# Queen’s Chem Eng at a glance...

- 14 professors
  - » expanding to 17
- Chemical Engineering and Engineering Chemistry undergraduate programs
- 60 graduate students - 25% PhD
- 200+ undergraduate students
- Research groupings (for accreditation)
  - » Biochemical Engineering
  - » Polymers and Reaction Engineering
  - » Process Systems Engineering
    - – control/applied statistics

# Nonlinearity in Estimation and Control

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# Nonlinearity in Estimation and Control

Statistical Estimation

Control

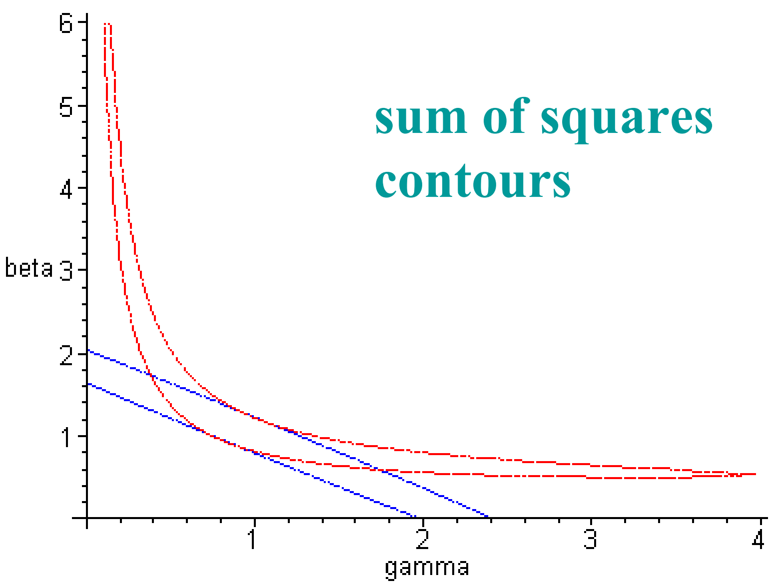
# Motivation

*Statistical Inference*

*Issue - reliability of conclusions*

- given estimated model for 1st order dynamic step response
- what is the plausible range for the gain, reciprocal time constant?
- linearization-based vs. likelihood interval
- different interpretation for example of Ross (1970)

$$Y = \beta\,(1 - e^{-\gamma\, t}) + \varepsilon$$



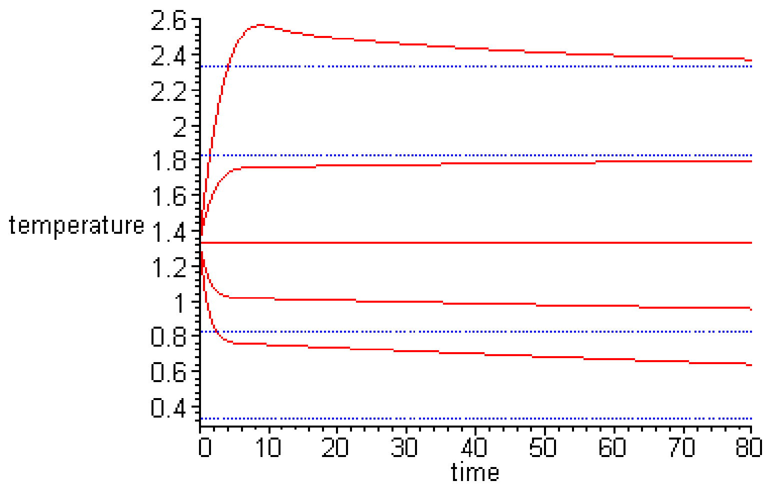

**sum of squares contours**

# Motivation

***Process Control***

*Issue - reliability of performance*

- linear controller on nonlinear process - proportional-integral controller - adjustments proportional to past and present tracking errors
- examine performance over range of setpoint changes




*variable setpoint tracking performance*

# Linearity

… is characterized by

Additivity

$$L(v_1 + v_2) = L(v_1) + L(v_2)$$

Scaling

$$L(k\,v) = k\,L(v)$$

**Nonlinearity is characterized by the *absence* of these properties.**

# Nonlinearity

…arises naturally in chemical process behaviour

» bulk flow - frequent source of bilinear terms

- energy $\propto$ flow * temperature
- material $\propto$ flow * composition

» chemical kinetics

- exponential dependence of rate on temperature - Arrhenius relationship
- polynomial dependence on composition - mass action kinetics

» saturation - reaching limits

- input - valve 100% open
- output - mole fraction of 1

# Questions

*1) What is the impact of nonlinearity on estimation and control?*

*2) How can we characterize the extent of nonlinearity in estimation and control?*

# Perspective

*At the statistical model-building stage, how does the model structure influence the final use of the model?*

- *parameters*
- *inputs*

# Outline

- Motivating Examples and Preliminaries
- Models in Statistical Inference and Process Control
- Nonlinearity and Its Impact in Statistical Inference, Estimation
- Nonlinearity and Its Impact in Process Control
- Summary

# The Model

Consider a general process model:

$$\mathbf{y} = \mathbf{F}(\mathbf{u},\theta) + \varepsilon$$

- **y** - response variables $\Leftrightarrow$ output variables - possibly functions of time
- **u** - explanatory variables $\Leftrightarrow$ inputs ("regressors") - possibly functions of time
- $\theta$ - parameters
- $\varepsilon$ - random shocks (noise) - e.g., i.i.d. normal but not necessarily
- **F(y,u,**$\theta$**)** may be a system of algebraic equations, or represented by a system of differential equations

# Roles of Models

***Statistical Inference***

- regressors (inputs) are fixed at a given design
- focus is on parameter-response (output) relationship

$$\mathbf{y} = \mathbf{F}(\mathbf{u},\theta) + \varepsilon$$

***Process Control***

- focus is on input-output (regressor-response) relationship
- parameters are considered fixed

$$\mathbf{y} = \mathbf{F}(\mathbf{u},\theta) + \varepsilon$$

# How Do We Select Model Structure?

- Frequently on the basis of physical understanding - mechanistic models
- use of empirical models guided by physical understanding, and empirical understanding of behaviour
  - e.g., yield relationship exhibits a maximum
    - » quadratic model required
  - e.g., process exhibits overdamped dynamic behaviour
    - » 1st order or higher-order overdamped model required

# How Do We Select Model Parameterizations?

- Parameterization selection frequently guided by physical understanding
  - » parameters that have a direct physical interpretation
- statistical inference
  - » model parameterization more flexible (!! or ??)
  - » e.g., Watts (1994) - issues in chemical eng. models
- process control
  - » model parameterization in the manipulated variable inputs strongly governed by MV's available
    - » **must be adjustable in plant**

# Example - Impact of Model Representation on Control

*The choice of variables used to model a stirred-tank reactor can have a significant impact on the* **internal** *behaviour, with significant implications for control design…*

# Example - Stirred Tank Reactor

- with first-order reaction
- non-isothermal with rapid temperature control - jacket temperature is manipulated variable input
- Calvet and Arkun (1988)

