Estimating Dynamic Models (Excerpted from a paper to be read to the Royal Statistical Society May 9, 2007)

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Outline

Overview

- We want to fit data by a solution to a system of nonlinear differential equations (DIFE's).
- We ignore DIFE's so simple that they can be solved, such as linear constant coefficient systems. These are already well taken care of.
- Our approach is a generalization of smoothing methods combined with a computational approach involving a modification of profiling.
- We will show results for simulated data from two test-bed problems.
- Data from a chemical reactor producing nylon is analyzed to estimate parameters defining equations for reaction kinetics.

Outline

The FitzHugh-Nagumo model

- This simple two-component system is widely used to model properties of actual neural networks.
- They describe the reciprocal dependencies of the voltage V across an axon membrane and a recovery variable R reflecting outward currents, and
- the impact of a time-varying external excitation E.
- In the typical experiment only V will be measured, but we will consider both to be available.

The FitzHugh-Nagumo equations

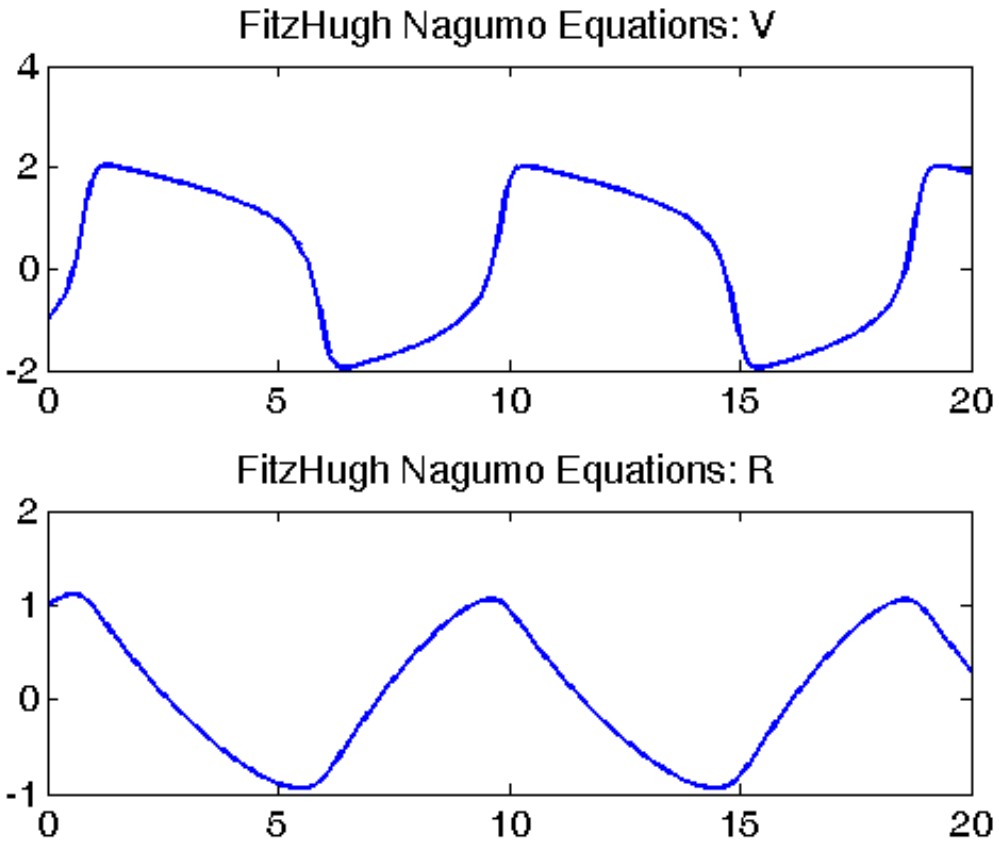
- Here is the system:

$$DV = c\left(V - \frac{V^3}{3} + R\right) + E(t)$$

$$DR = -\frac{1}{c}(V - a + bR)$$

- V is voltage across axon membrane
- R reflects outward currents
- E reflects external excitation
- The dynamics of the system are controlled by parameters a, b and c.
- The system would be linear except for the V^3 term.

