Identification of Non-linear Dynamical Systems

Lennart Ljung

Linköping University

Sweden

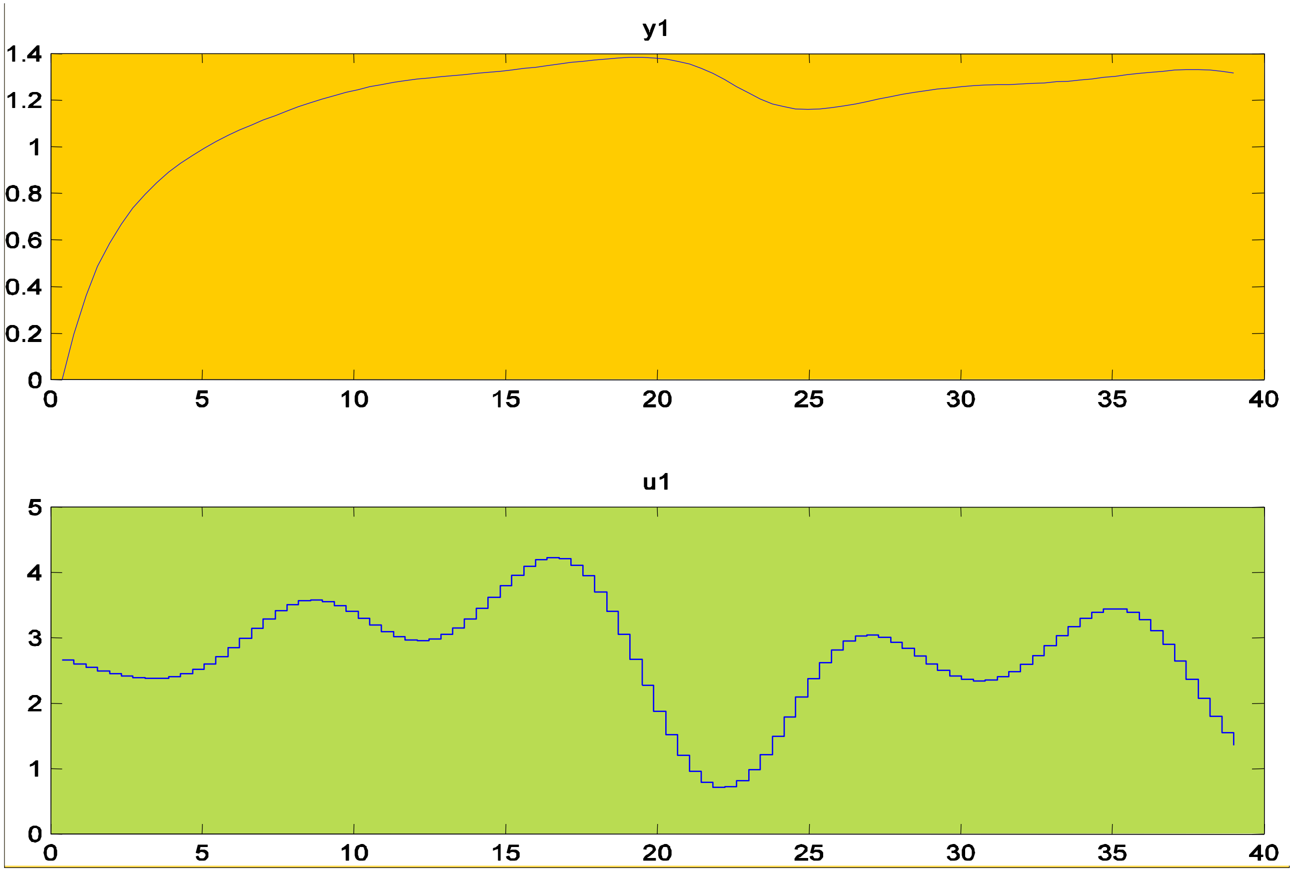
Prologue

Prologue

The PI, the Customer and the Data Set

- C: I have this data set. I have collected it from a cell metabolism experiment. The input is Glucose concentration and the output is the concentration of G6P. Can you help me building a model of this system?

The Data Set



Output

Input

A Simple Linear Model

Try the simplest model

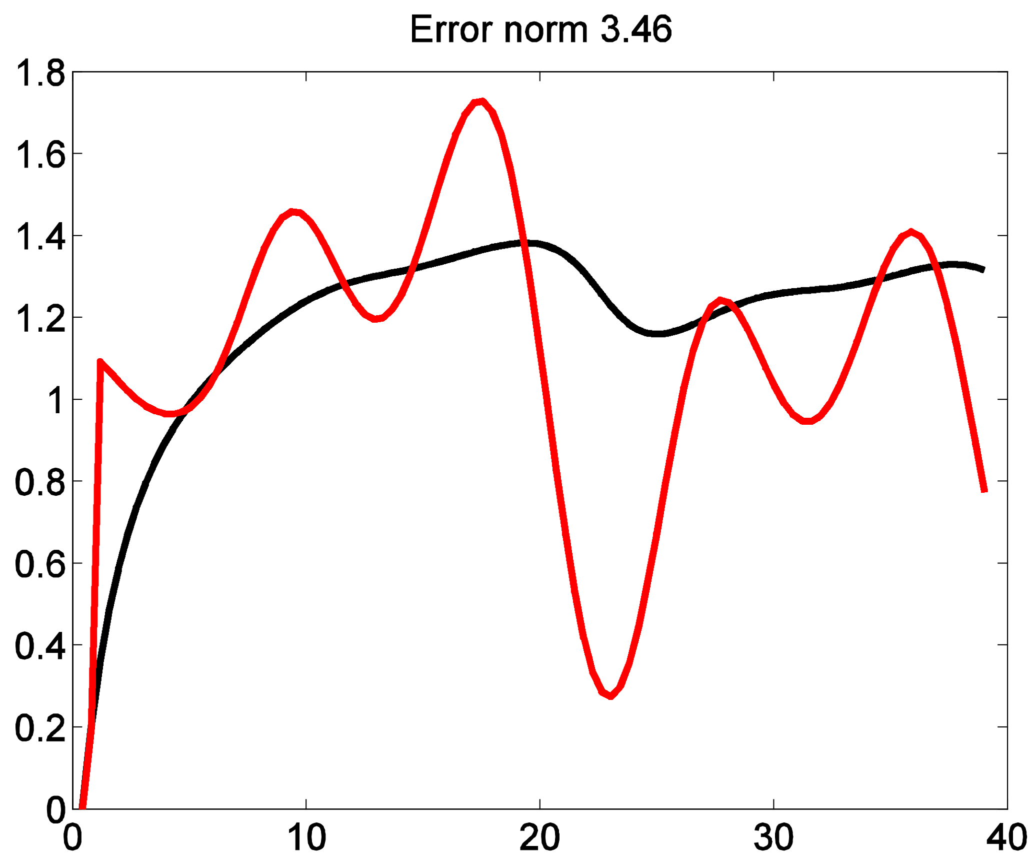
y(t) = a u(t-1) + b u(t-2)

Fit by Least Squares:

m1=arx(z,[0 2 1])

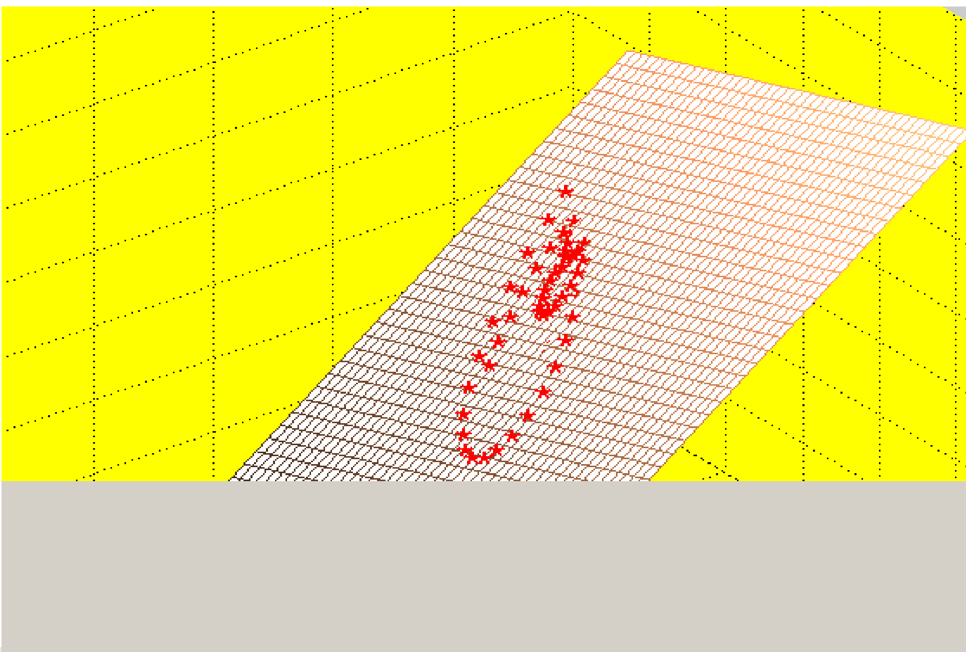
compare(z,m1)

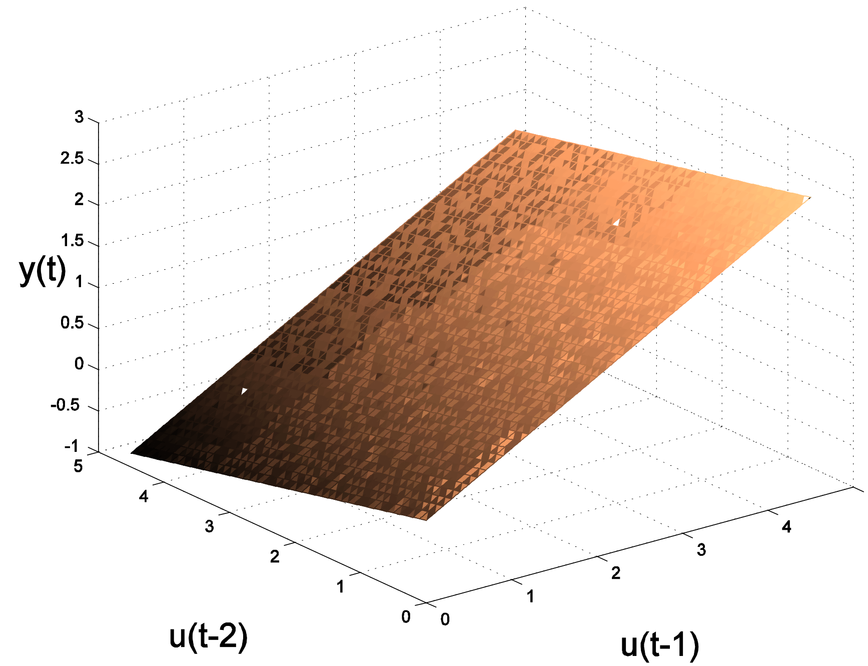
Red: Model
Black: Measured



A Picture of the Model

Depict the model as y(t) as a function of u(t-1) and u(t-2)