*parameterization in inputs and model parameters motivated by desire for dimensionless responses - conversion and dimensionless T*

$$\frac{dx_1}{dt} = -x_1 + Da(1-x_1)e^{\left(\frac{x2}{1+x2/\gamma}\right)} = r(x_1, x_2)$$

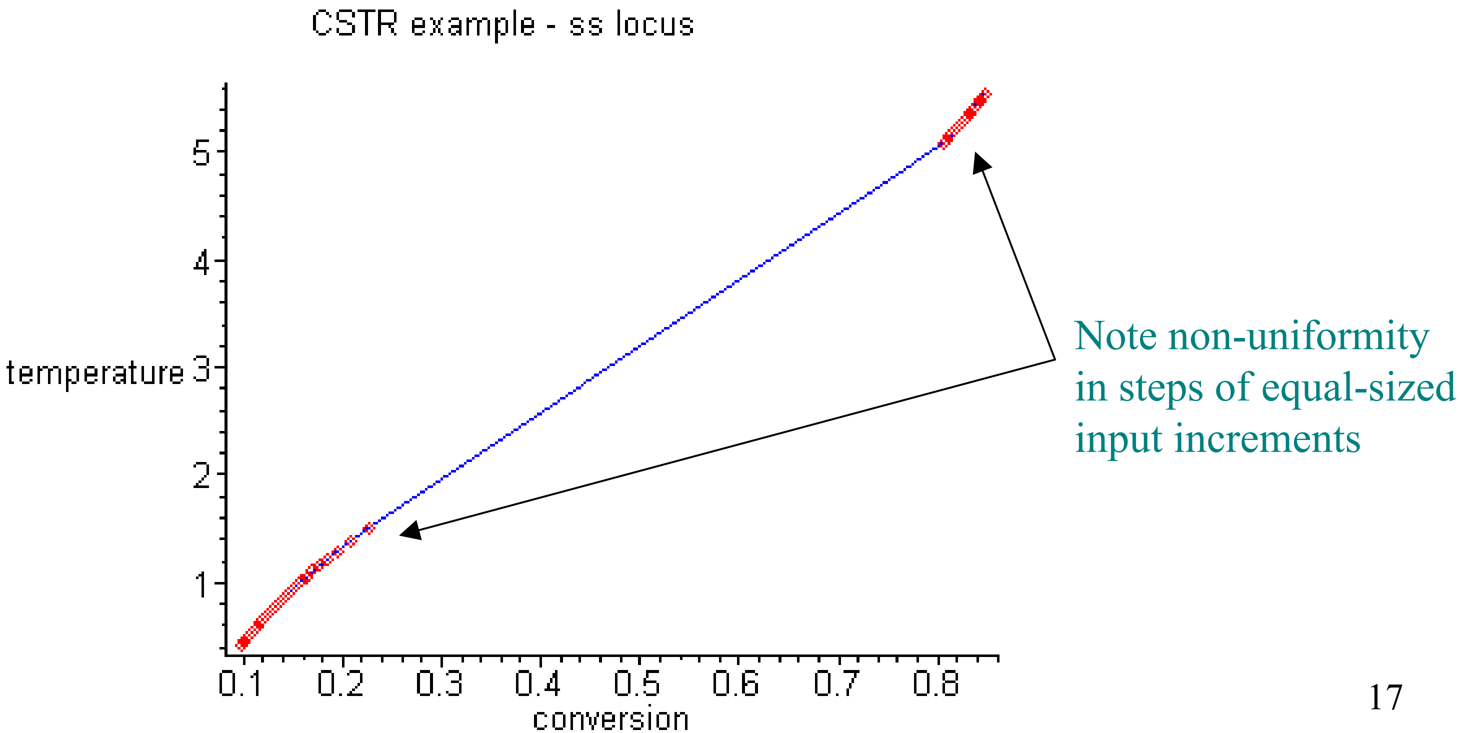
$$\frac{dx_2}{dt} = -x_2 + B\ Da(1-x_1)e^{\left(\frac{x2}{1+x2/\gamma}\right)} - \beta\,(x_2 - x_{2c0}) + \beta\ u$$

$$= enerbal(x_1, x_2, u)$$

# Stirred Tank Reactor

*Steady-state behaviour*

… through the coordinates of conversion and dimensionless temperature



## Stirred Tank Reactor - Alternative Representation

- conversion is a natural output
- how is conversion achieved?
  - » Instantaneous rate of conversion can be changed in time by adjusting the jacket temperature

*rate of conversion*

*change in rate of conversion with time*

$$\frac{dx_1}{dt} = r$$

$$\frac{dr}{dt} = \frac{\partial r}{\partial x_1} r(x_1, x_2) + \frac{\partial r}{\partial x_2} enerbal(x_1, x_2, u)$$

  - » temperature is expressed in terms of $x_1$, r

**Consider this as a change of coordinates...**

# Stirred Tank Reactor - Alternative Representation

- represents a transformation of response space

$$(conversion, temperature) \rightarrow (conversion, rate\, of\ \ conversion)$$

- dynamic structure of model is converted to an integrating form *however* **behaviour** remains the same

**behaviour** $\equiv$ **u** $\rightarrow$ **conversion**

*cf., natural integrating structure of mechanical systems:*
*- force→ acceleration-velocity-position*

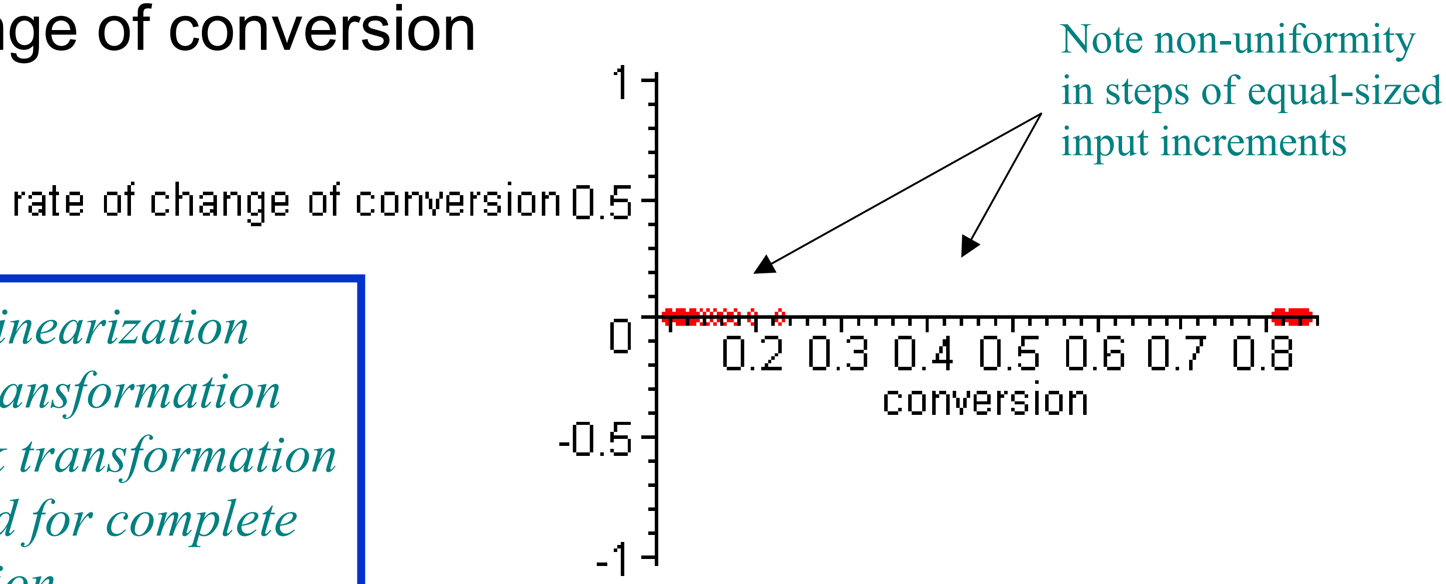
» internal variables have changed

- cf., realizations of dynamic systems

# Stirred Tank Reactor

*Steady-state behaviour*

… through the coordinates of conversion and rate of change of conversion




*(partial) linearization by state transformation - feedback transformation is required for complete linearization*