A FitzHugh-Nagumo solution



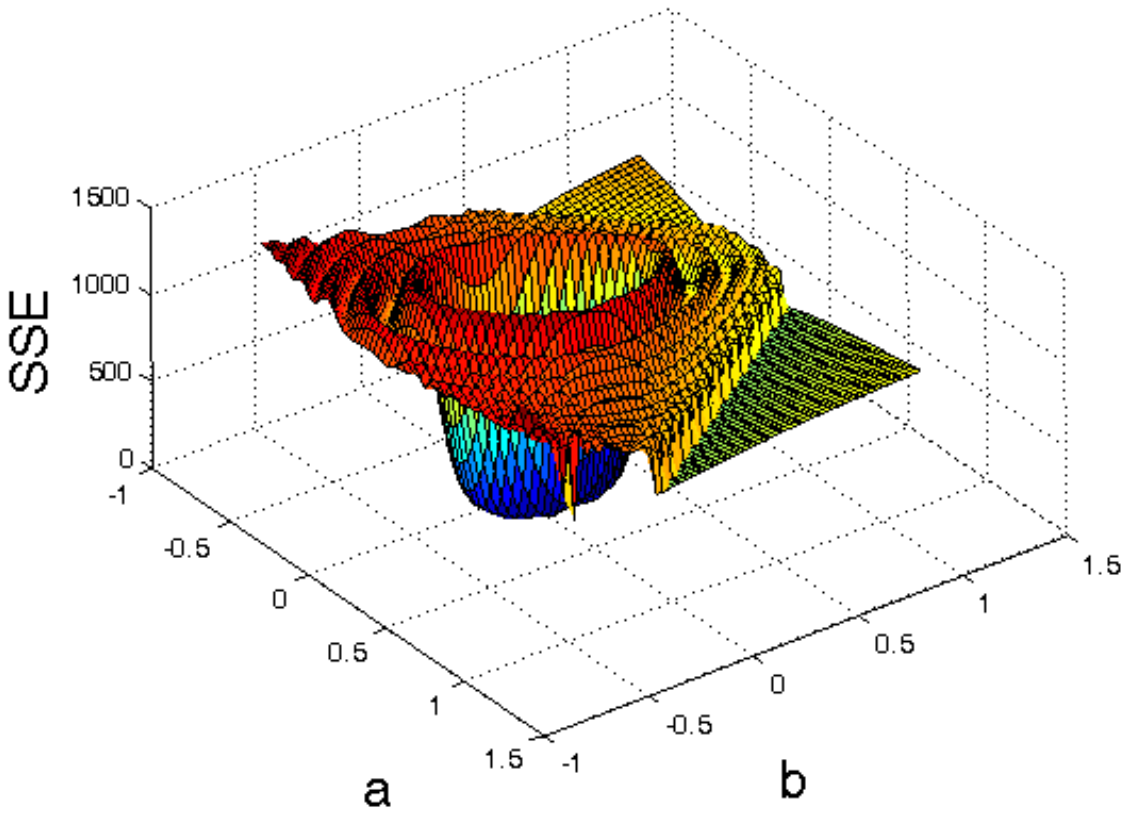
What we see

- The solution quickly reaches a steady state where it is periodic with an asymmetric pattern.
- The parameters control the amplitude and period of the response.
- The second order van der Pol equation is a closely related system.

The response surface can be complex

- Differential equations be simple, and yet define extremely complex behavior.
- This is reflected in the response surface of these equations as a functions of parameters a and b.

A FitzHugh-Nagumo response surface



The tank reactor model

- A continuously stirred tank reactor *CSTR* consists of a tank surrounded by cooling jacket and an impeller which stirs the contents.
- It is a basic piece of equipment for a chemical engineer.

The tank reactor variables

- A fluid is pumped into the tank containing a reagent with concentration C_{in} at a flow rate F_{in} and temperature T_{in}.
- Inside the tank a reaction takes place, producing a product that leaves the tank with concentration C_{out} and temperature T_{out}.
- A coolant enters the cooling jacket with temperature T_{cool} and flow rate F_{cool}.
- Temperature T_{out} is can be cheaply measured with little delay and considerable accuracy, but concentration C_{out} requires time and money.

The tank reactor equations

$$\begin{aligned} DC_{out} &= -\beta_{CC}(T_{out})C_{out} + F_{in}C_{in} \\ DT_{out} &= -\beta_{TT}(F_{cool}, F_{in})T_{out} + \beta_{TC}(T_{out})C_{out} \\ &\quad + F_{in}T_{in} + \alpha(F_{cool})T_{cool}. \end{aligned}$$

- The concentration equation is linear and forced by C_{in}.
- The temperature equation is nonlinear because of the role of T_out in coefficient $\beta_{TC}(T_{out})$ multiplying C_{out}.

