consider n differently parameterized versions of an assimilation model $\dot{x} = f(x, p)$

$$\begin{aligned} \dot{x}^1 &= f(x, p_1) \\ \dot{x}^2 &= f(x, p_2) \\ &\vdots \\ \dot{x}^n &= f(x, p_n) \end{aligned}$$

Given a training sequence of the unmodeled variable S_t, form the approximation

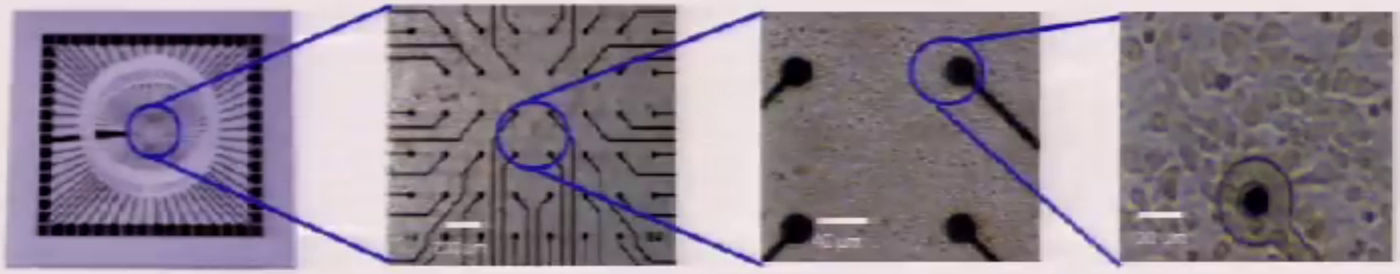
$$S_t \approx \sum_{i,j} c_j^i x_j^i + d$$

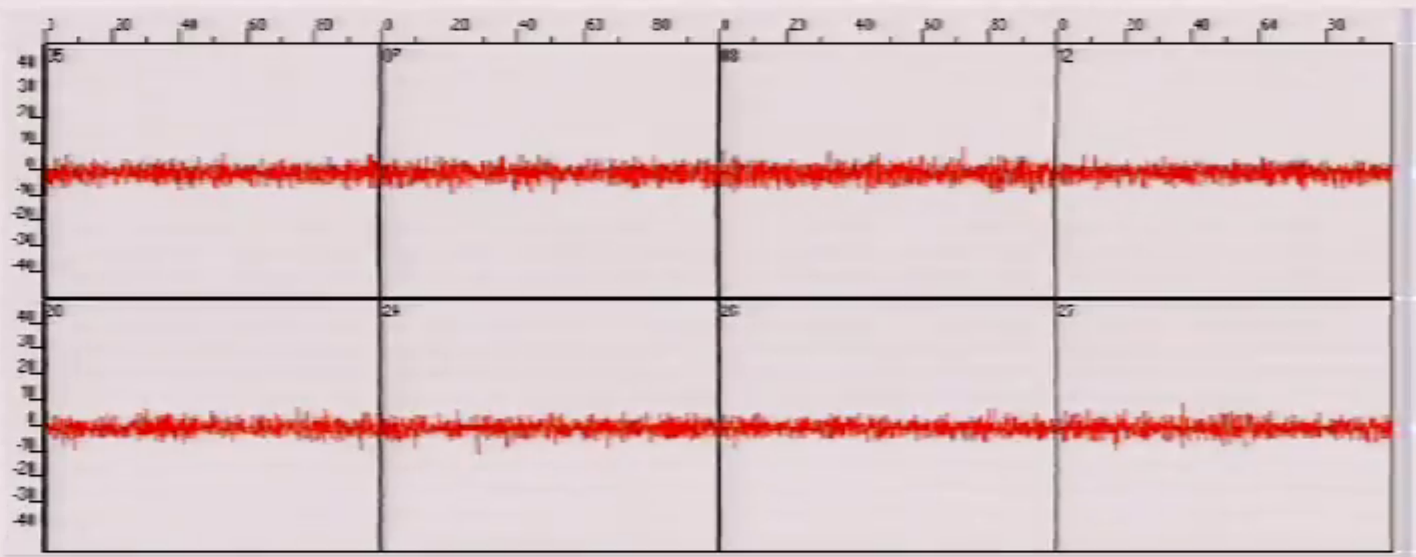
Using Multiple Models

1. Continuously observe some variables (the observables)

2. Observe **unmodeled** variables during a training period, form their reconstruction using all **modeled** variables

3. Once training is over, predict the unmodeled quantity while assimilating the observable





- Assume a generic spiking neuron model (Hindmarsh-Rose)

$$\begin{aligned}\dot{\mathbf{V}} &= \mathbf{y} - a\mathbf{V}^3 + b\mathbf{V}^2 - \mathbf{z} + I \\ \dot{\mathbf{y}} &= c - d\mathbf{V}^2 - \mathbf{y} \\ \dot{\mathbf{z}} &= \tau(s(\mathbf{V}+1) - \mathbf{z})\end{aligned}$$