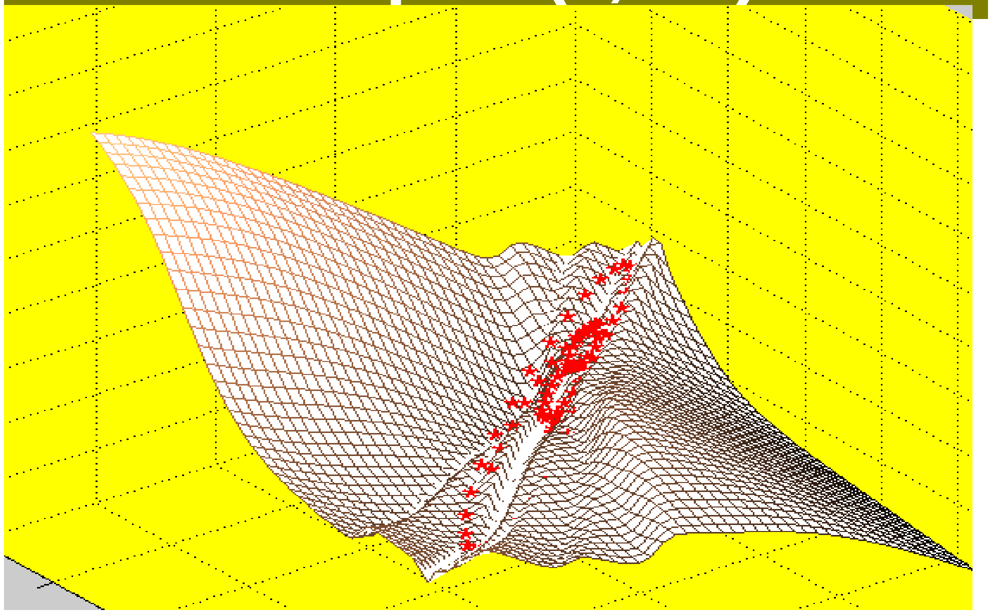
A Nonlinear Model

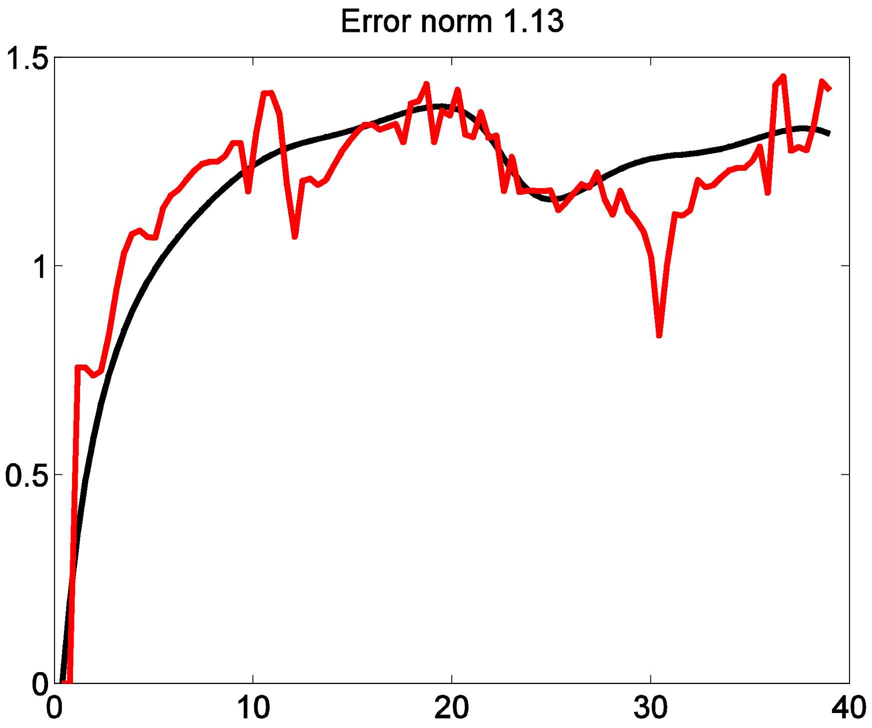
Try a nonlinear model

y(t) = f(u(t-1),u(t-2))

m2 = arxnl(z,[0 2 1],'sigm')

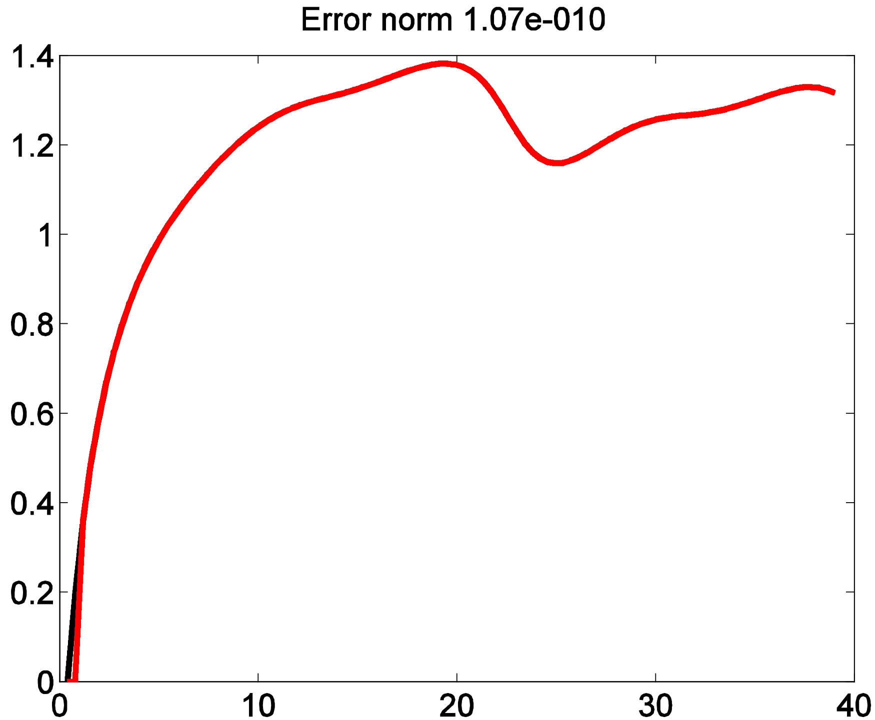
compare(z,m2)