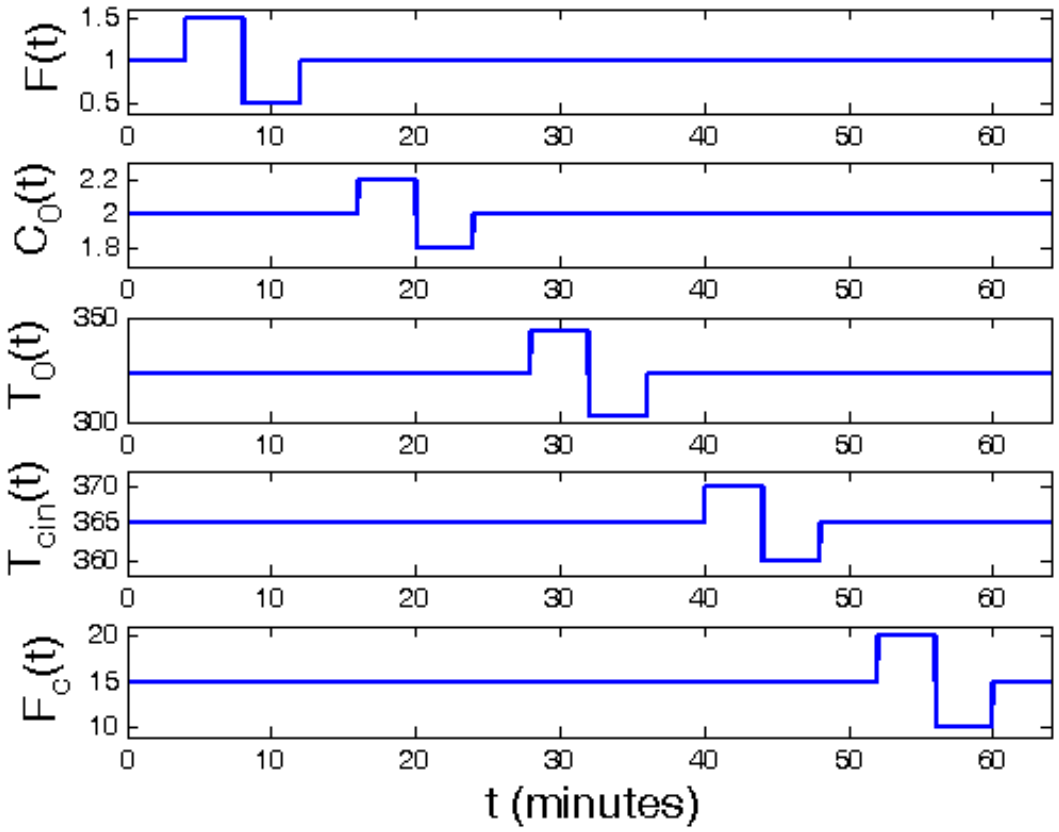
The tank reactor coefficients

- The dynamics of the system are controlled by these four coefficient functions:

$$\begin{aligned}
\beta_{CC}(T_{out}, F_{in}) &= \kappa \exp[-10^4 \tau(1/T_{out} - 1/T_{ref})] + F_{in} \\
\beta_{TT}(F_{cool}, F_{in}) &= \alpha(F_{cool}) + F_{in} \\
\beta_{TC}(T_{out}) &= 130\beta_{CC}(T_{out}, F_{in}) \\
\alpha(F_{cool}) &= aF_{cool}^{b+1}/(F_{cool} + aF_{cool}^{b}/2),
\end{aligned}$$