  V neuron potential, **y** fast scale dynamics, **z** slow scale dynamics

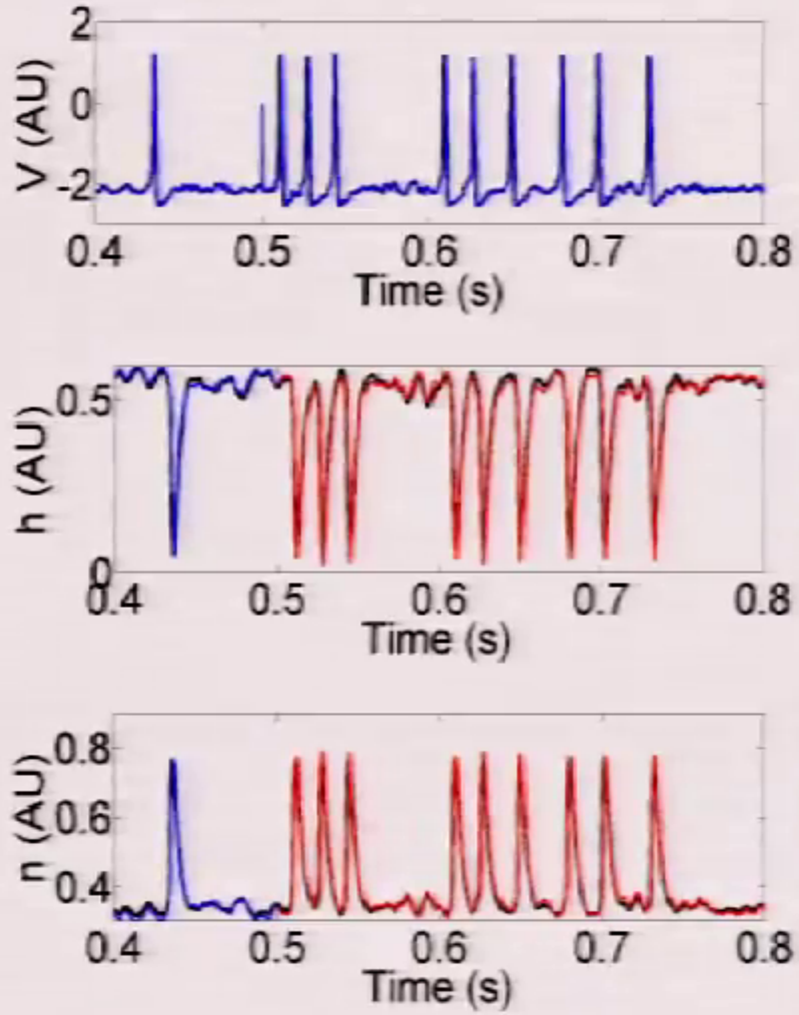
- **Goal:** Use multiple parameterized Hindmarsh-Rose models to reconstruct unmodeled neuronal quantities while assimilating recorded neuron potential

J. Hindmarsh and R. Rose, Proc. Roy. Soc., **221**, 87 (1984).

Reconstructing Unmodeled Gating Variables

Observing Hodgkin-Huxley voltage, reconstruct unmodeled gating variables (assimilation model is Hindmarsh-Rose)

A. Hodgkin and A. Huxley, J. Physiology **117**, 500 (1952).

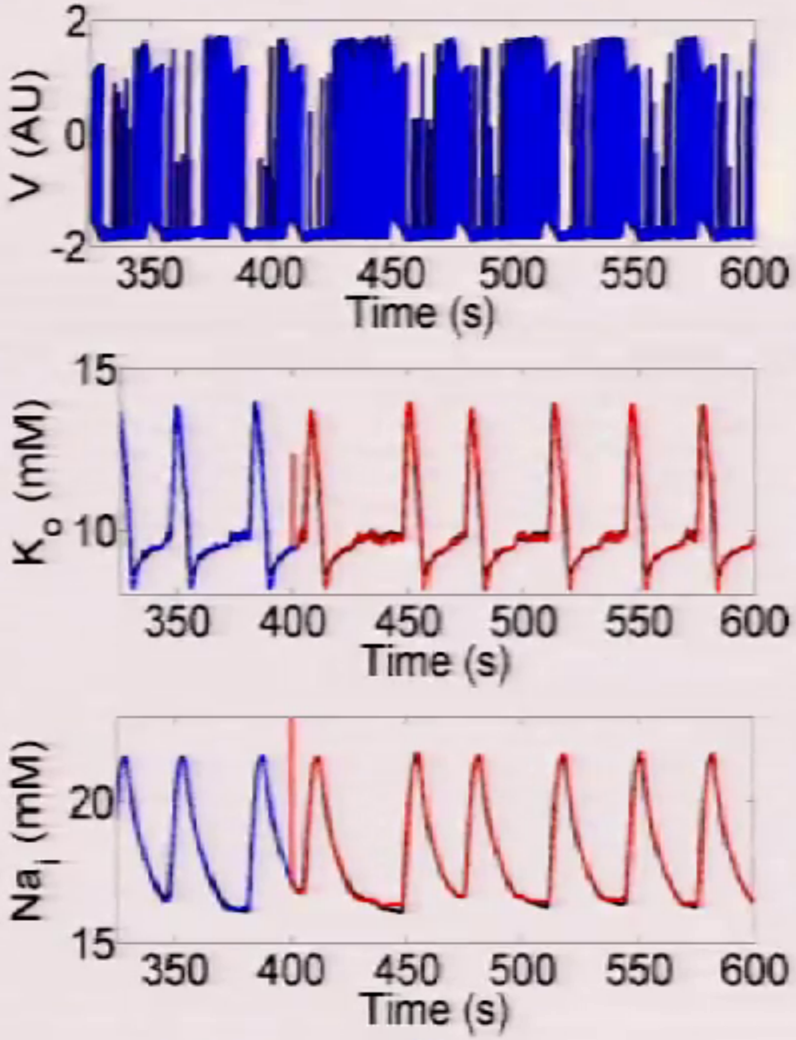


Actual **Observed** **Predicted**

Reconstructing Unmodeled Ionic Dynamics

Observing seizure voltage, reconstruct unmodeled potassium and sodium dynamics (assimilation model is Hindmarsh-Rose)