*Conclusion - coordinates in which physical behaviour is described influence degree of nonlinearity in model behaviour description.*


Nonlinearity in
Statistical Inference

# Statistical Inference

Interested in:

- ***inferences about parameters***

  » range of plausible values

  » explanatory power of associated model term

  – inclusion in model?

  » Physical interpretation of parameter estimate

  – e.g., adsorption constant in reaction kinetic scheme

# Statistical Inference

- ***inferences about model predictions***
  - » precision of predictions
  - » assessment of plausible values
    - – e.g., efficacy of a treatment
  - » generalization -functions of parameters
- ***inferences about model structure***
  - » finding the correct structure to explain behaviour
  - » model discrimination - link to regressors
- ***impact of model structure on estimation***
  - » identifiability / estimability

# Impact of Nonlinearity on Statistical Inference

Focus - nonlinearity in the parameters (regressors are fixed)

Possible points of impact:

- estimation - numerical conditioning - convergence
- inference
  - reliability of linear approximation methods
  - rate at which asymptotic properties are achieved
- identifiability/estimability
- distinctions - intrinsic and parameter-effects curvature

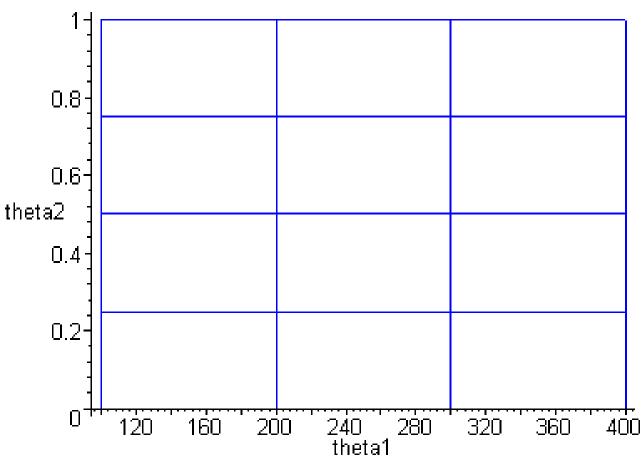
*Nonlinearity in the parameters is reflected in the curvature of the expectation surface...*

# Expectation Surface

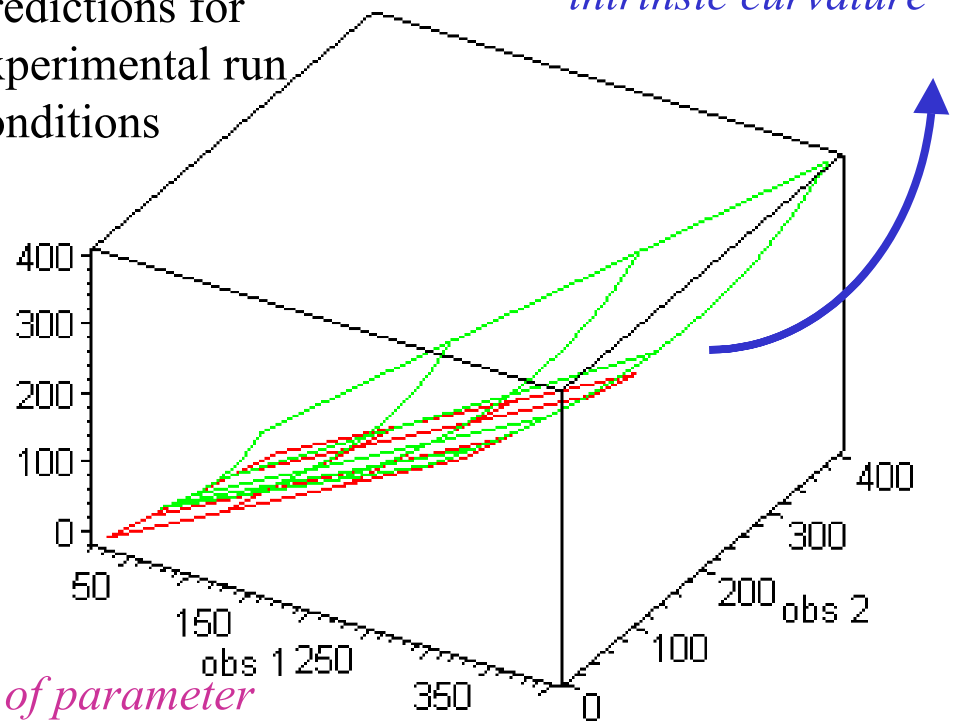
… in observation space

*bending of surface associated with intrinsic curvature*

Parameters




Predictions for experimental run conditions



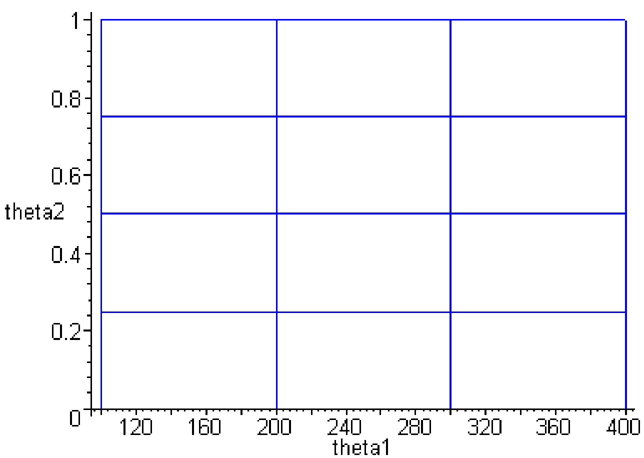

*non-uniformity of parameter lines on surface associated with parameter-effects curvature*