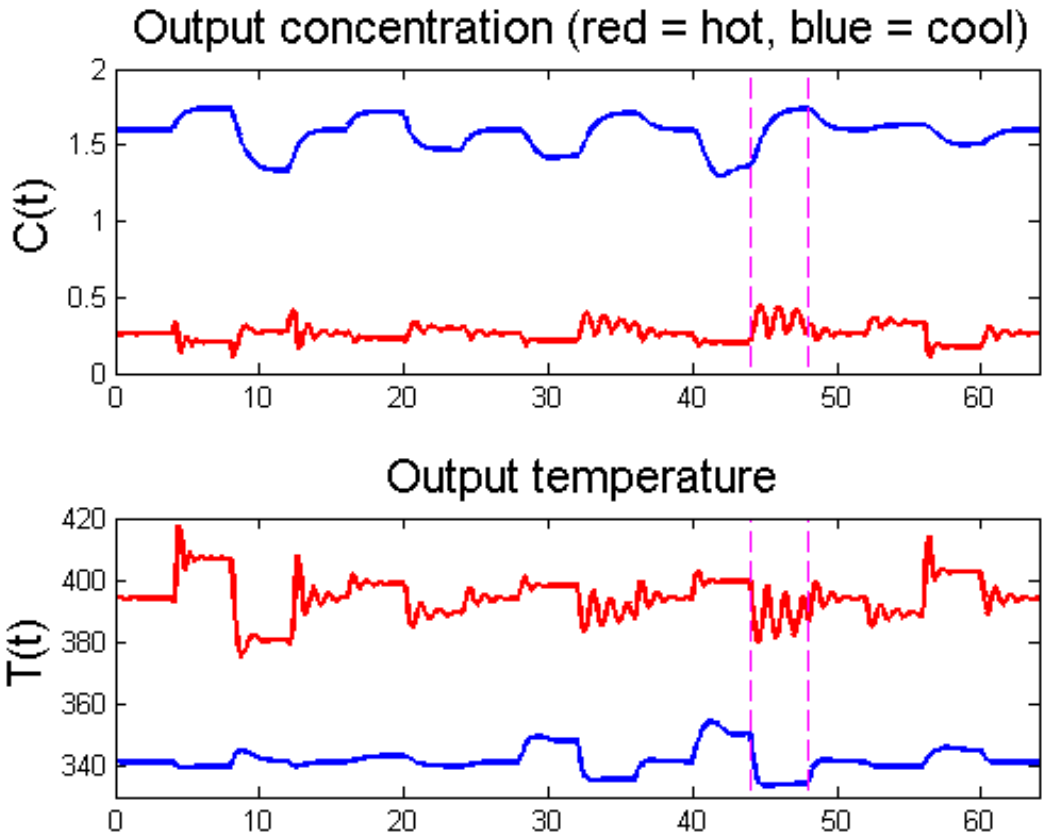
- These functions depend on two paired unknown parameters:
  - κ and τ
  - a and b

Tank reactor inputs



Each input in turn is stepped up, down and back to baseline.

Tank reactor outputs



The experiment is run at two coolant temperatures: hot and cool.

What we see

- When temperatures are moderate, the reactor responds smoothly to changes in input.
- But when temperatures are higher, sharp high frequency oscillations emerge, and are particularly troublesome for a change in coolant temperature.
- Can we predict reactor response at high temperatures from data collected and parameters estimated under the safer cool regime?
- Can we do this using only temperature measurements?

Outline

Results for the Fitzhugh-Nagumo equations

- The solution to be estimated was determined by $\{a, b, c\} = \{0.2, 0.2, 3\}$ and initial values $\{V(0), R(0)\} = \{-1, 1\}$.
- The paths were measured at 0.05 time units on the interval [0,20].
- Noise was then added to these values with standard deviation 0.5.
- 500 simulated samples were analyzed.