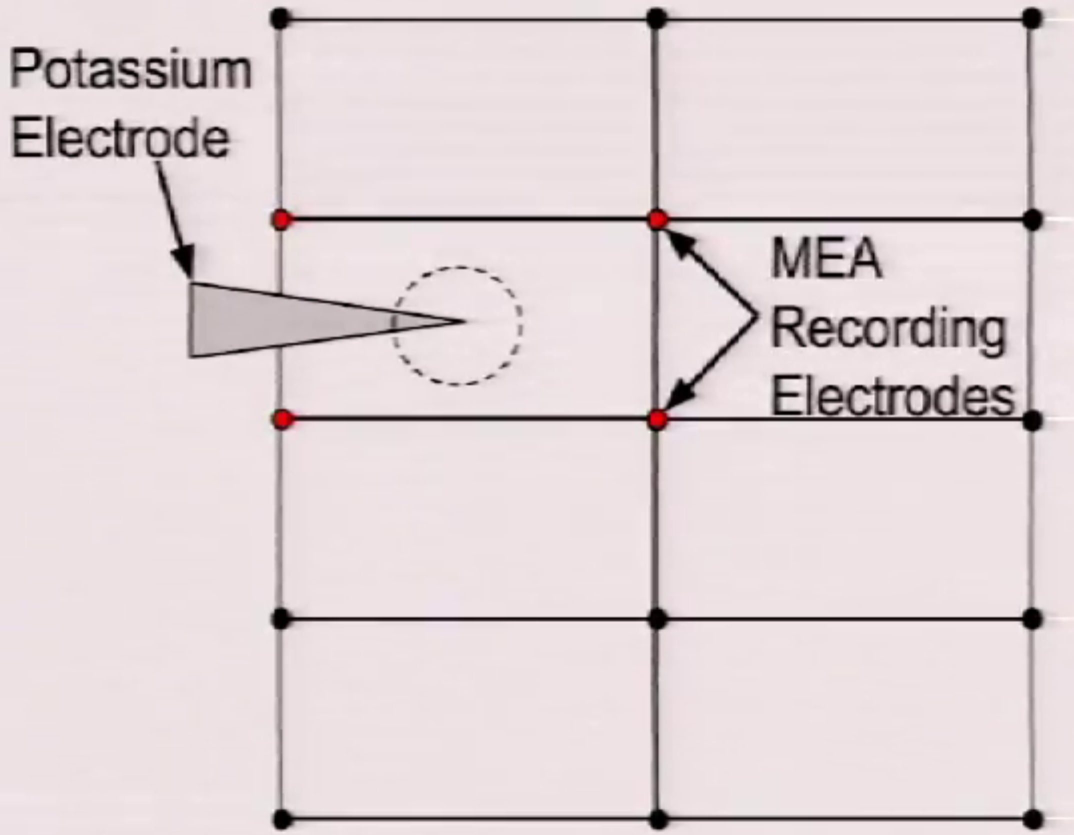
J. Cressman, G. Ullah, J. Ziburkus, S. Schiff, and E. Barreto, Journal of Comp. Neuroscience 26, 159 (2009).



Actual **Observed** **Predicted**

Potassium from an *In Vitro* Network

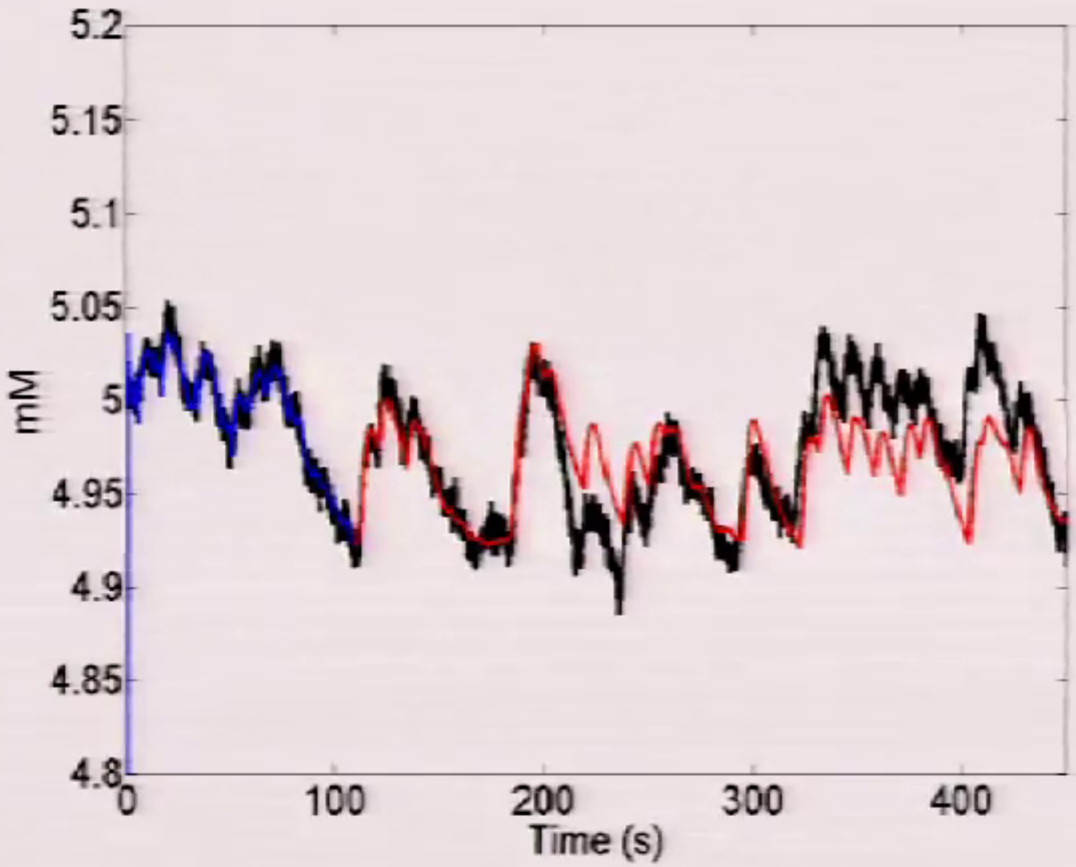
We want to track extracellular potassium dynamics in a network but measurements are difficult and spatially limited