# Nonlinear Least Squares Estimation

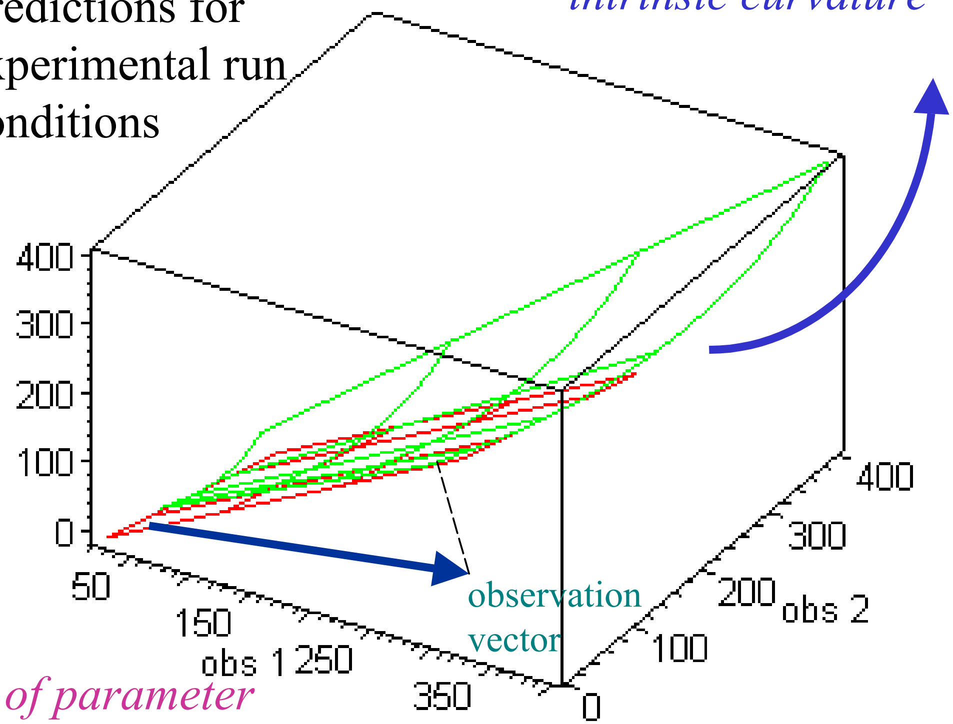
… relies on projection of observation vector to expectation surface

*bending of surface associated with intrinsic curvature*

Parameters




Predictions for experimental run conditions




*non-uniformity of parameter lines on surface associated with parameter-effects curvature*

# Linear Approximation

Success will depend on

» extent to which tangent plane approximates surface

- depends on bending of surface in observation space

» uniformity of coordinatization on surface

- link back to parameter space
- depends on uniformity of spacing and bending of coordinate lines on the surface

## Example - Impact of Parameterization on Statistical Inference

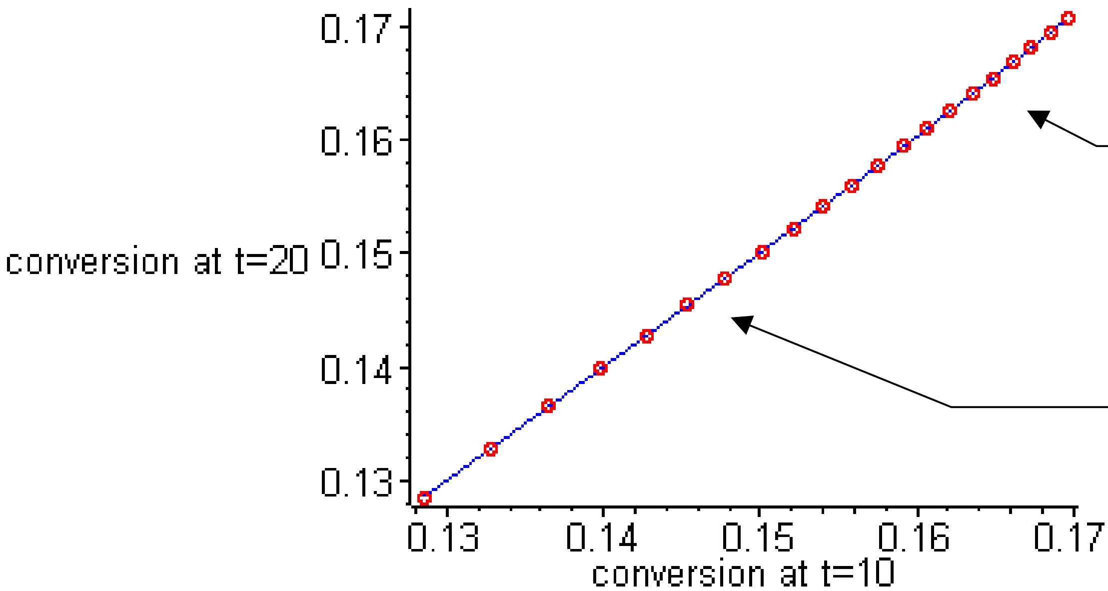
*The choice of parameters for estimation in a stirred-tank reactor can have a significant impact on the* **expectation surface** ...

# Example - Stirred Tank Reactor

Expectation surface for responses at time = 10, 20

» parameter varied is $\gamma$

expectation surface parameterized by gamma (t=10,20)