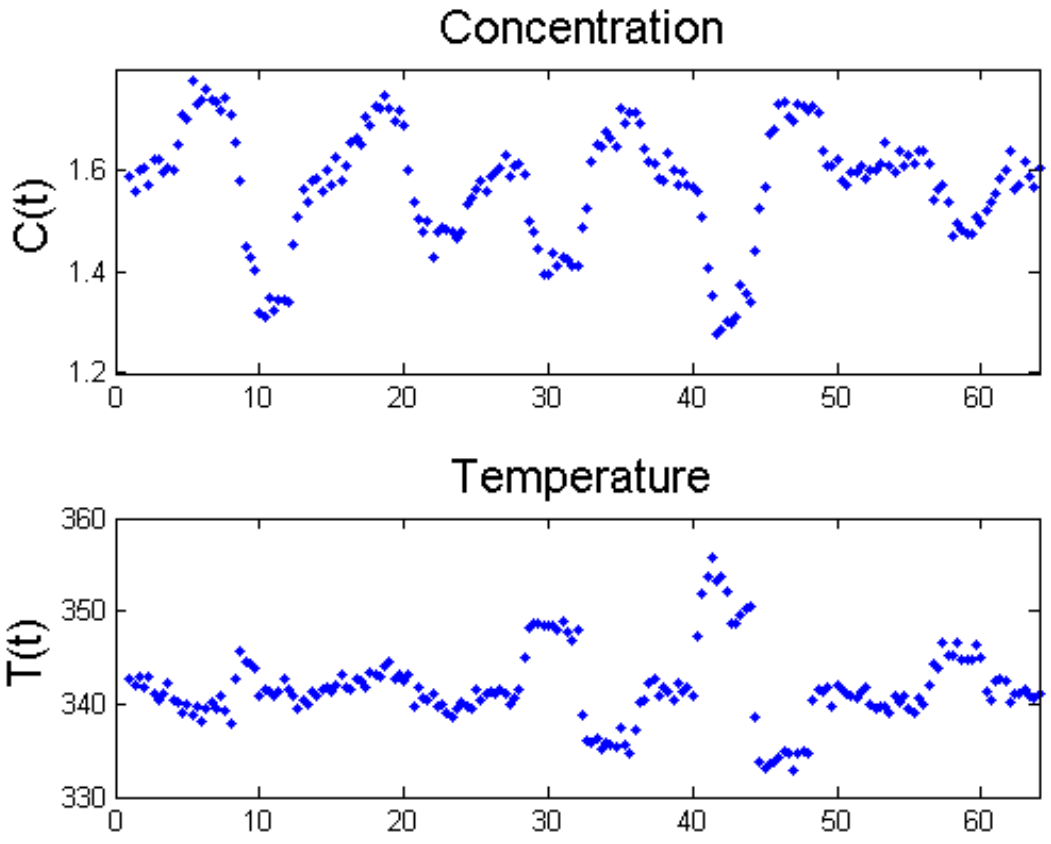
Summary statistics for parameter estimates

	a	b	c
True value	0.2000	0.2000	3.0000
Mean value	0.2005	0.1984	2.9949
Std. Dev.	0.0149	0.0643	0.0264
Est. Std. Dev.	0.0143	0.0684	0.0278
Bias	0.0005	-0.0016	-0.0051
Std. Err.	0.0007	0.0029	0.0012

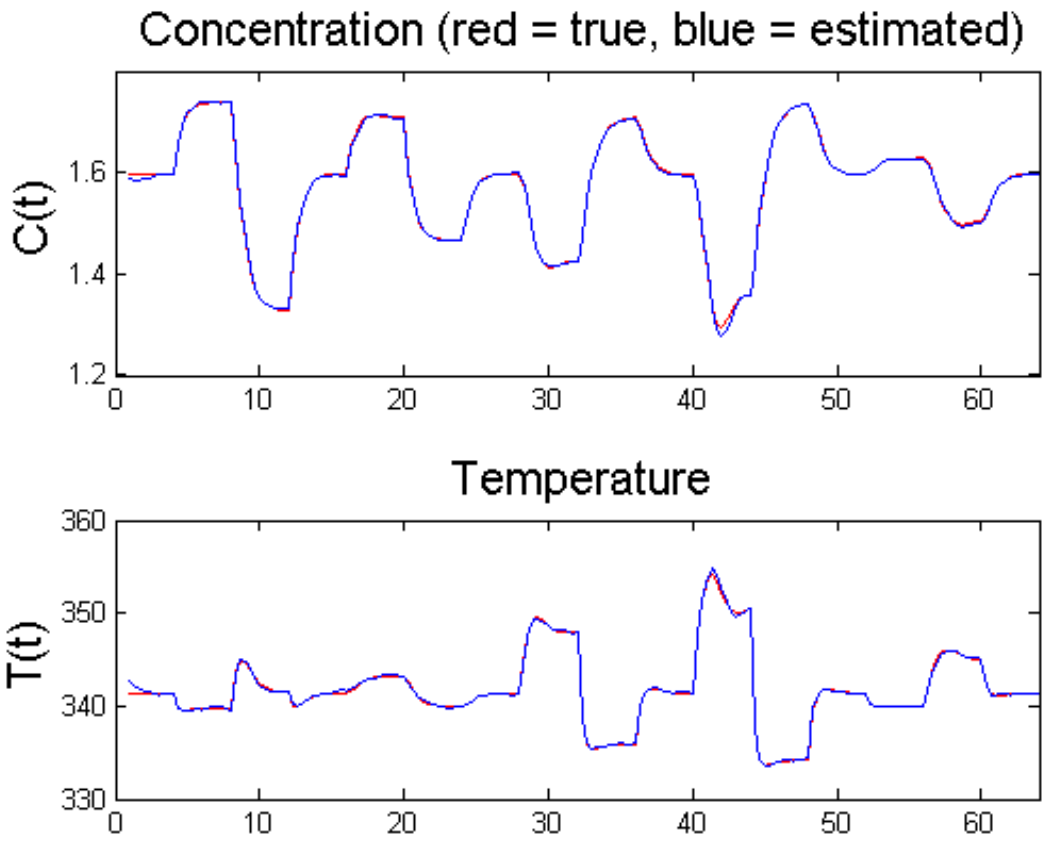
Simulations for the tank reactor equations