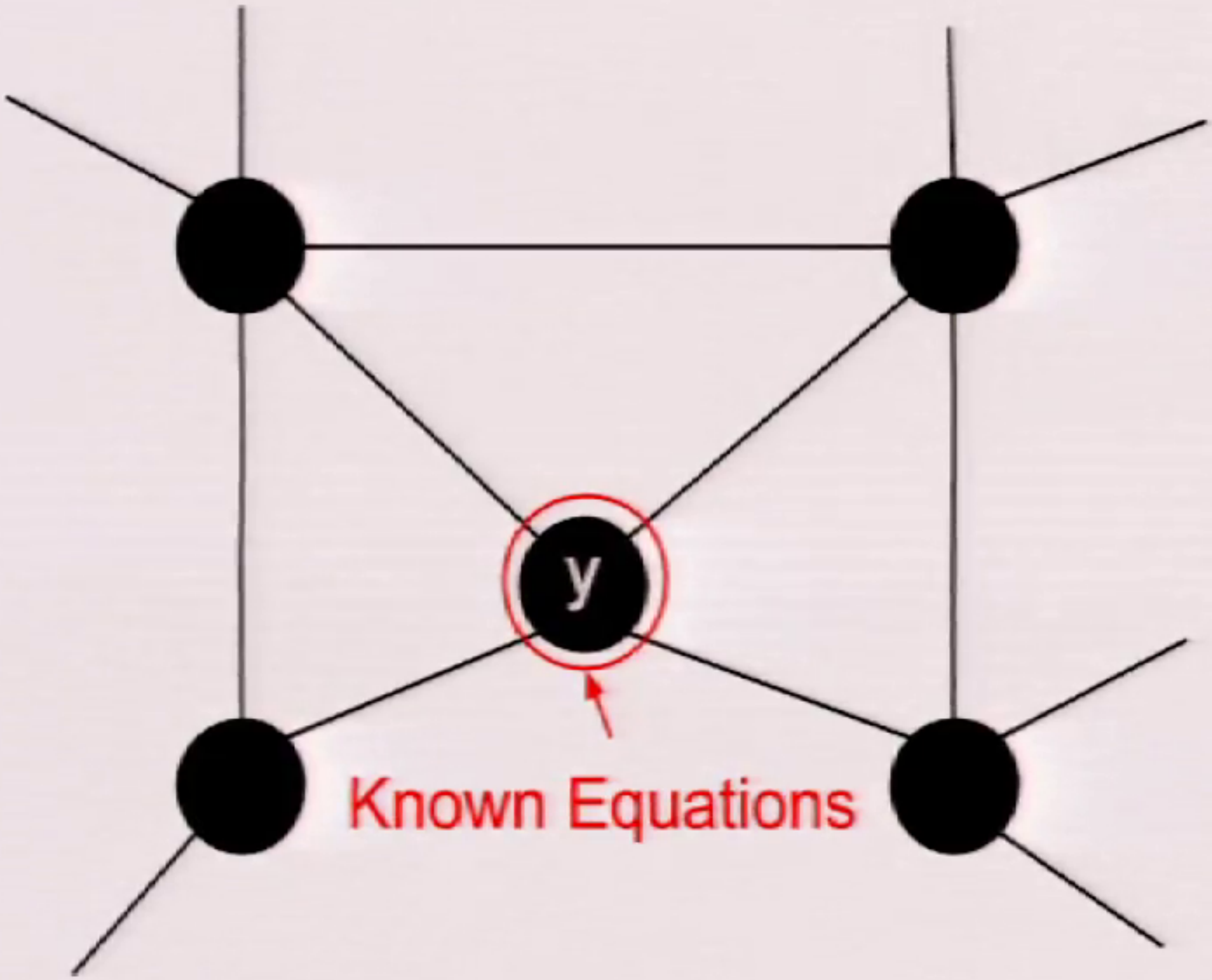
Extracellular potassium is an **unmodeled variable**

Potassium from an *In Vitro* Network

The local extracellular potassium in an MEA network can be reconstructed and predicted using our approach (assimilation model is Hindmarsh-Rose)