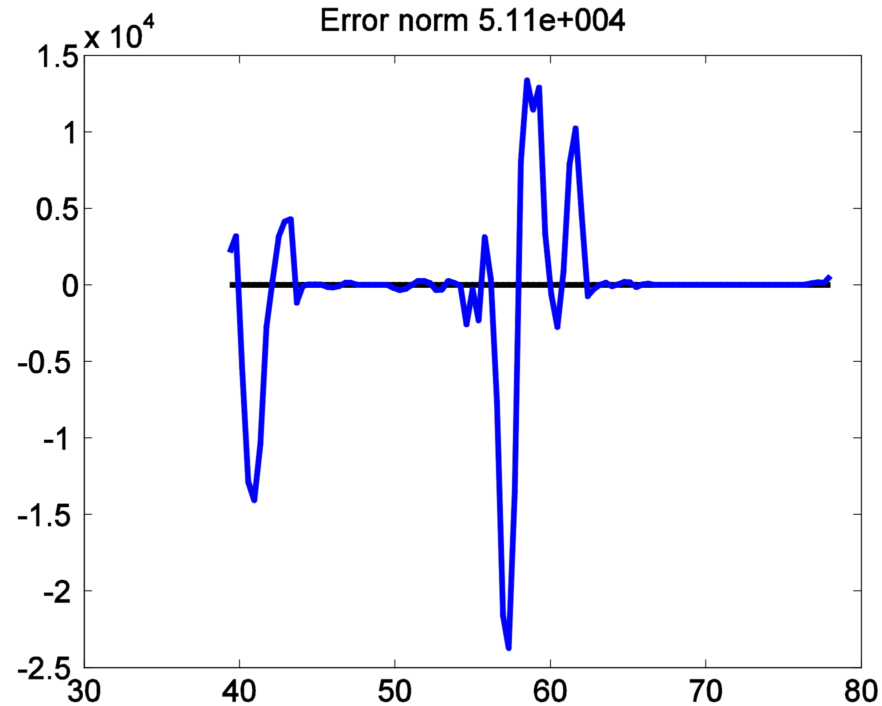




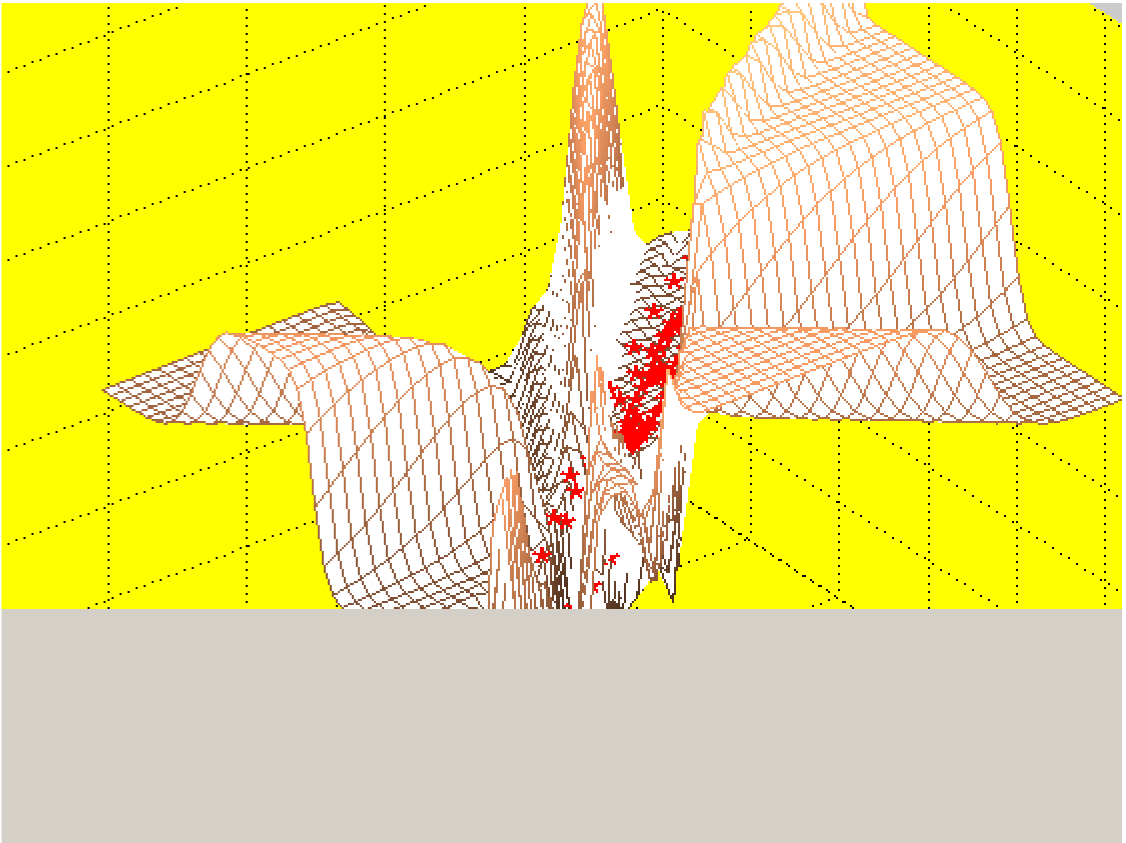
More Flexibility

A more flexible, nonlinear model
y(t) = f(u(t-1),u(t-2))
m3 = arxnl(z,[0 2 1],’sigm’,’numb’,100)
compare(z,m3)
compare(zv,m3)



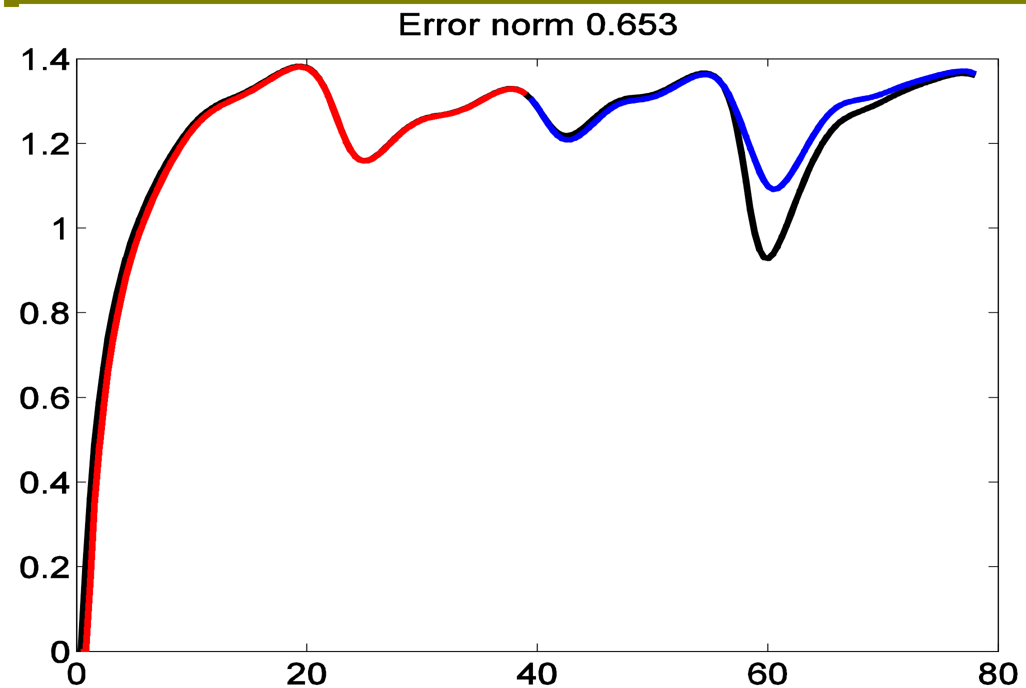


The Fit Between Model and Data



More Regressors

Try other arguments:
y(t) = f(y(t-1),y(t-2),u(t-1),u(t-2))
m4 = arxnl(z,[2 2 1],'sigm')
compare([z;zv],m4)



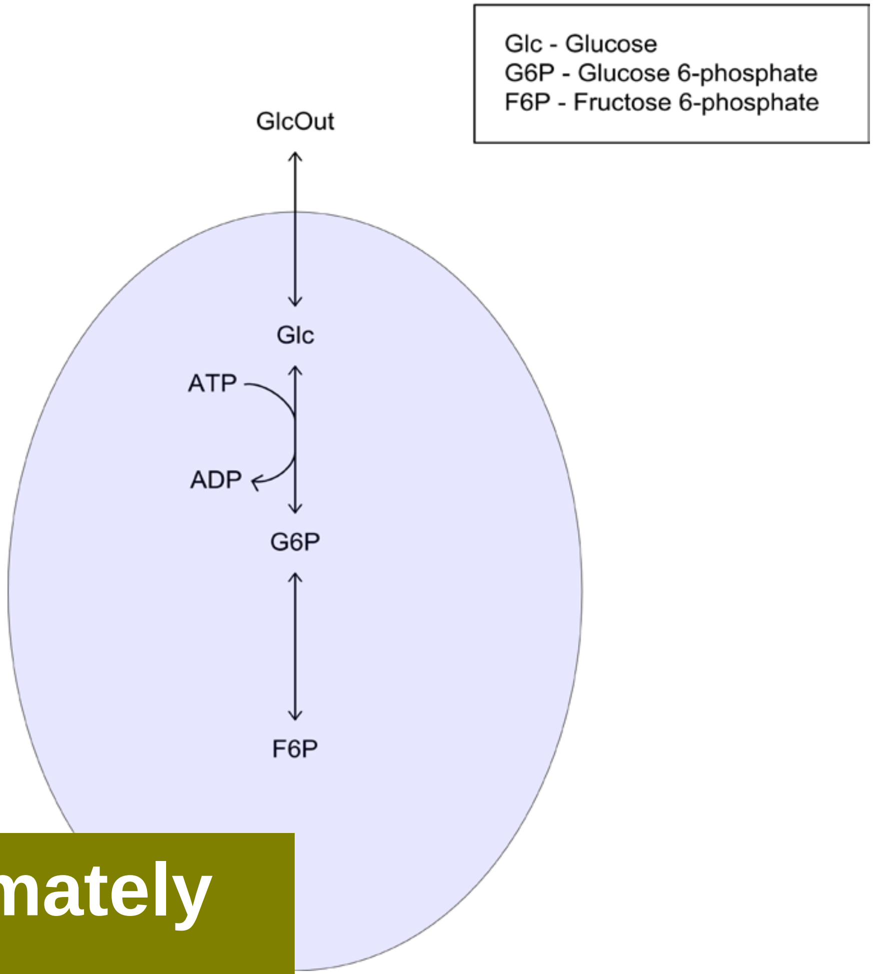
Biological Insight

Pathway diagram

$$\dot{x}_1 = -\theta_1 \frac{x_1/\theta_2 - x_2/\theta_3}{1 + x_1/\theta_2 + x_2/\theta_3} + \theta_4 \frac{u - x_1}{1 + u/\theta_5 + x_1/\theta_5 + x_1 u/\theta_5^2}$$

$$\dot{x}_2 = \theta_1 \frac{x_1/\theta_2 - x_2/\theta_3}{1 + x_1/\theta_2 + x_2/\theta_3} - \theta_6 \frac{x_2/\theta_7 - \theta_8}{1 + x_2/\theta_7 + \theta_8}$$

$$y = x_2$$

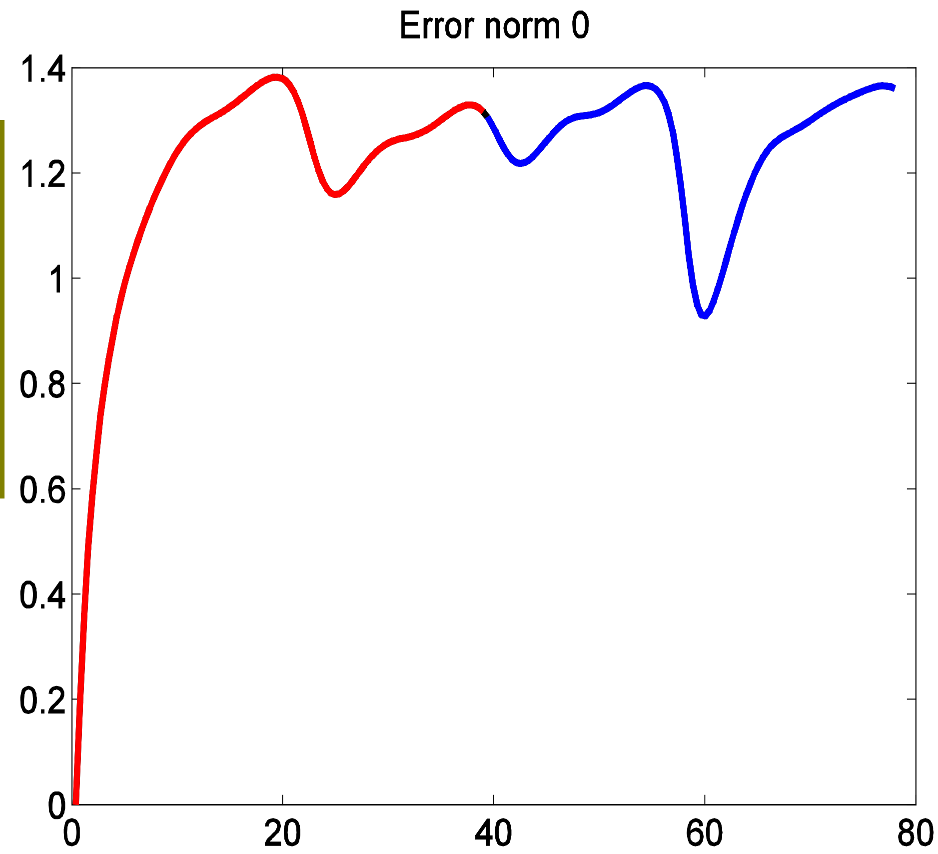


For sampled data, approximately

y(t) = f(y(t-1),y(t-2),u(t-1),u(t-2),θ)