- Parameters and initial values for paths were set to those provided by a well known text on control engineering, T. E. Marlin (2000) *Process Control*. New York: McGraw-Hill.
- Parameter b is impossible to estimate because of its correlation with a, and therefore was fixed 0.5.
- 1000 simulated samples were analyzed.

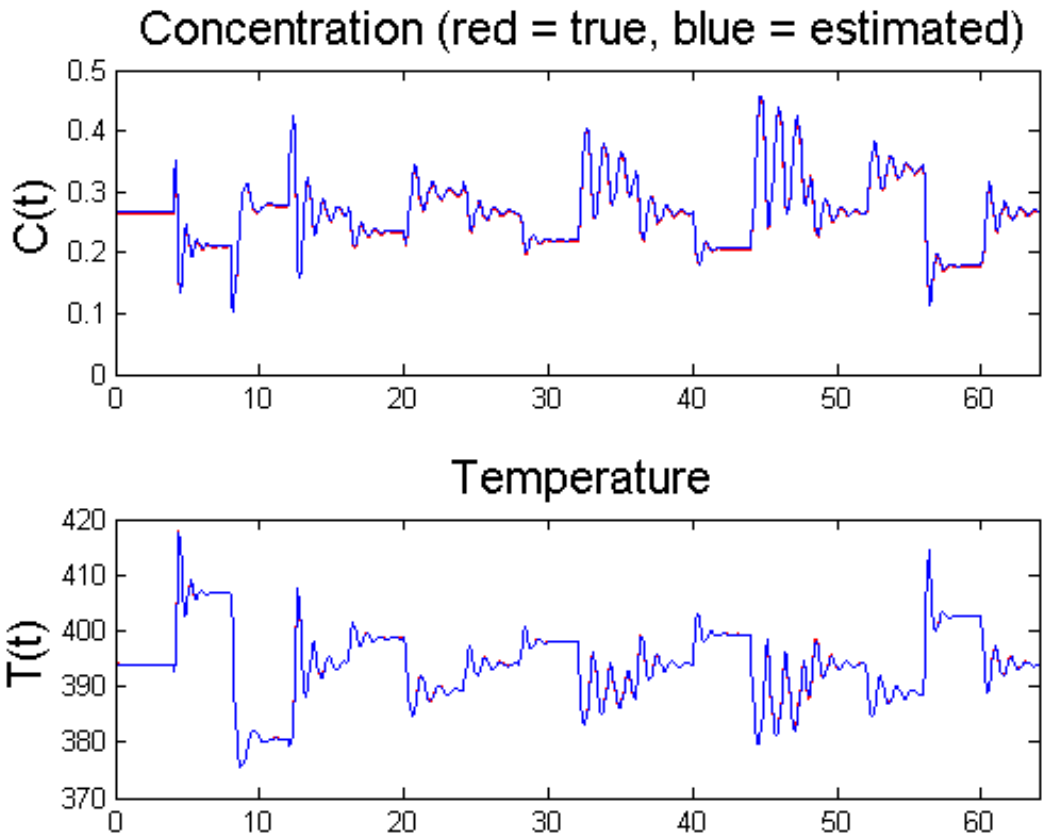
A typical set of tank reactor data



Path estimations, cool mode



Path estimations, hot mode



Data for only temperature collected in the cool mode were used.

Summary statistics for parameter estimates

	κ	τ	a
True value	0.4610	0.8330	1.6780
Mean value	0.4610	0.8349	1.6745
Std. Dev.	0.0034	0.0057	0.0188
Est. Std. Dev.	0.0035	0.0056	0.0190
Bias	0.0000	0.0000	-0.0001
Std. Err.	0.0002	0.0004	0.0012

Outline

The nylon experiment

- Nylon and other polymers are created by a chemical reaction in which molecules with two special types of endings chain together to form long molecules.
- The reaction requires water to form the molecules.
- The long molecules can also be broken up, releasing water.
- Temperature and water are critical control variables.
- There were five runs of the experiment at different temperature settings.
- These data were collected in the laboratory of Prof. K. MacAuley of the Dept. of Chemical Engineering at Queen's University, Kingston, Canada.
- The concentration measurements for variables A and C cost about \$30,000 to obtain.