Actual **Observed** **Predicted**


y
Known Equations

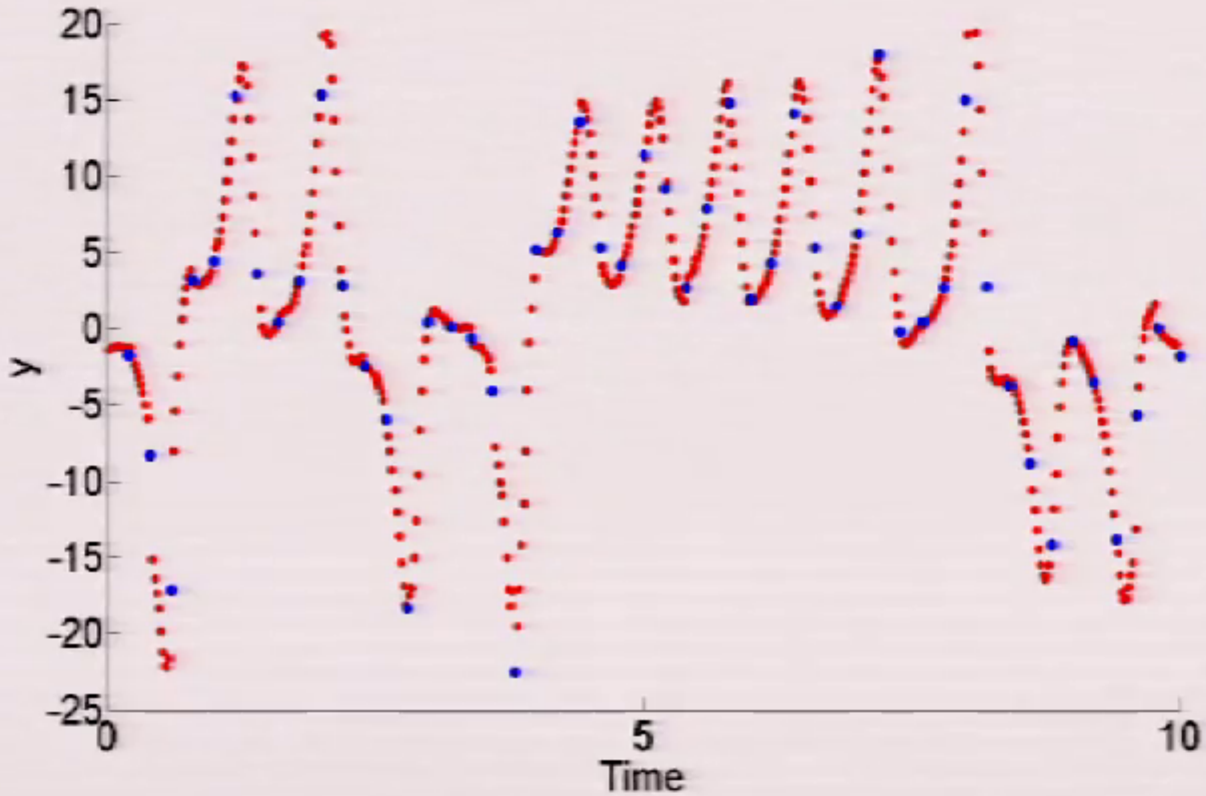
- Assume we have multivariate time series data from a system
  - E.g. x, y and z variables of Lorenz-63 system observed at $dt = h$ time units
- How can we forecast, or predict, the system at future time points?

- Parametric- full model available: Estimate parameters and free-run system

$$\begin{aligned}\dot{x} &= \sigma(y-x)\\ \dot{y} &= x(\rho - z) - y\\ \dot{z} &= xy - \beta z\end{aligned}$$

- Nonparametric- no model available: Use delay embedding with direct prediction
- **Semiparametric- partial model available**:

$$\dot{y} = x(\rho - z) - y$$

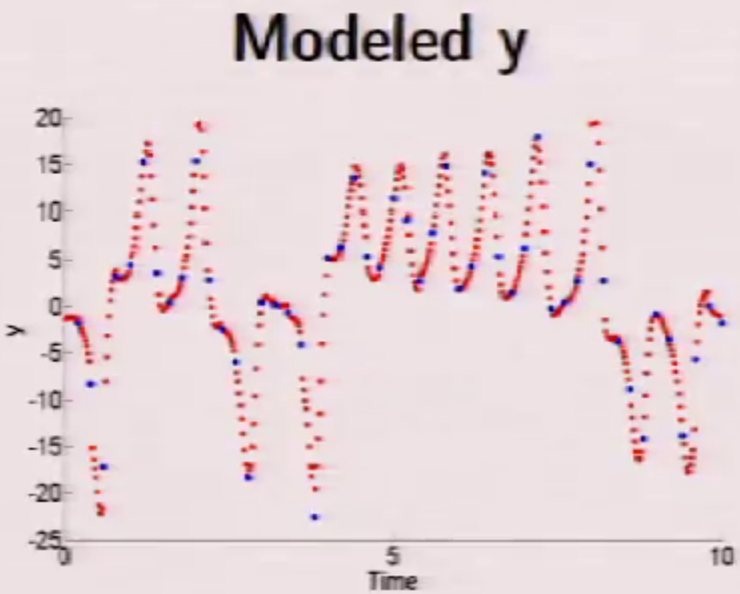


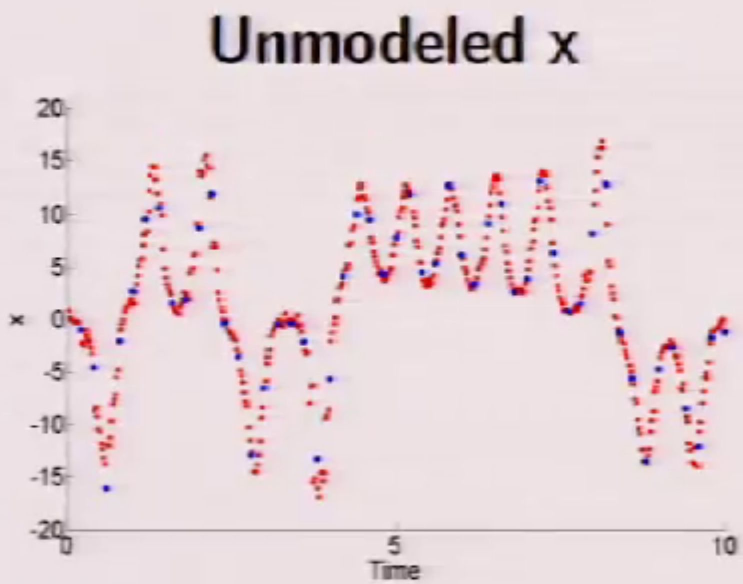
$$\dot{y} = x(\rho - z) - y$$

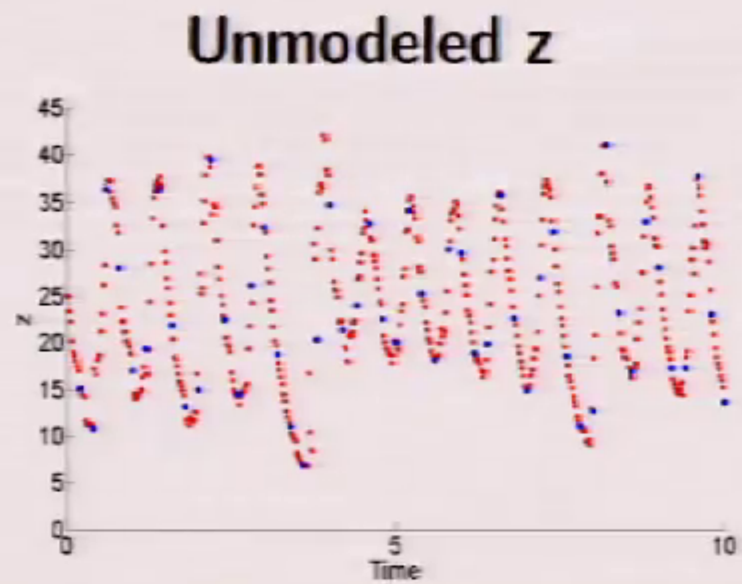
Goal: Use the equation to interpolate the attractor at a finer resolution $k = h/m$

- Collect multivariate time series sampled at rate h
- Select subsample rate $k = h/m$
- At a given sample time t_i
  1. Using **partial model**, apply fractional-step multistep method to advance modeled variables to $t_i + k$
  2. Given modeled variables at time $t_i + k$, find nearest neighbors in **Takens delay-coordinate space** and build **local reconstruction** of unmodeled variables at $t_i + k$
  3. Given modeled and unmodeled variables at $t_i + k$, apply modified fractional-step multistep method to advance modeled variables to $t_i + 2k$
  4. ...