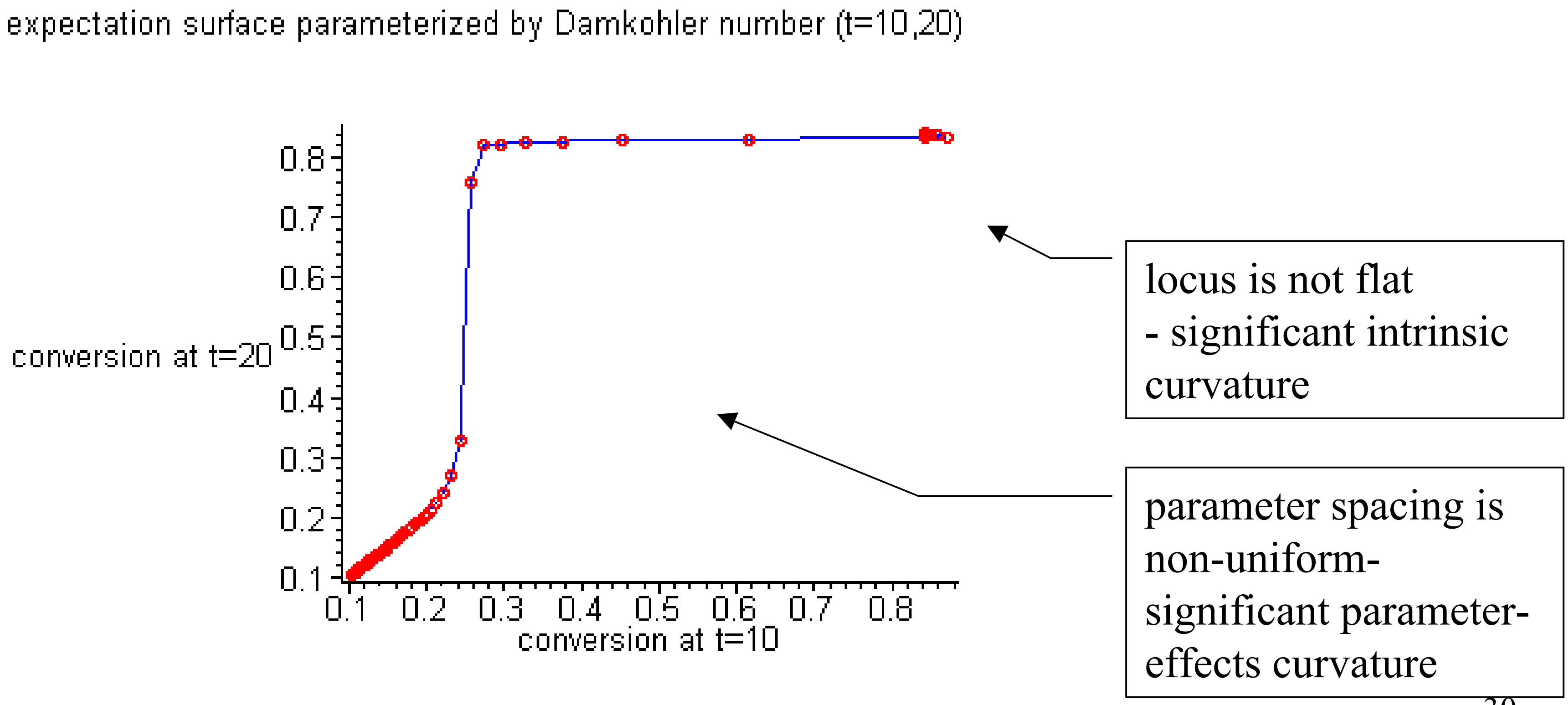

locus is almost flat - negligible intrinsic curvature

parameter spacing is non-uniform- significant parameter-effects curvature

# Example - Stirred Tank Reactor

Expectation surface for responses at time = 10, 20

» parameter varied is Da



# Example - Stirred Tank Reactor

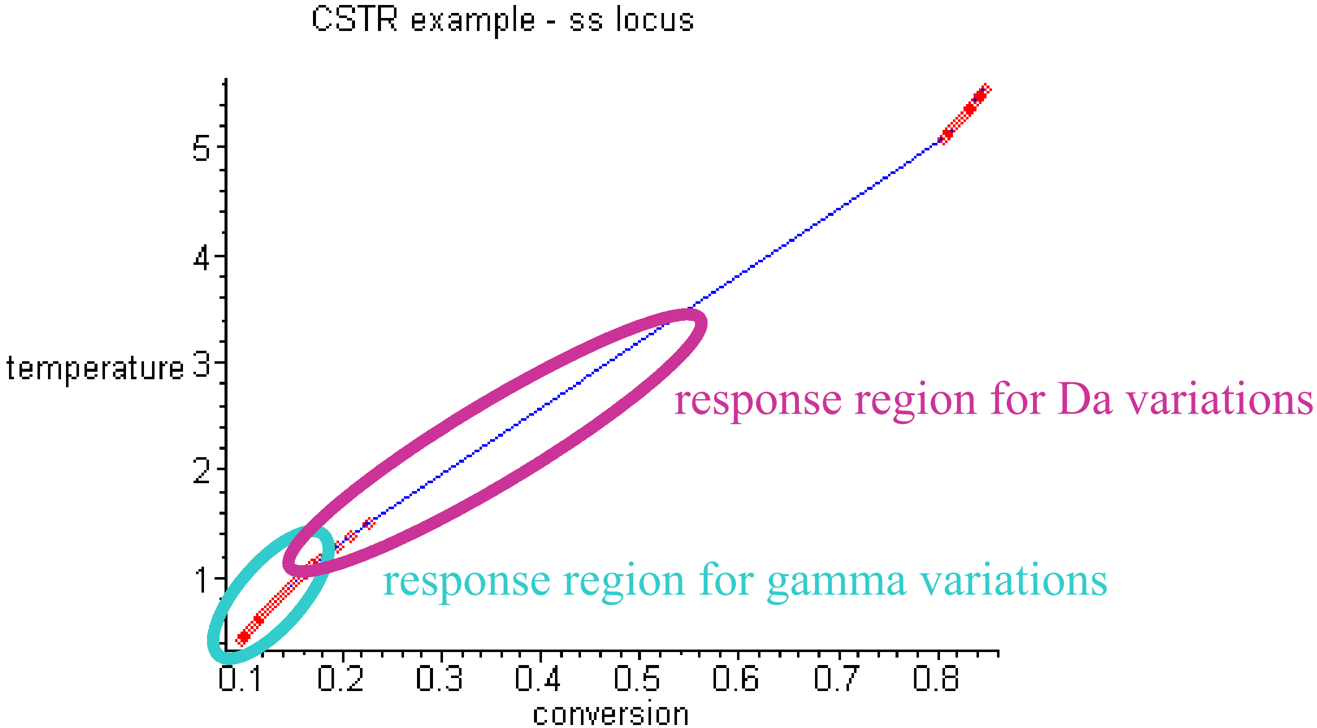
$$\frac{dx_1}{dt} = -x_1 + Da(1 - x_1)e^{\left(\frac{x_2}{1 + x_2/\gamma}\right)} = r(x_1, x_2)$$

$$\frac{dx_2}{dt} = -x_2 + B\ Da(1 - x_1)e^{\left(\frac{x_2}{1 + x_2/\gamma}\right)} - \beta(x_2 - x_{2c0}) + \beta u$$

$$= enerbal(x_1, x_2, u)$$

# Example - Stirred Tank Reactor

- Issue - change in characteristics of steady-state
  - » solution now tends to significantly different equilibrium