Tailor-made Model Structure

```
cell = nlgrey(eqns,nom_pars)
m5 = pem(z,cell);
compare([z;zv],m5)
```



End of Prologue

Outline

- Problem formulation
- How to parameterize black box predictors
- Using physical insight
- Initialization of parameter search
- LTI approximation of non-linear systems

The Basic Picture

Input u, Output y, $Z^t = \{u(1), y(1), \dots u(t), y(t)\}$

- State-Space

$$\dot{x} = g(x, u, w)$$

$$y = h(x, u, e)$$

w and e noises

$$\hat{y}(t|t-1) = E(y(t)|Z^{t-1})$$

- Output predictor

$$\hat{y}(t|t-1) = f_0(Z^{t-1})$$

The Predictor Function

General structure $\hat{y}(t|t-1) = f_0(Z^{t-1})$

Common/useful special case:

$$\hat{y}(t|t-1) = f_0(Z^{t-1}) = f_0(\phi(t))$$

$\phi(t) = \phi(Z^{t-1})$ of fixed dimension m (”state”, ”regressors”)

Think of the simple case

$$\phi(t) = \left[y(t-1) \quad \ldots \quad y(t-n_a) \quad u(t-1) \quad \ldots \quad u(t-n_b) \right]$$

The Predictor Function

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Think of the simple case

$$\phi(t) = \left[y(t-1) \quad \dots \quad y(t-n_a) \quad u(t-1) \quad \dots \quad u(t-n_b) \right]$$

The Data and the Identification Process

The observed data

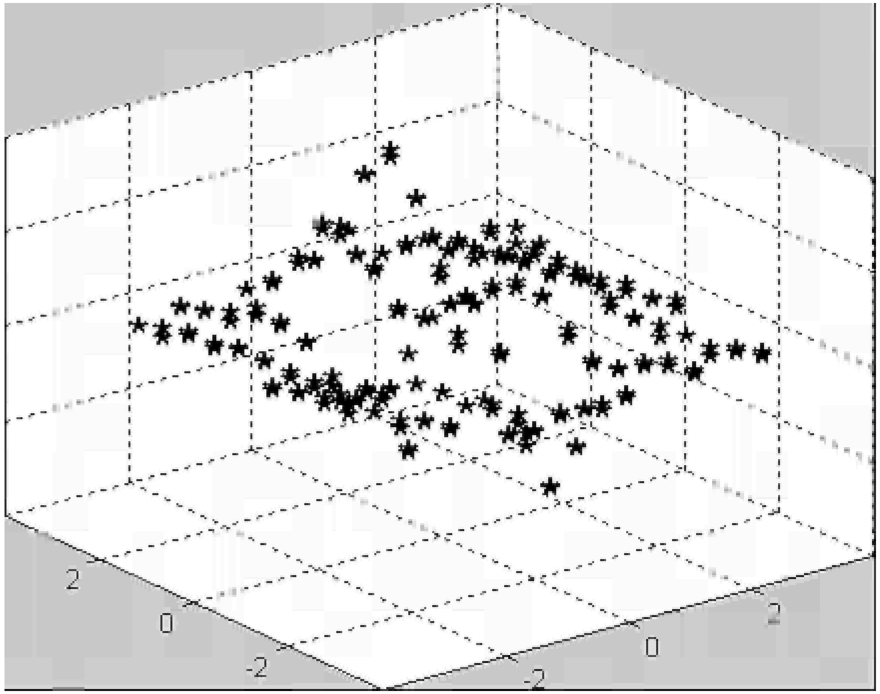
$Z^N=[y(1),\phi_1,\ldots y(N),\phi_N]$

are N points in $\mathbb{R}^{m+1}$

The predictor model

$$\hat{y} = f_0(\phi)$$

is a surface in this space



Identification is to find the predictor surface from the data:

Mathematical Formulation

- Collect observations: Z^N , $y(t)=f_0(\phi(t))$+noise
- Non-parametric: Smooth the y(t)'s locally over selected $\phi(t)$-regions
- Parametric:
  - Parameterize the predictor function: $f(\theta,\phi)$, $f \in \mathcal{F}$ when $\theta \in D$
  - Fit the parameters to the data:

$$\hat{\theta}_N = \arg\min_{\theta \in D} V_N(\theta, Z^N)$$

$$V_N(\theta, Z^N) = \sum_{t=1}^{N} \ell(y(t) - f(\theta, \phi(t))) = \sum_{t=1}^{N} \|y(t) - f(\theta, \phi(t))\|^2$$

- Use model $\hat{f}_N(\phi) = f(\hat{\theta}_N, \phi)$

Outline

- Problem formulation
- Parameterizing black box predictors
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Predictor Function Parameterization

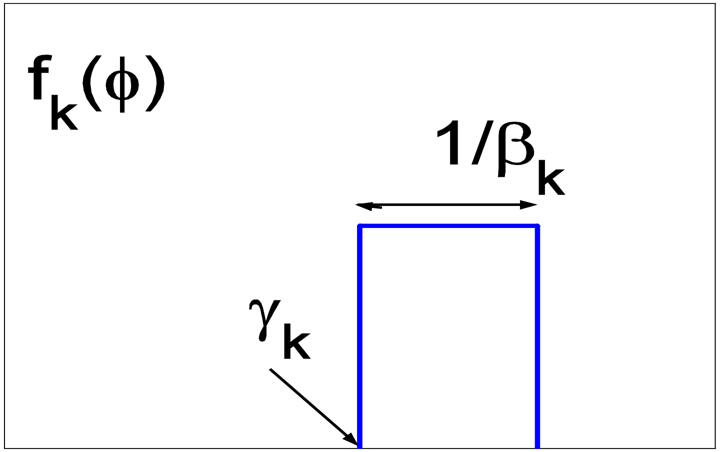
- How to parameterize the predictor function $f(\theta,\phi)$?
  - Grey-box (Physical insight of some sort)
  - Black-box (Flexible function expansions)

$$f(\theta,\phi) = \sum_{k=1}^{n} \theta_k f_k(\phi)$$

General case: $f_k(\phi) = f_k(\phi(\theta),\theta)$

Choice of Functions: Methods

- Neural Networks
- Radial Basis Neural Networks
- Wavelet-networks
- Neuro-Fuzzy models
- Spline networks
- Support Vector Machines
- Gaussian Processes
- Kriging



$$\gamma_k = \phi(k)$$

$$\kappa = \text{GaussianBell}$$

ALL THESE USE

$$f(\theta,\phi) = \sum_{k=1}^{n} \alpha_k \kappa(\beta_k(\phi - \gamma_k))$$

Several layers….

$$\theta = \{\alpha_k, \beta_k, \gamma_k\}$$

An Aspect for Dynamical Systems

- Let $\phi(t) = [y(t-1), u(t-1)]^T$
- (One-step ahead) predicted output:

$$\hat{y}_p(t|\theta) = f(\theta, [y(t-1), u(t-1)]^T)$$

- This is normally what is fitted to data.
- A tougher test for the model is to simulate the output from past inputs only:

$$\hat{y}_s(t,\theta) = f(\theta, [\hat{y}_s(t-1,\theta), u(t-1)]^T)$$

- Stability issues!

The Basic Challenge

- Non-linear surfaces in high dimensions can be very complicated and need support of many observed data points.
- How to find parameterizations of such surfaces that both give a good chance of being close to the true system, and also use a moderate amount of parameters?
- The data cloud of observations is by necessity sparse in the surface space.

How to Deal with Sparsity

- Need ways to interpolate and extrapolate in the data space
- Leap of Faith: Search for global patterns in observed data to allow for data-driven interpolation
- Use Physical Insight: Allow for few parameters to parameterize the predictor surface, despite the high dimension.

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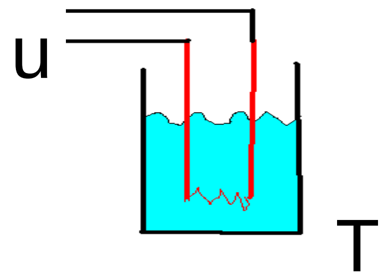
Using Physical Insight: Light Version