As we interpolate, reconstruct unmodeled variables using a local regression







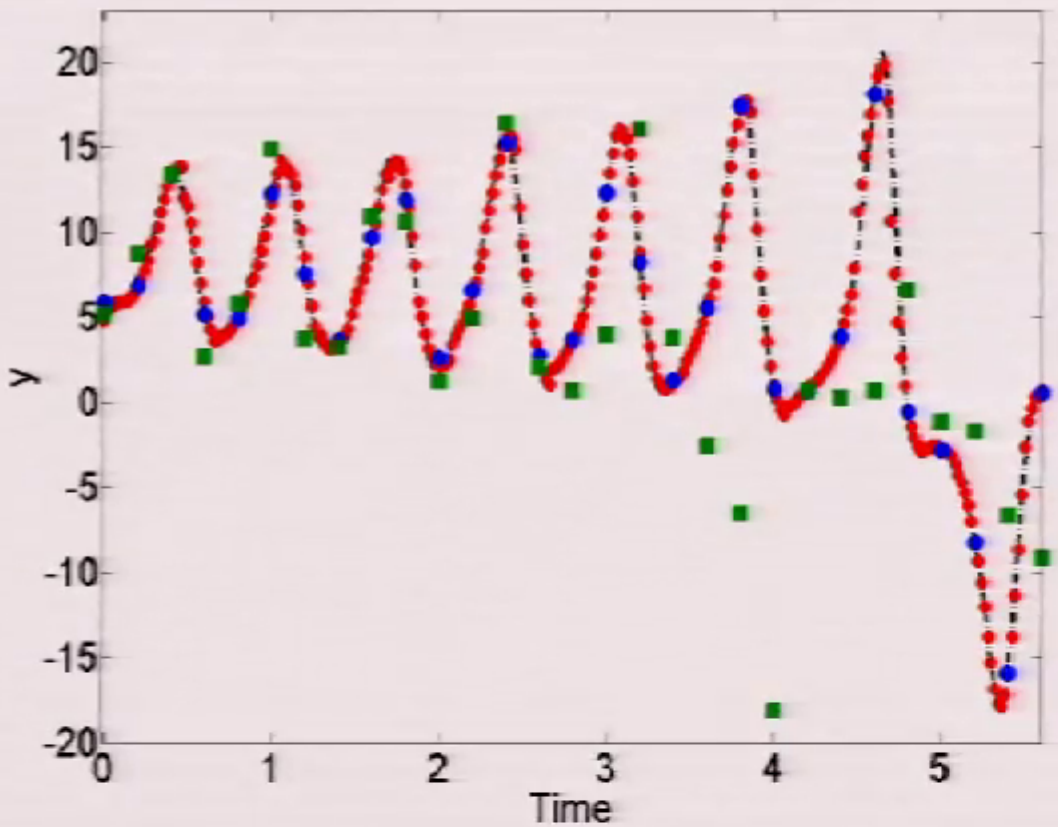
Nonparametric vs. Semiparametric

1. Build delay-coordinates of variables ✓ ✓

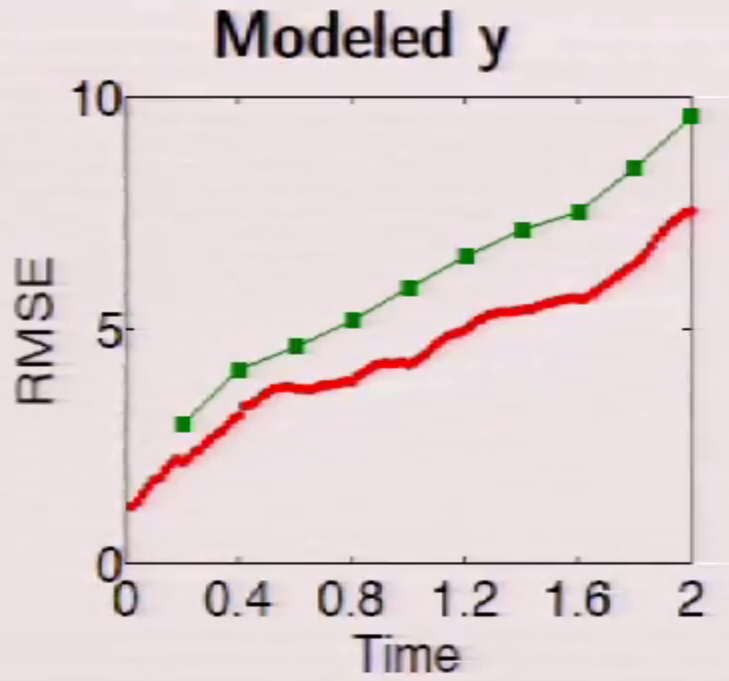
2. Use partial model to interpolate date ✓

3. Find nearest neighbors and build local forecast ✓ ✓

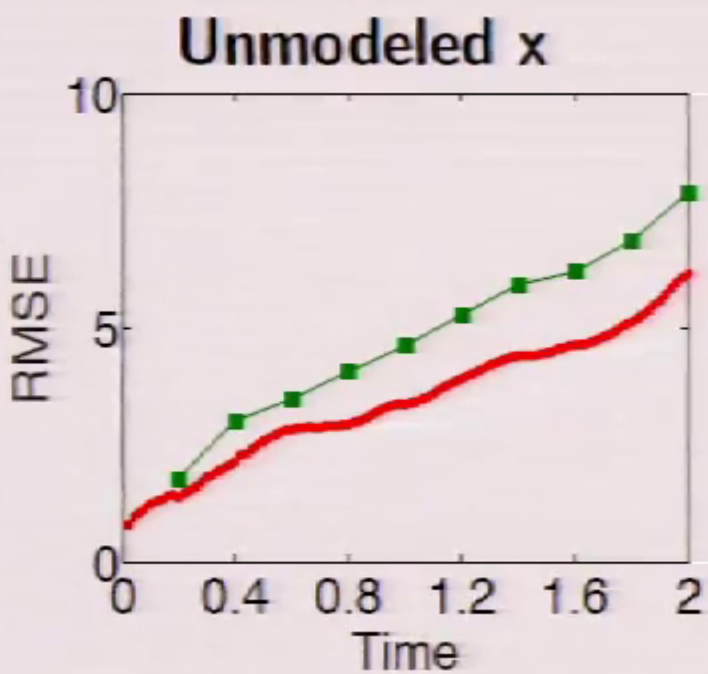
Can direct predict with original data set or interpolated data



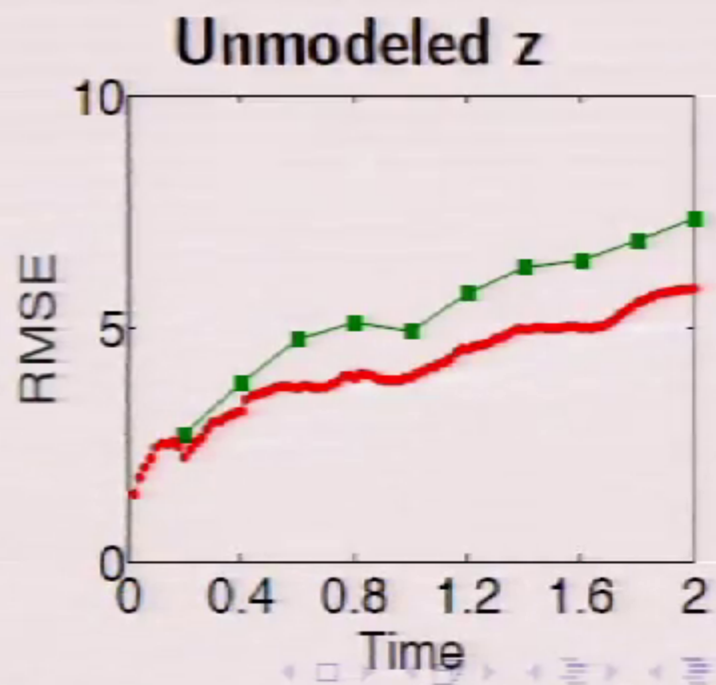
Actual **Nonparametric** **Semiparametric**