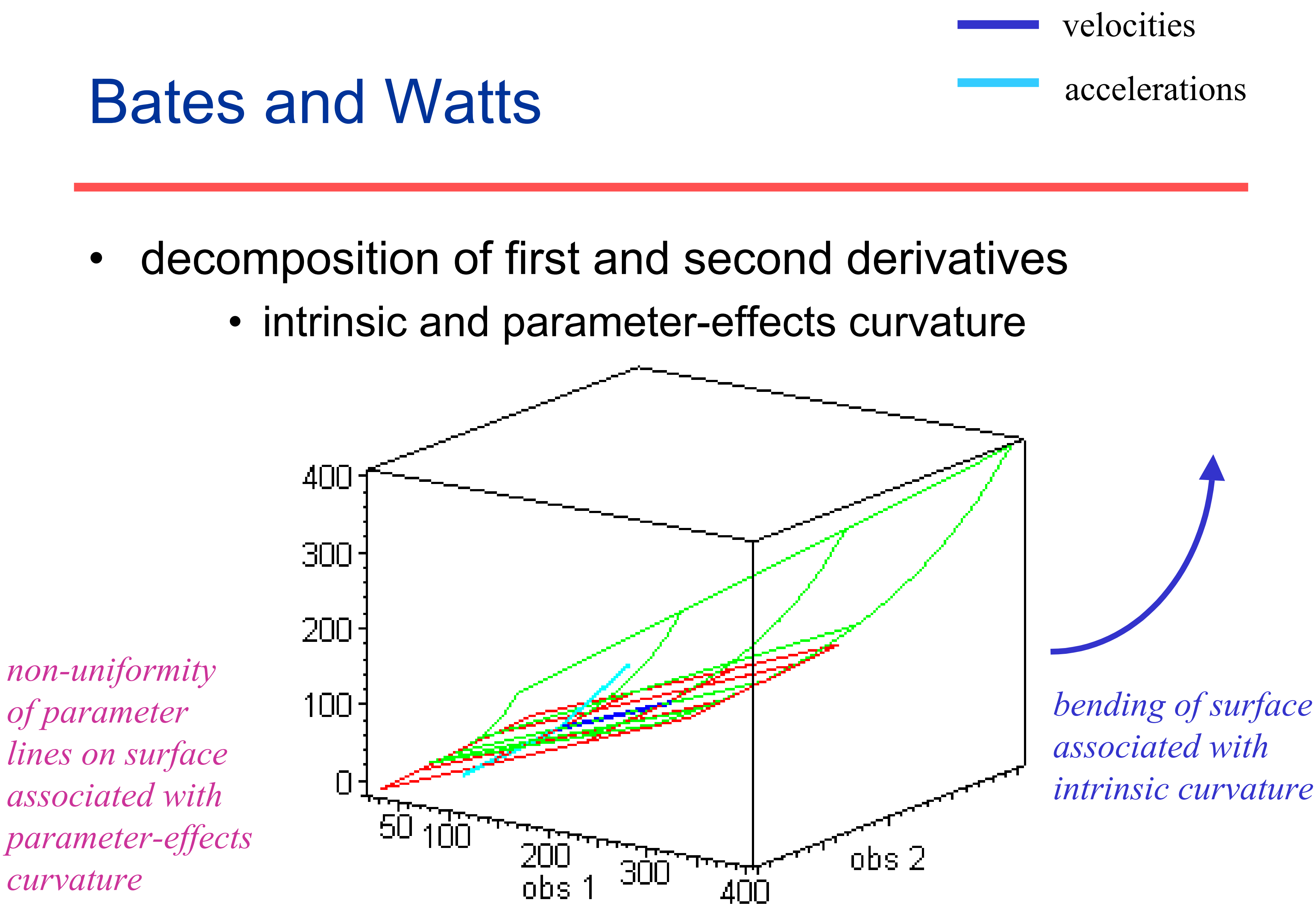


# Quantifying Nonlinearity in Statistical Inference

- Beale (1960)
  - » examine difference between linear approximation, nonlinear model
  - » 4 measures
- Bates and Watts (1980, 81)
  - » derivative-based methods - dissection of derivatives
  - » profile t-plots and traces
- Cook and Weisberg (1990) - confidence curves
- M.J. Box - bias (1971)
- Efron/Amari - statistical manifolds

# Bates and Watts

- decomposition of first and second derivatives
  - intrinsic and parameter-effects curvature



# Bates and Watts Curvature Measures

- based on decomposition of second derivative information
- given expectation surface mapping

$$\eta(\theta) = \begin{bmatrix} f(\mathbf{x}_1, \theta) \\ \vdots \\ f(\mathbf{x}_N, \theta) \end{bmatrix}$$

- velocity vectors span tangent plane approximating surface

$$\mathbf{V} = \frac{\partial \eta(\theta)}{\partial \theta'}$$

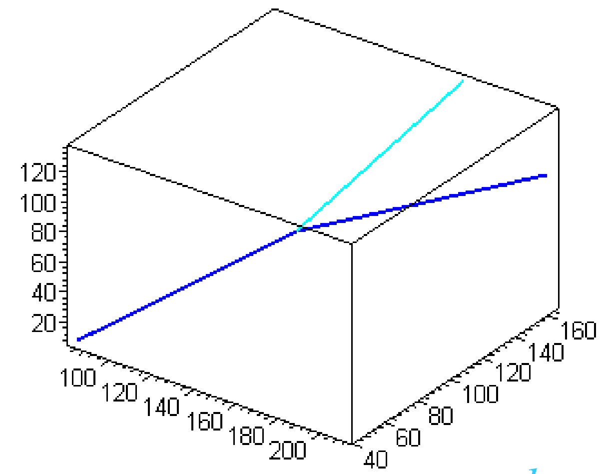
- acceleration vectors contain information about both parameter-effects and intrinsic curvature

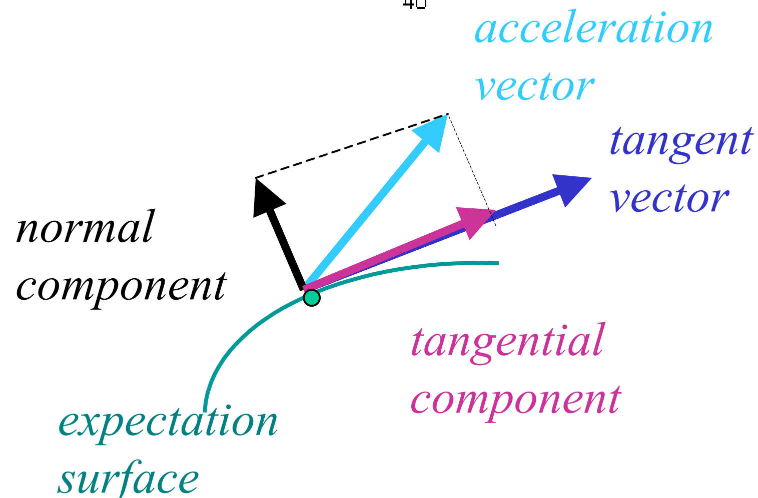
$$\ddot{\mathbf{V}} = \frac{\partial \eta(\theta)}{\partial \theta \, \partial \theta'}$$

# Bates and Watts Curvature Measures

Decompose acceleration vectors into components tangential and normal to the surface

- » apply a QR decomposition to velocity and acceleration vectors - achieve orthogonal basis
- » first p columns span tangent plane
- » first p coordinates of transformed acceleration vector represent tangential component of given acceleration
- » next p(p+1)/2 components represent normal component of given acceleration



# Bates and Watts Curvature Measures

- parameter-effects curvature
  - » associated with tangential curvature
  - » assess from tangential component of accelerations
- intrinsic curvature
  - » associated with normal curvature
  - » assess from normal component of accelerations
  - » independent of model parameterization
- these curvatures can be assessed in specific directions, or over all directions - RMS curvature
- normalize against first-order effects - Jacobian
- benchmark - RMS curvature
  - » value of 0.3 represents significant curvature - 15% deviation 1 unit away from point of linearization

$$\frac{\left\| \mathbf{h}' \ddot{\mathbf{V}} \mathbf{h} \right\|}{\left\| \dot{\mathbf{V}} \mathbf{h} \right\|^2}$$

# Bates and Watts Curvature Measures

## Scaling

- natural scaling implied by variance of random shocks (normally distributed)
- multivariate normal distribution justifies use of standard (Euclidean) metrics
- scaling becomes a significant issue in control nonlinearity assessment

# Extensions

- Subset curvatures - Cook and Goldberg (1986)
  - » restriction to subsets of parameters
- Marginal curvatures - Kang and Rawlings (1998)
  - » individual parameters
- nonlinearity of time series models
  - » Lam and Watts (1991) - profile plots
  - » Ravishanker (1994) - relative curvatures
  - » proximity of roots to stability/inversion boundary - Quinn, Bacon and Harris (1999)
- graphical tools
  - » profiling (Bates and Watts, 1988), and others