Semiphysical Modeling



Input: heater voltage u

Output: Fluid temperature T

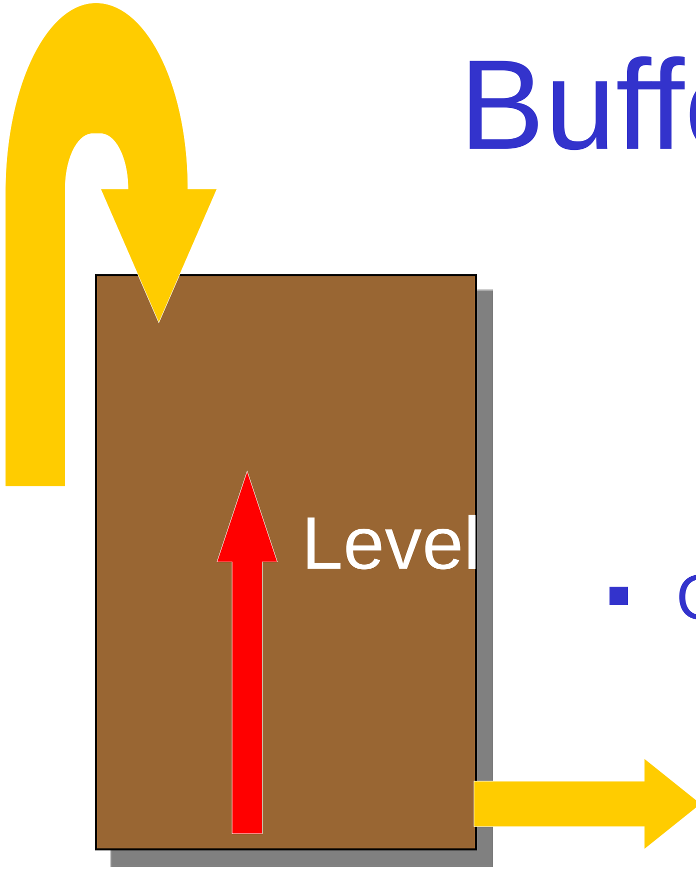
Square the voltage: $u \rightarrow u^2$

Example: Semiphysical Modeling

Buffer Vessel for Pulp

Inflow

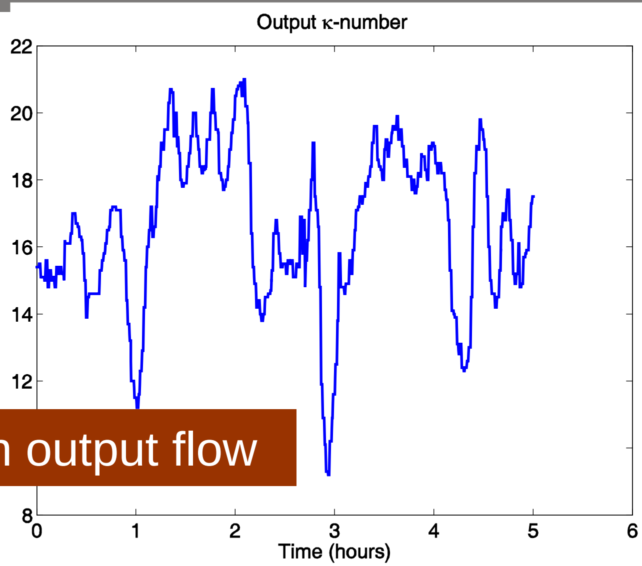
κ-number



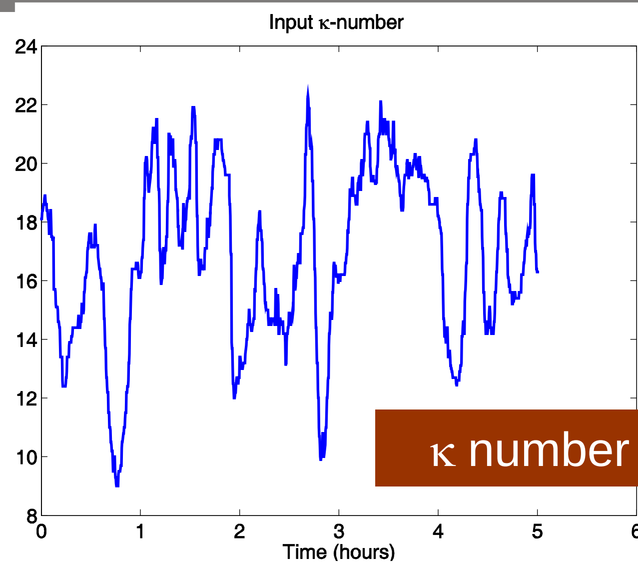
- Outflow
  - Flow
  - κ-number

Find the dynamics of this process!