Modeled y
10
5
0
RMSE
0 0.4 0.8 1.2 1.6 2
Time



Unmodeled x
10
5
0
RMSE
0 0.4 0.8 1.2 1.6 2
Time



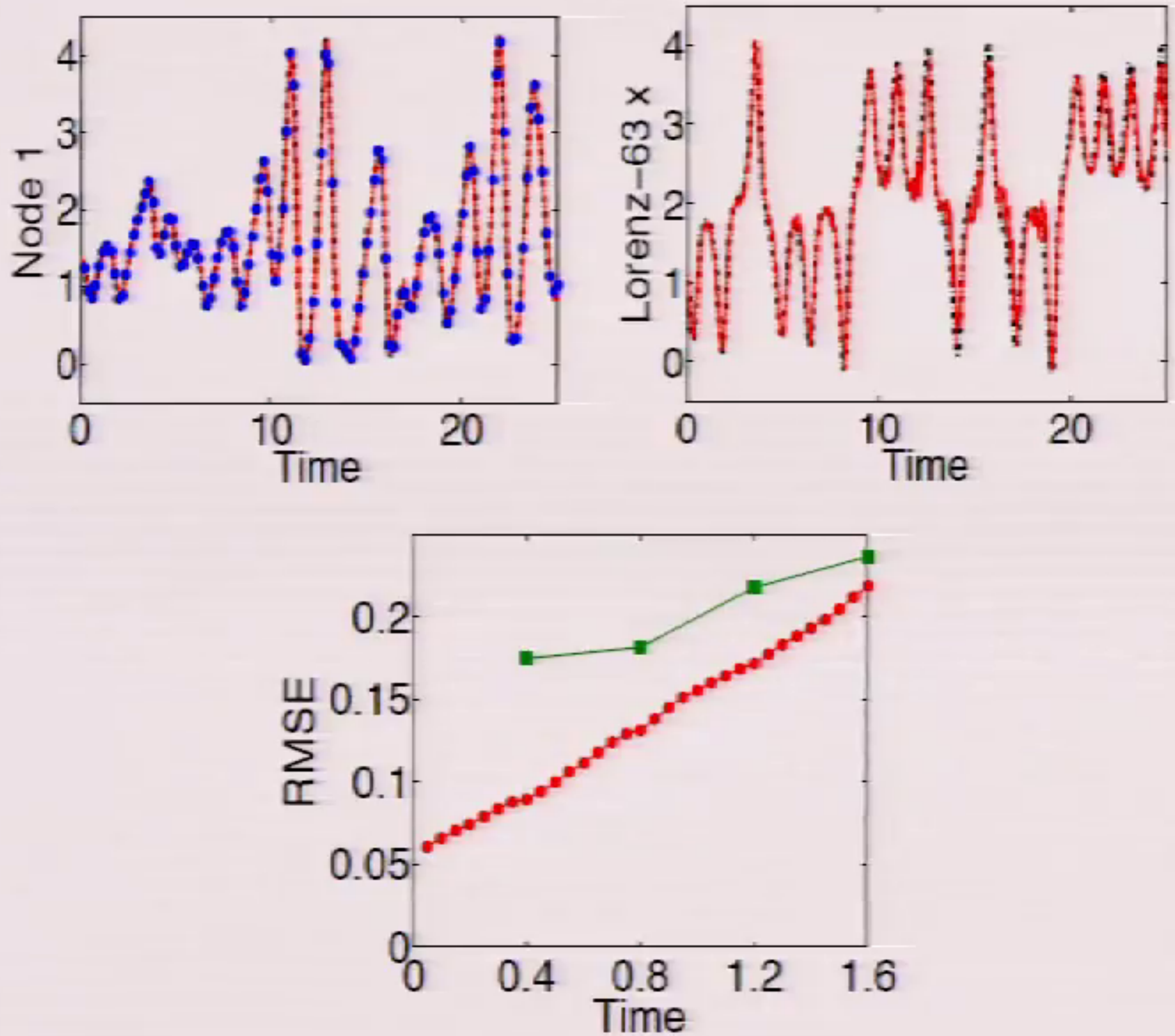
Unmodeled z
10
5
0
RMSE
0 0.4 0.8 1.2 1.6 2
Time

Consider the Lorenz-96 network

$$\dot{x}_i = (x_{i+1} - x_{i-2})x_{i-1} - c_i x_i + F_i + b_i x^1_{p+1}$$

driven by a Lorenz-63 attractor where $i = 1, \ldots, N$

Can we extend these ideas to this high dimensional system?


Node 1
Time
Lorenz-63 x
Time
RMSE
Time

1. Proposed a new approach to data assimilation for reconstructing unmodeled variables
    - F. Hamilton, J. Cressman, N. Peixoto, T. Sauer. Reconstructing neural dynamics using data assimilation with multiple models. Europhysics Letters, 107, 68005 (2014)

2. Utilized a partial model and delay-coordinate reconstruction of unmodeled variables for improved forecasting
    - F. Hamilton, T. Berry, T. Sauer. Predicting chaotic time series with a partial model (*preprint*)

- This work was supported by the National Science Foundation grants CMMI-1300007 and DMS-1216568
- People
  - Nathalia Peixoto, Ph.D
  - John Cressman, Ph.D
  - Tyrus Berry, Ph.D
  - Robert Graham