# Using these tools

- Guides - reliability of linearization-based inference
- possible reparameterization
  - » reduce parameter-effects nonlinearity - impact on parameter inference regions
- corrections for intrinsic curvature
- investigation of small-sample behaviour
  - » e.g., bias


Nonlinearity in
Process Control

# Process Control

Interested in :

- ***Stability***
  - » does the response of the process stay within limits when bounded changes are introduced?
- ***Impact***
  - » how sensitive are the outputs to changes in inputs
- ***Control Configuration***
  - » how are manipulated variables to be used to adjust responses?
- ***Control Algorithms***
  - » computation of MV adjustments given measurements

# Impact of nonlinearity on process control

***Safety***

» qualitative nature of dynamics can change - stable/unstable points of operation

- e.g., fluidized-bed ethylene reactor

» gain reversals - direction of response to mv actions changes

***Performance***

» degradation - with linear controller, consistent performance may not be achievable over operating range

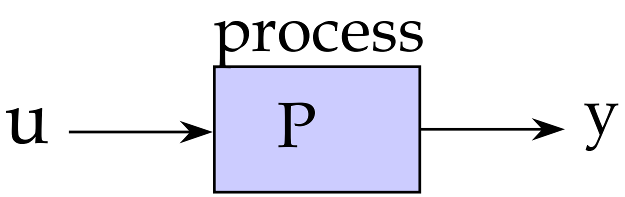
- e.g., batch reactors, multi-grade processes

# Control Relationships of Interest

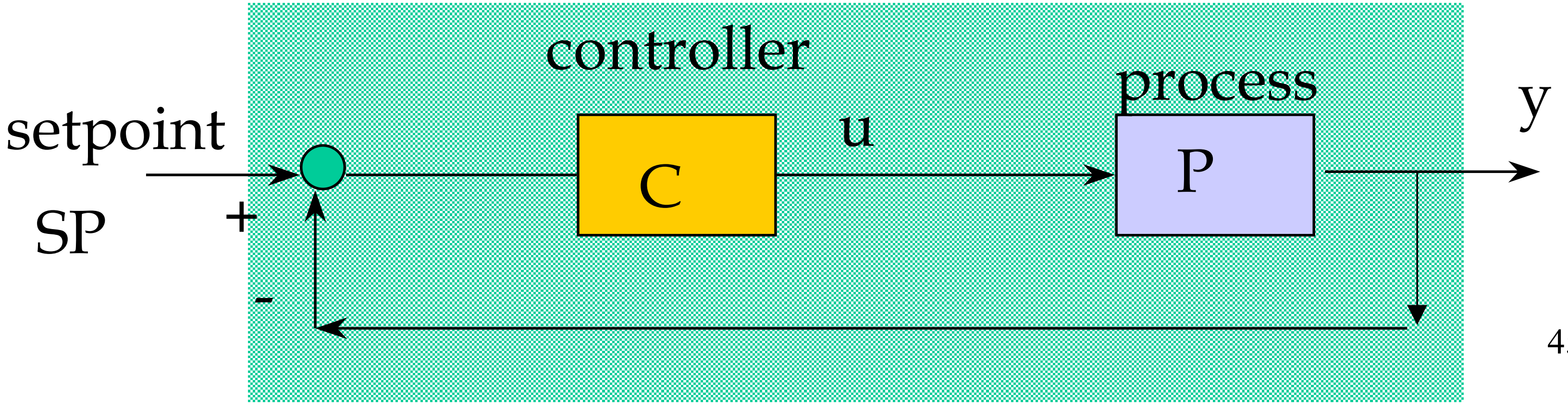
- Manipulated variable input - output
- disturbance input-output
- setpoint-output - ***closed-loop***
  - » inherently linear ***steady-state*** relationship, since ideally it is the identity relationship - we get what we ask for

# Approaches for Assessing Control Nonlinearity

Open-Loop Process




Closed-Loop Process



# Approaches for Assessing Control Nonlinearity

***Open-Loop***

- focus on MV input - CV output behaviour without control present

***Closed-Loop***

- focus on behaviour with controller present
  - » output measurement to MV
  - » setpoint target to output

# Focusing on Process Behaviour

Steady state

- ultimate goal in many instances
- exception - batch operation

Dynamic

- transition from one operating point to another
- particularly important for multi-product plants
- safety considerations - stability - change in approximate relationship that can lead to closed-loop instability
- disturbance rejection

# Open-Loop Assessment of Nonlinearity

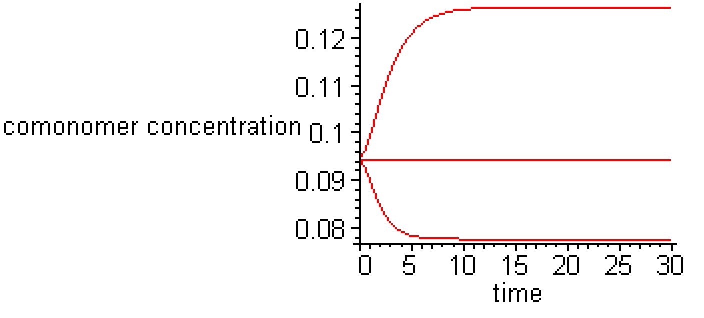
Approaches

- linearity properties -
  - » scaling and additivity
- changes in linear approximations
  - » Ogunnaike et al. (1993)
- deviations of linear approximations from full nonlinear behaviour
- curvature assessment using derivative information

# Open-Loop Assessment of Nonlinearity

Visual confirmation - *Response Symmetry*

- study process response to set of symmetric input changes - e.g., step inputs
- consequence of scaling property




- indication of
  - » gain nonlinearity - ultimate change - steady state behaviour
  - » dynamic nonlinearity - e.g., in speed of response or character - over/under-damped

# Open-Loop Assessment of Nonlinearity

Correlation properties

- » higher-order moments
- » spectral behaviour
- » necessary conditions, but not sufficient to guarantee nonlinearity

Changes in Linear Approximations

- » Ogunnaike et al. (1993) - for steady state problems
- » examine changes in linear approximations (gains) over operating region
- » infer nonlinearity from extent of changes in local linear behaviour