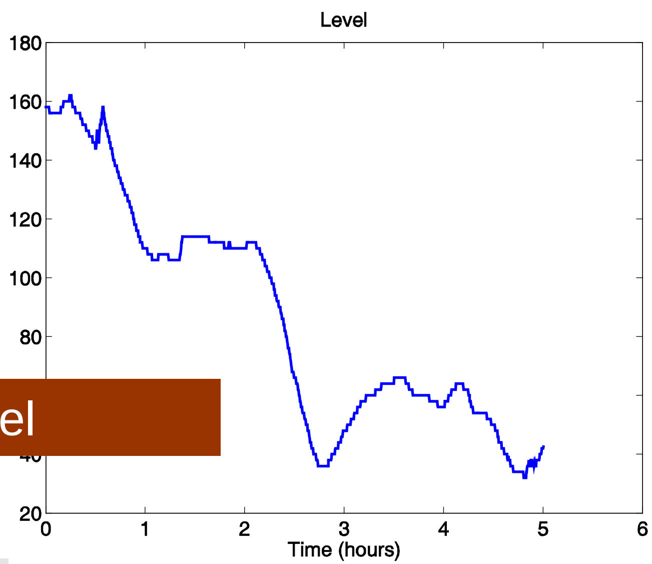
Measured Data from the Vessel



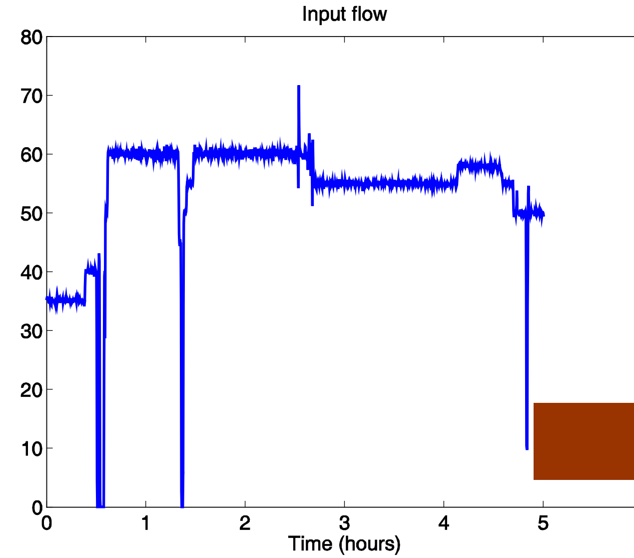
κ number in output flow



κ number in input flow

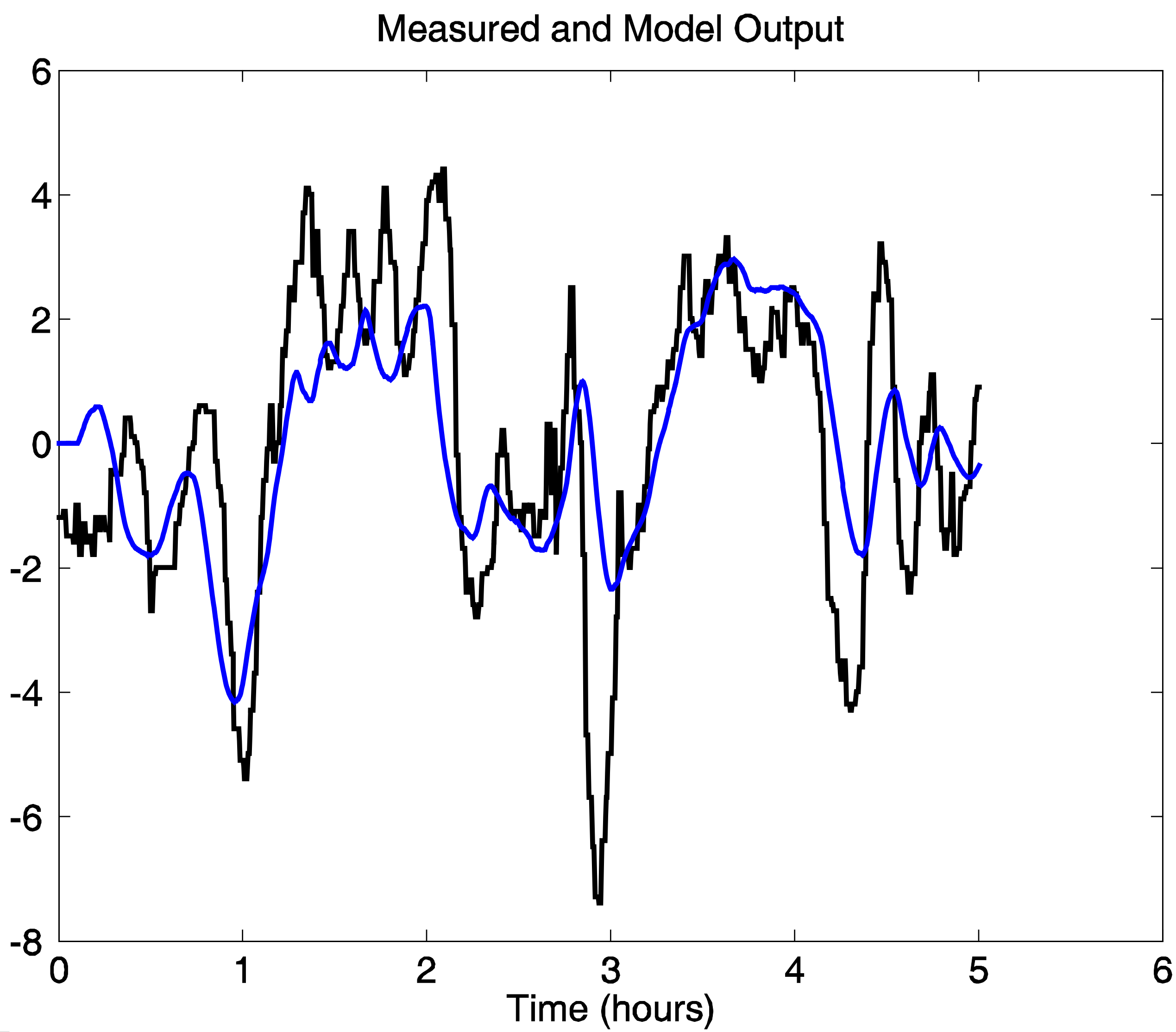


Level

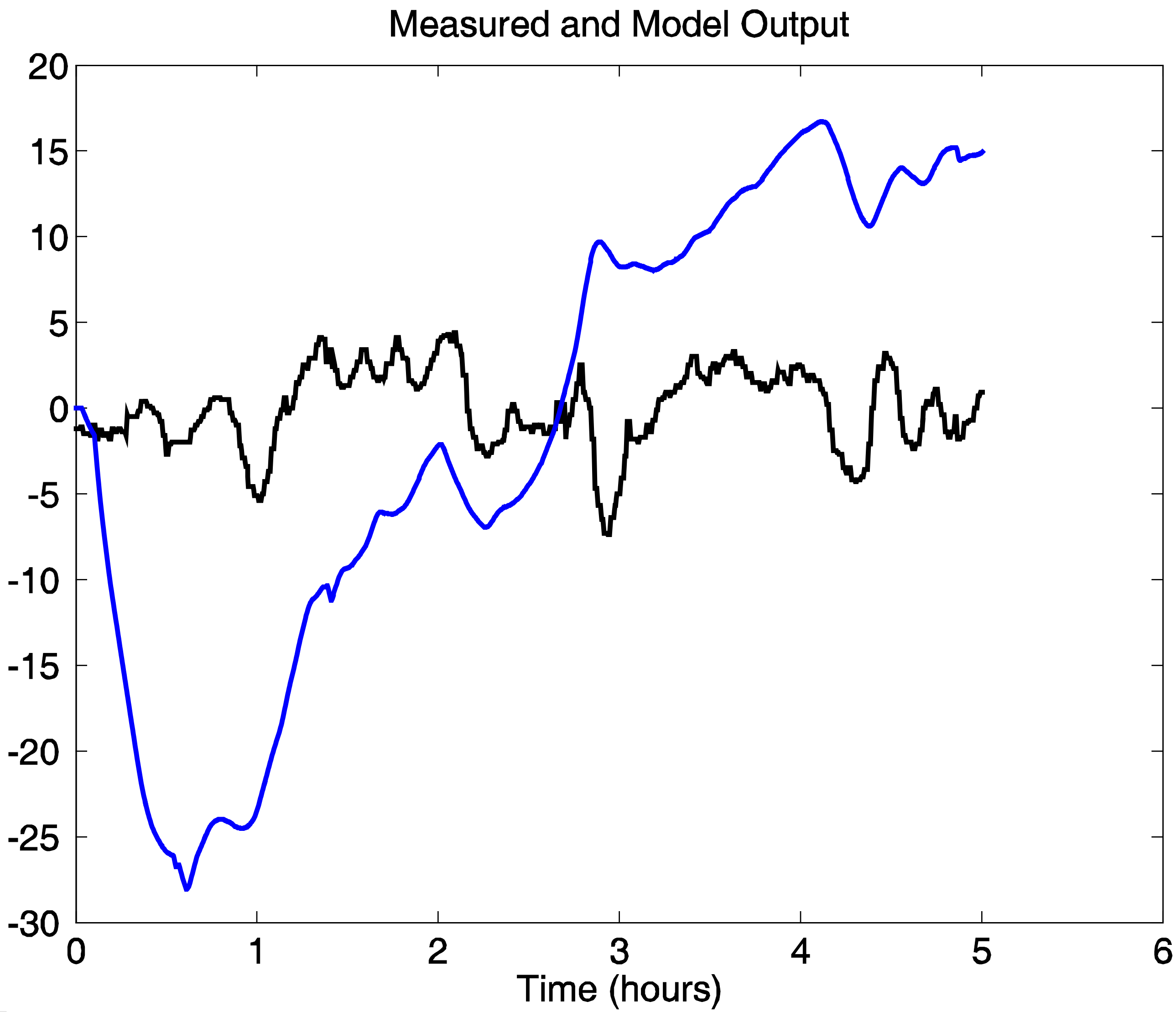


Flow

Fit a Linear Model to Data



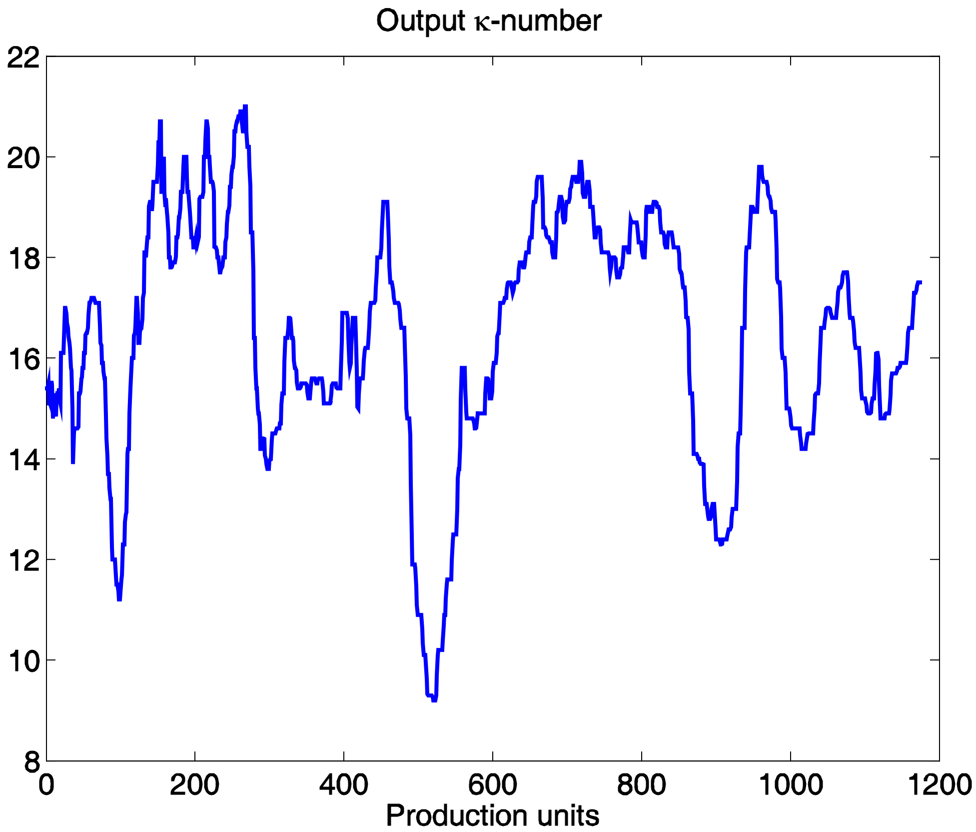
Using All 3 Inputs to Predict the Output

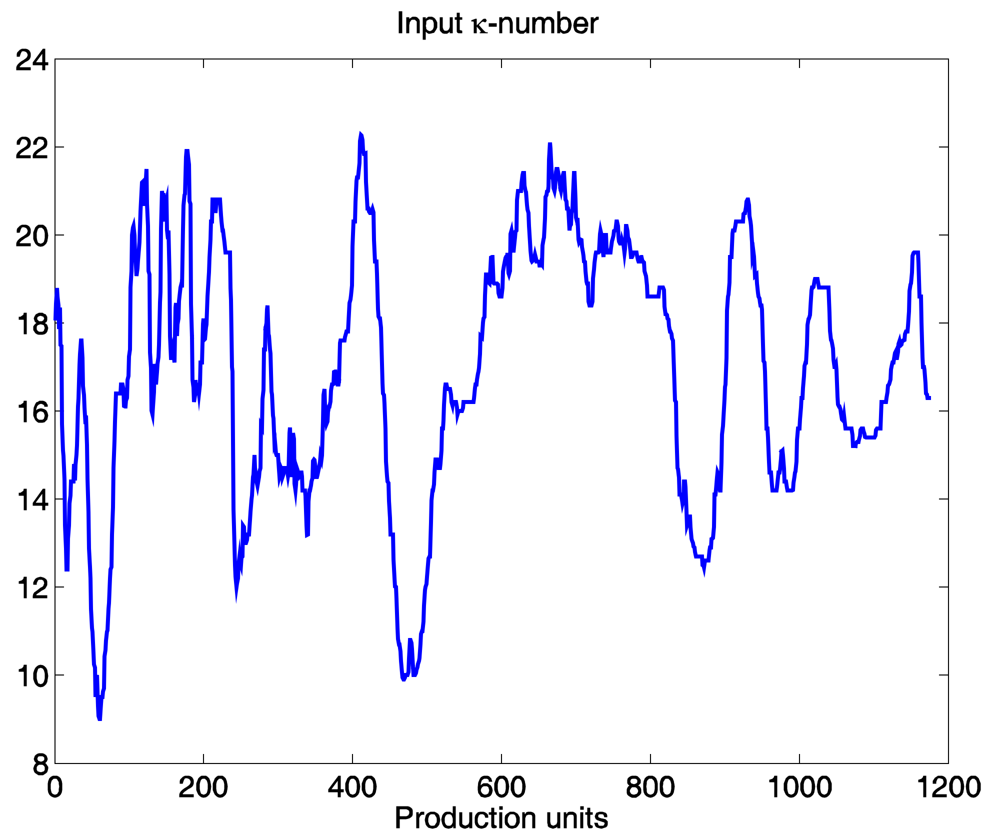


Think …

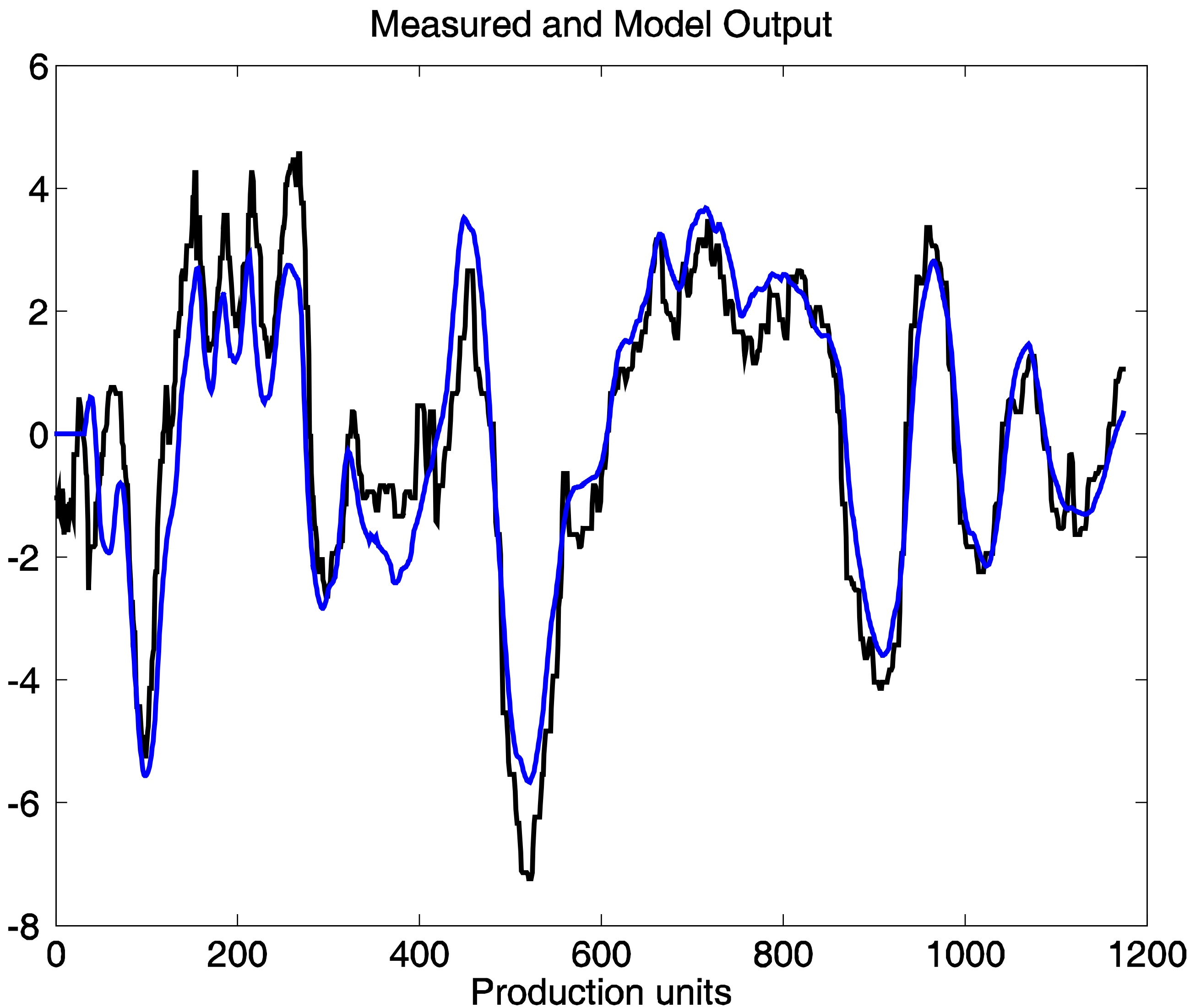
- Plug Flow: The system is a pure time delay of Volume/Flow
- Perfectly stirred tank: First order system with time constant = Volume/Flow
- Natural Time variable: Volume/Flow
- Rescale Time:
- `Pf = Flow/Level`
- `Newtime = interp1(cumsum(Pf),time,[Pf(1):sum(Pf)]);`
- `Newdata = interp1(Time,Data,Newtime);`