The variables in the nylon equations

- A: molecules with an amine group end (measured)
- C: molecules with a carboxyl group end (measured)
- L: Nylon, a long chain of molecules (a polymer) (not measured)
- W: Water, indirectly adjusted in the experiment
- The variables are related by the mass balance equation

$$A + C \rightleftharpoons L + W$$

Nylon equations

$$DA = DC = -k_p(T)\left(CA - \frac{LW}{K_a(T)}\right)$$

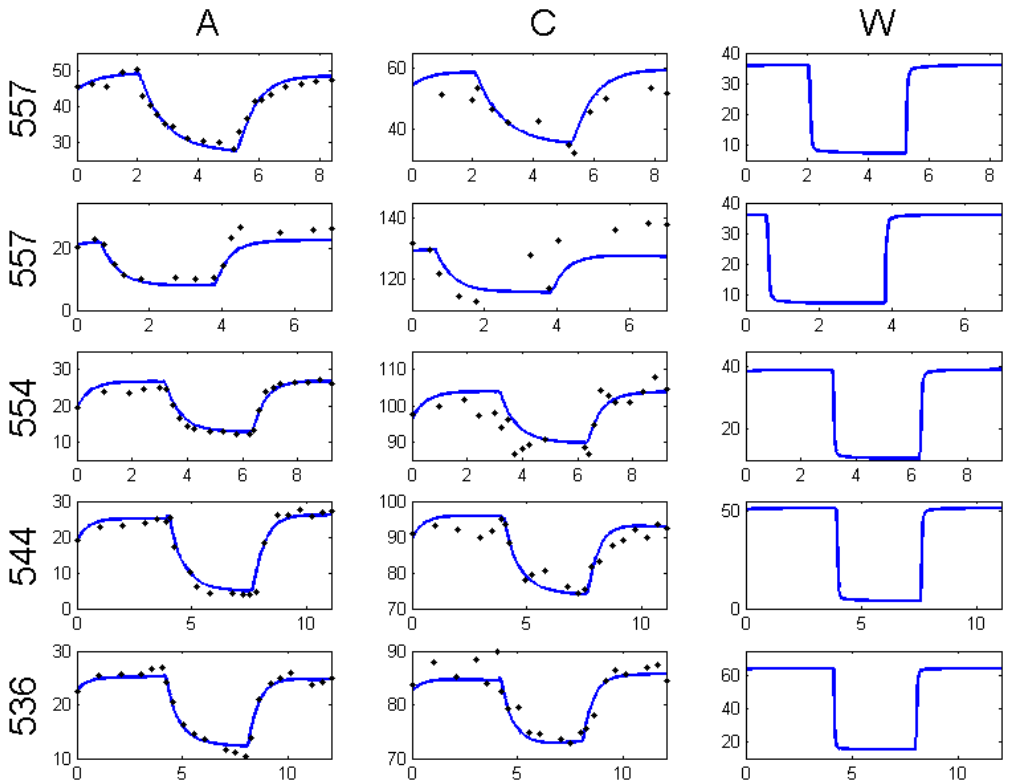
$$DW = k_p(T)\left(CA - \frac{LW}{K_a(T)}\right) - k_m\left(W - W_{eq}\right)$$

$$k_p(T) = k_{p0} \exp\left[-\frac{E}{R}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right]$$

$$K_a(T) = \left[\frac{1 + \alpha W_{eq}}{\gamma_w/\gamma_{w0}}\right] K_{a0} \exp\left[-\frac{\triangle H}{R}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right]$$

- variables and known constants are black
- parameters to be estimated are in red
- experimentally manipulated and measured constants and variables are in blue

Fits to the data



Outline

Software and resources

- All the results were computed in Matlab.
- Matlab functional data analysis software was also used. These and a set of software routines that may be applied to any differential equation is available from the URL: http://www.functionaldata.org.
- A paper is available from the URL: http://www.functionaldata.org.
- J. O. Ramsay and B. W.Silverman (2005) *Functional Data Analysis*, Second Edition. New York: Springer.