The Data with a New Time-scale





Simple Linear Model for Rescaled Data



Using Physical Insight: Serious Version

- Careful modeling leading to systems of Differential Algebraic Equations (DAE) parameterized by physical parameters.
- Support by modern modeling tools.
- The ”statistically correct” approach is to estimate the parameters by the Maximum Likelihood method.

Local Minima of the Criterion

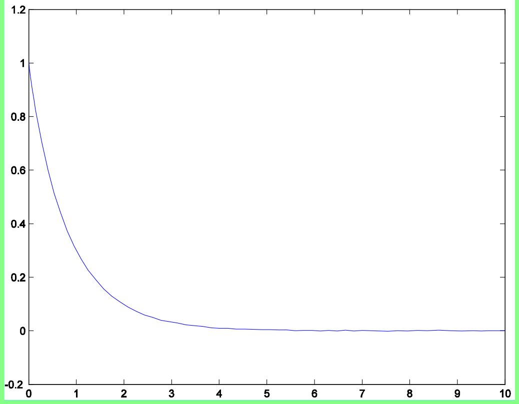
- This sounds like a general and reasonable approach
- Are there any catches?
- Well, to minimize the criterion of fit (maximizing the likelihood function) could be a challenge.
- Can be trapped in local minima….

Maximum Likelihood: The Solution?

- Example: A Michaelis-Menten equation:

$$\dot{x} = \theta_1 \frac{x}{\theta_2 + x} - x + u$$
$$y = x + e$$
$$u = \text{impulse}$$

- The output:

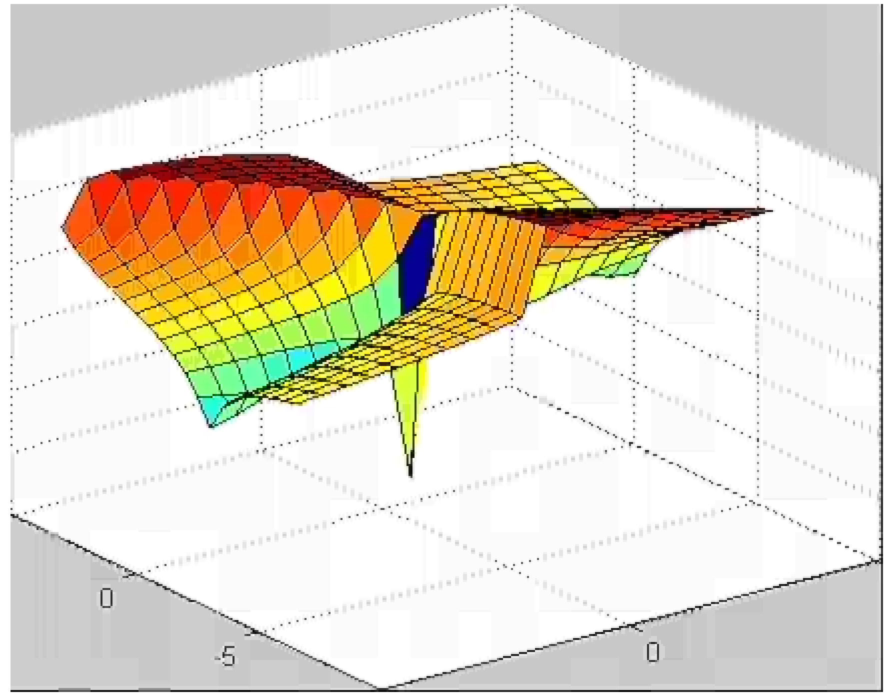


The ML Criterion (Gaussian Noise)

$$V(\theta) = \sum_{k=1}^{100} \|y(t_k) - x(t_k, \theta)\|^2$$

$$\dot{x}(t,\theta) = \theta_1 \frac{x(t,\theta)}{\theta_2 + x(t,\theta)} - x(t,\theta) + u(t)$$

V(θ) as a function of θ



Outline

- Problem formulation
- How to parameterize black box predictors
- Using physical insight
- Initialization of parameter search
- LTI approximation of non-linear systems

Can We Handle Local Minima ?

- Can the observed data be linked to the parameters in a different (and simpler) way?
- Manipulate the equations …

Ex: The Michaelis-Menten Equation

- In our case (noisefree)

$$\dot{y} = \frac{\theta_1 y}{y+\theta_2} - y + u$$

$$\dot{y}y + \theta_2\dot{y} = \theta_1 y - y^2 - \theta_2 y + uy + \theta_2 u$$

$$\dot{y}y + y^2 - uy = \begin{bmatrix}\theta_1 & \theta_2\end{bmatrix}\begin{bmatrix} y \\ u - \dot{y} - y \end{bmatrix}$$

For observed y and u this is a linear regression in the parameters. With noisy observations, the noise structure will be violated, though, which could lead to biased estimates.

Identifiability and Linear Regression

Crucial Challenge for physically parameterized models: Find a good initial estimate

- Result of conceptual interest: (Ljung, Glad, 1994)

A parameterized set of DAEs is globally identifiable

if and only if

the set can be rearranged as a linear regression

Ritt's algorithm from differential algebra provides a finite procedure for constructing the linear regression

Example of Ritt's Algorithm

Original equations

$$\dot{x}_1 = \theta x_2^2$$
$$\dot{x}_2 = u$$
$$y = x_1$$

Differentiate y twice

$$\dot{y} = \dot{x}_1 = \theta x_2^2$$
$$\ddot{y} = 2\theta x_2 \dot{x}_2 = 2\theta x_2 u$$

Square the last expression

$$\ddot{y}^2 = 4\theta\theta x_2^2 u^2 = 4\theta \dot{y} u^2$$

which is a linear regression

Challenge for Parameter Initialization

- Only small examples treated so far. Make the initialization work in bigger problems.
- Potential for important contributions:
  - Handle the complexity by modularization
  - Handle the noise corruption so that good quality initial estimates are secured
- Room for innovative ideas using algebra and semidefinite programming!

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A Control Aspect

- Despite all the work and results on non-linear models, the most common situation will still be

How to live with an estimated LTI model approximation of a Non-linear system.

Outline

- Problem formulation
- Generalization properties
- How to parameterize black box predictors
- Using physical insight
- Initialization of parameter search
- LTI approximation of non-linear systems

Non-linear System Approximation

- Given an LTI Output-error model structure $y=G(q,\theta)u+e$, what will the resulting model be for a non-linear system?
- Assume that the inputs and outputs u and y are such that the spectra Φ_u and Φ_{yu} are well defined.
- Then the LTI second order equivalent is

$$G_0 = \frac{1}{\lambda L(z)} \left[\frac{\Phi_{yu}(z)}{L(z^{-1})} \right]_{\text{causal}} \qquad \Phi_u(z) = \lambda L(z) L(z^{-1})$$

Note: G_0 depends on u

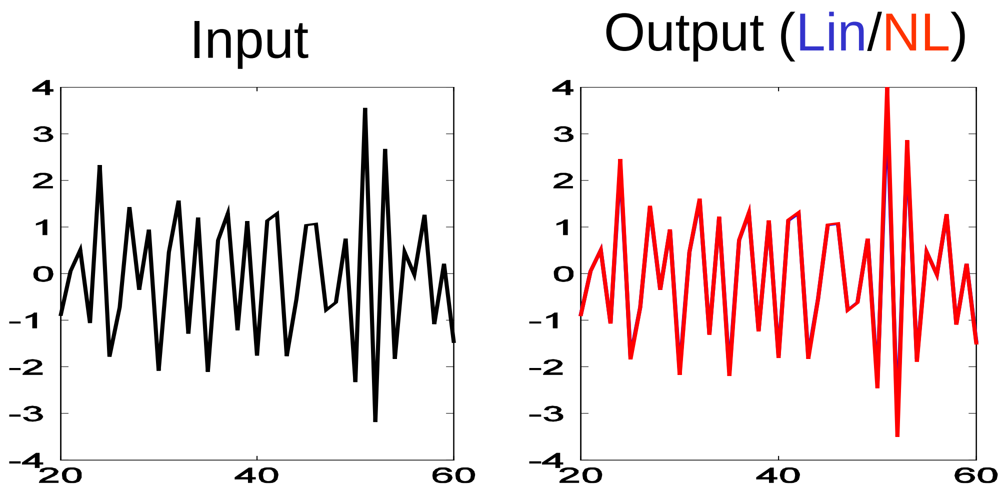
- The limit model will be

$$\min_\theta \int |G(z,\theta) - G_0(z)|^2 \Phi_u(z) dz$$

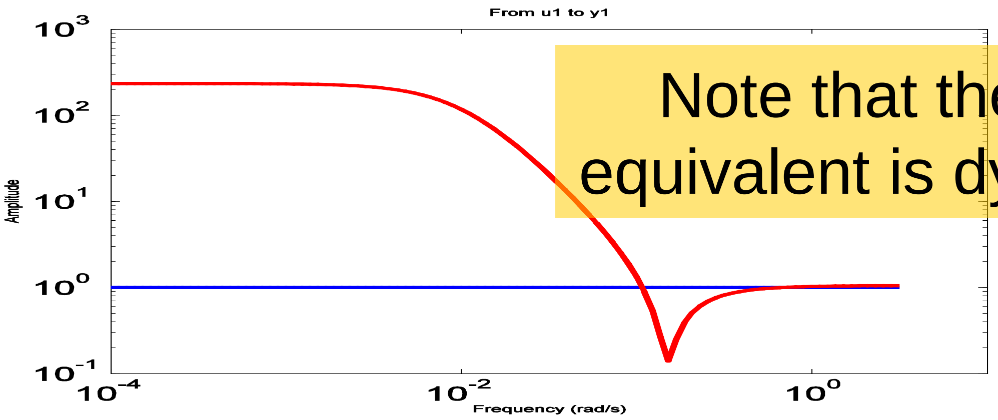
An Example

- Two data sets
- Input u and output y
- $y = u$
- $y = u + 0.01u^3$

(Enqvist, 2003)



The corresponding LTI equivalents (amplitude Bode plot)



Note that the LTI equivalent is dynamic!

An Example

- Two data sets
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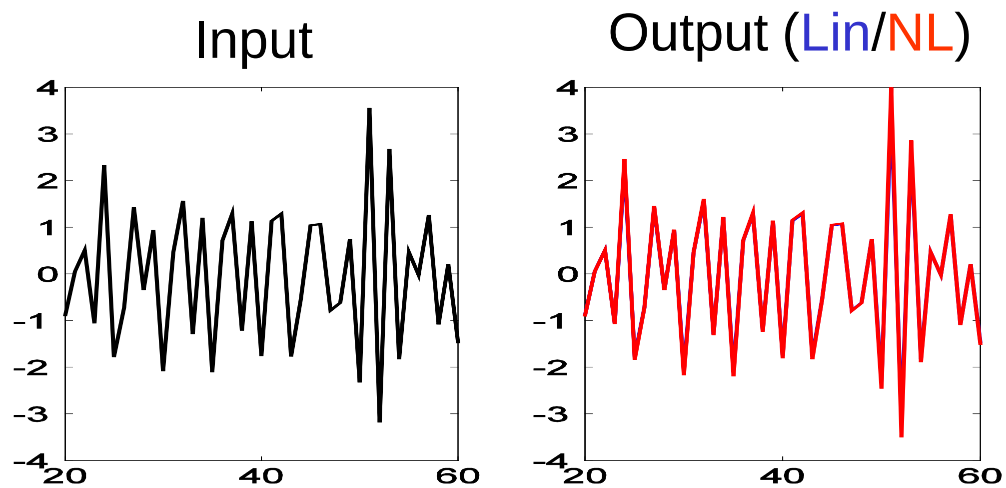
- y = u
- $y = u + 0.01u^3$

(Enqvist, 2003)



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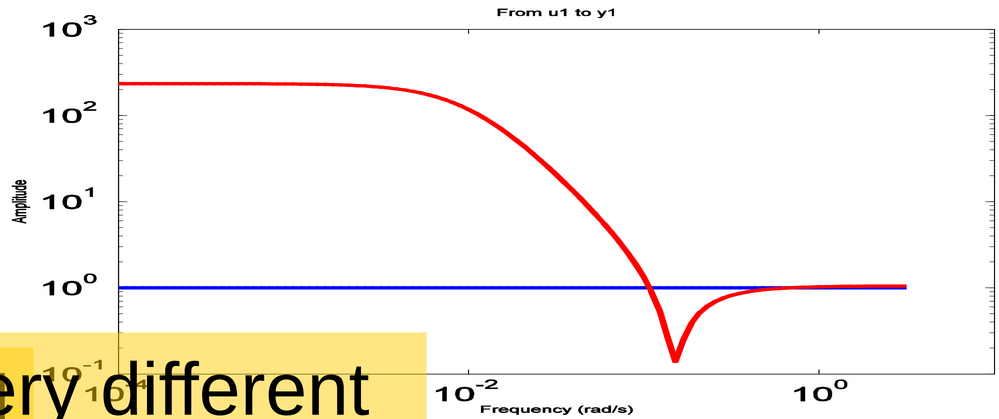

Is the red Bode plot a good basis for control design?

So, oe(z,[2 2 1]) give very different results for the two data sets!

S

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- Problem formulation
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- LTI approximation on non-linear systems
- Generalization properties

Model Quality

Model quality $|f_0(\phi) - f(\theta, \phi)|$. Average over a selected sequence of regressors $\tilde{\phi}_t$:

$$W_N(\theta) = \frac{1}{N} \sum_{t=1}^{N} |f_0(\tilde{\phi}_t) - f(\theta, \tilde{\phi}_t)|^2$$

Good model: One that makes $W_N(\theta)$ small.
Best possible model and fit in model set:

$$\theta_N^* = \arg\min W_N(\theta), \qquad W_N(\theta_N^*)$$

Evaluating Quality From Data

Estimation Data $Z_e: \; y(t) = f_0(\phi_t) + e(t)$

Validation Data $Z_v: \; y(t) = f_0(\tilde{\phi}_t) + v(t)$

$$V_N(\theta, Z_e) = \frac{1}{N}\sum_{t=1}^{N} |y(t) - f(\theta, \phi_t)|^2, \quad V_N(\theta, Z_v) = \ldots$$

$\hat{\theta}_N = \arg\min V_N(\theta, Z_e)$. What does $V_N(\hat{\theta}_N, Z_e)$ tell us?

$$V_N(\hat{\theta}_N, Z_e) = \frac{1}{N}\sum |f_0(\phi_t) - f(\hat{\theta}_N, \phi_t)|^2 + \frac{1}{N}\sum e^2(t) + \frac{2}{N}\sum (f_0(\phi_t) - f(\hat{\theta}_N, \phi_t))e(t)$$

Difficult to interpret, since the last term does not tend to zero.

Evaluating Fit Using Validation Data

What does $V_N(\hat{\theta}_N, Z_v)$ tell us?

$$
\begin{aligned}
V_N(\hat{\theta}_N, Z_v) =& \frac{1}{N}\sum |f_0(\tilde{\phi}_t) - f(\hat{\theta}_N, \tilde{\phi}_t)|^2 + \frac{1}{N}\sum v^2(t) \\
&+ \frac{2}{N}\sum (f_0(\tilde{\phi}_t) - f(\hat{\theta}_N, \tilde{\phi}_t))v(t) \\
&\to W_N(\hat{\theta}_N) + \sigma_v^2
\end{aligned}
$$

Gives a good grip on the interesting quality measure $W_N(\hat{\theta}_N)$

Asymptotic Theory

In case $\phi_t = \tilde{\phi}_t$ we have the asymptotic results

$$\hat{\theta}_N - \theta_N^* \to 0 \text{ as } N \to \infty$$
$$EW_N(\hat{\theta}_N) = W_N(\theta_N^*) + \frac{d}{N}\sigma_e^2$$

Here *d* is the number of parameters, regardless of the parameterization!

Bias – Variance Trade-off

Akaike-type result. Similar in Learning Theory.

Epilogue: Tasks for the Control Community

- Black-box models
  - Working stability theory: Prediction/Simulation
- Semiphysical Models
  - Tools to generate and test non-linear transformations of data
- Fully integrated software for modeling and identification
  - Object oriented modeling
  - Differential Algebraic Equations – including disturbance modeling
  - Robust parameter initialization techniques
- Understand LTI approximation of nonlinear dynamic systems

Epilogue

- Challenges for the Control Community:

1) Black-box models
   - ✓ A working stability theory: Prediction/Simulation
2) Semiphysical modeling

1) Fully integrated software for modeling and identification
   - ✓ Object oriented modeling
   - ✓ Differential algebraic equations
   - ✓ Full support of disturbance models
2) Robust parameter initialization techniques
   - ✓ Algebraic/Numeric

Mathematical Formulation

- Collect observations: Z^N , $y(t)=f_0(\phi(t))$+noise
- Non-parametric: Smooth the $y(t)$'s locally over selected $\phi(t)$-regions
- Parametric:
  - Parameterize the predictor function: $f(\theta,\phi)$, $f \in \mathcal{F}$ when $\theta \in D$
  - Fit the parameters to the data:

$$\hat{\theta}_N = \arg\min_{\theta \in D} V_N(\theta, Z^N)$$

$$V_N(\theta, Z^N) = \sum_{t=1}^{N} \ell(y(t) - f(\theta, \phi(t))) = \sum_{t=1}^{N} \|y(t) - f(\theta, \phi(t))\|^2$$

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- IMPORTANT PROBLEM
- The fit for estimation data $V_N(\hat{\theta}_N, Z^N)$ is known
- How to assess the fit for another (validation) data set?

Thanks to …

Coauthors (non-linear identification):

Alberto Bemporad * Albert Benveniste * Martin Braun * Torbjörn Crona * Bernard Delyon * Martin Enqvist * P-Y Glorennec * Markus Gerdin * Torkel Glad * Fredrik Gustafsson * Håkan Hjalmarsson * Anatoli Juditsky * Ingela Lind * David Lindgren * Peter Lindskog * Mille Millnert * Alexander Nazin * Alexander Poznyak * Pablo Parrilo * Dan Rivera * Jacob Roll * Jonas Sjöberg * Anders Skeppstedt * Anders Stenman * Jan-Erik Strömberg * Vincent Verdult * Michel Verhaegen * Qinghua Zhang *

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www.control.isy.liu.se/~ljung/bode

A Multitude of Concepts

Neural Networks * Support Vector Machines * Nonparametric Regression * Lazy Learning * Wavenet networks * Just-in-time Models * Local Polynomial Methods * Statistical Learning Theory * Multi-index Model Estimation * Kernel Methods * Fuzzy Modeling * Radial Basis Networks * Regression Trees * Differential Algebraic Equations * Model on Demand * Single-index Model Estimation Neuro-Fuzzy Approach * Least-squares Support Vector Machines * Reproducing Kernel Hilbert Spaces * SupAnova * Kriging * Gaussian Processes * Regularization Networks * Nearest Neighbor Modeling * Direct Weight Optimization * Bayesian Learning * Committee Networks * Nystrom Method *

Using Physical Insight I

Semiphysical Modeling

Hammerstein-Wiener

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Local Linear Models (also LPV)

$\phi = [\rho, \psi]$; $f(\theta,\phi)=f(\theta,\rho,\psi)$

Linear in ψ for fixed ρ (”regime variable”)

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