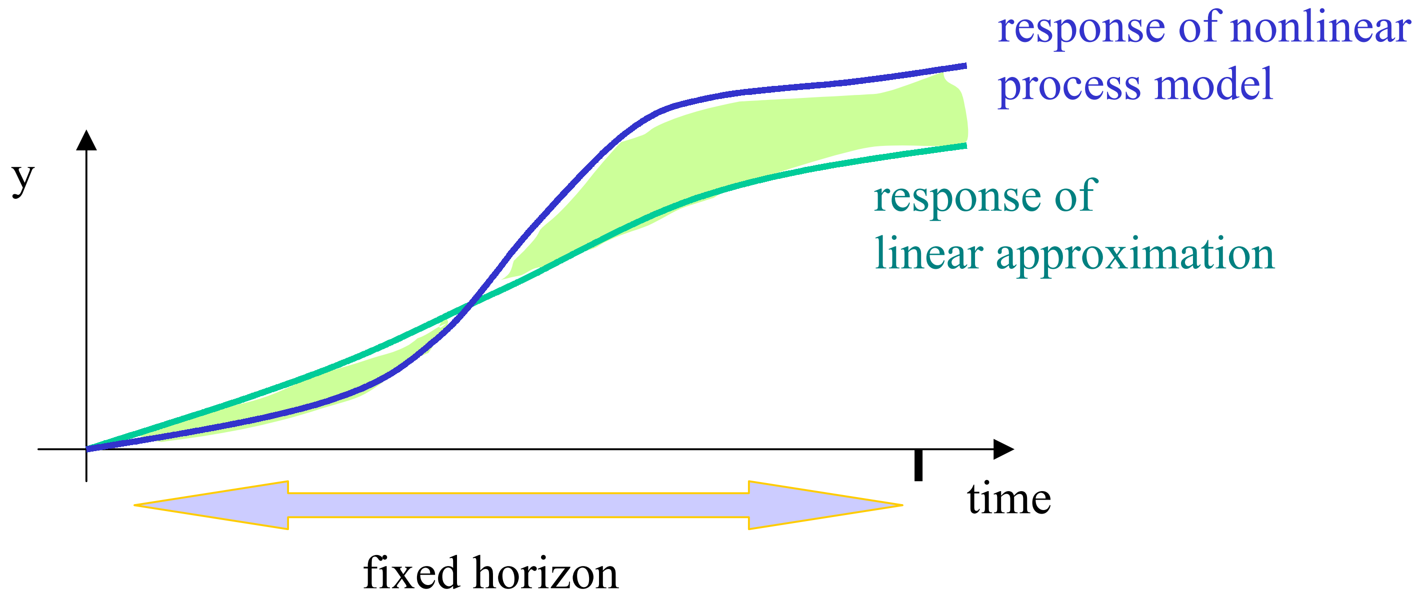
# Open-Loop Assessment

Closeness to Linear Systems

» systematic application by Allgower (1995)

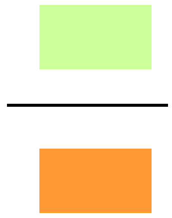
» based on measure of closeness proposed by Desoer and Wang (1981)

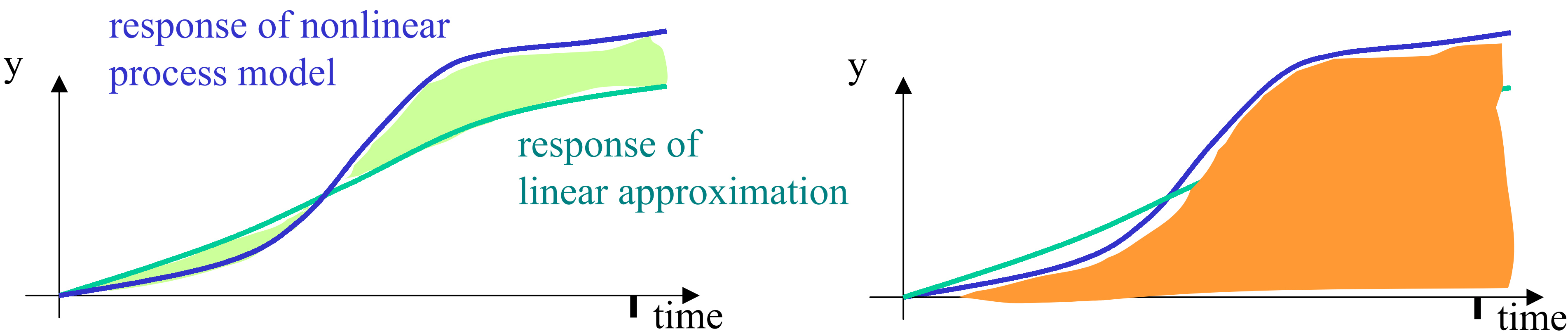
» similar definitions considered by Nikolaou (1994)



# Open-Loop Assessment

$$\underset{\substack{\text{all linear}\\ \text{approx.}}}{\text{smallest}} \left( \underset{\substack{\text{all input}\\ \text{signals}}}{\text{worst}} \frac{\left\| \text{linear approximation error} \right\|}{\left\| \text{size of process response} \right\|} \right) =$$





# Open-Loop Assessment

$$\inf_{g \in G} \sup_{u \in U} \frac{\left\| g(u) - P(u) \right\|_{py}}{\left\| P(u) \right\|_{py}}$$

- » normalization by response, or input
- » ***smallest approximation error over all linear approximations, for the worst-case input signal***
- » normalization by response or input
- » analogies to measures of Beale
- » departure from linear approximation (Taylor series)

# Open-Loop Assessment

Derivative-based approach

$$\frac{\left\| d^2 P(u) \right\|}{\left\| dP(u) \right\|^2}$$

- Guay, McLellan and Bacon 1996, 1997
- extension of Bates and Watt's methodology to control context
- decomposition of second-order derivative information, relative to first-order derivatives
- steady-state curvature - derivatives of steady-state map
- dynamic curvature - derivatives of process operator
- scaling - based on outputs or inputs
- interpretation - based on approximation deviation

# Open-Loop Assessment

Derivative-based approach

» **steady state**

- examine derivatives of steady state map

$$\frac{\left\|\mathbf{h}'\ddot{\mathbf{V}}\mathbf{h}\right\|}{\left\|\dot{\mathbf{V}}\mathbf{h}\right\|^2}$$

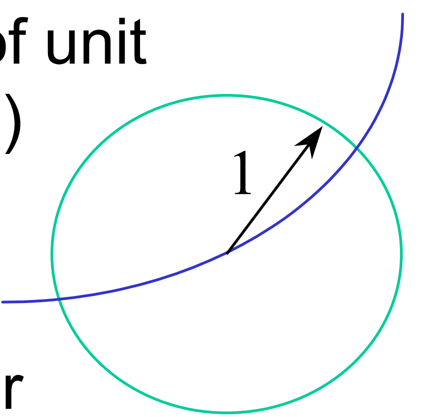
» **dynamic**

- compute over family of inputs - e.g., step changes
- use sensitivity differential equations to compute instantaneous first and second-derivatives of the states with respect to the inputs
- integrate instantaneous sensitivities to obtain dynamic curvature

$$\sqrt{T}\,\frac{\sqrt{\int_0^T \left\|\mathbf{h}^T \frac{\partial^2 \mathbf{y}(t)}{\partial \mathbf{u}\,\partial \mathbf{u}^T}\mathbf{h}\right\|^2 dt}}{\int_0^T \left\|\frac{\partial \mathbf{y}(t)}{\partial \mathbf{u}^T}\mathbf{h}\right\|^2 dt}$$

# Steady-state measure - scaling

- **magnitude of curvature depends on choice of scaling of outputs or inputs**
- output prescribed scaling
  - » implies an associated region in input space specified by inverse of process map
    - – identify through linearization - gain matrix
  - » measure RMS curvature relative to region of unit norm in output space (similarly, input space)
    - • value of 0.3 ⇔15% deviation



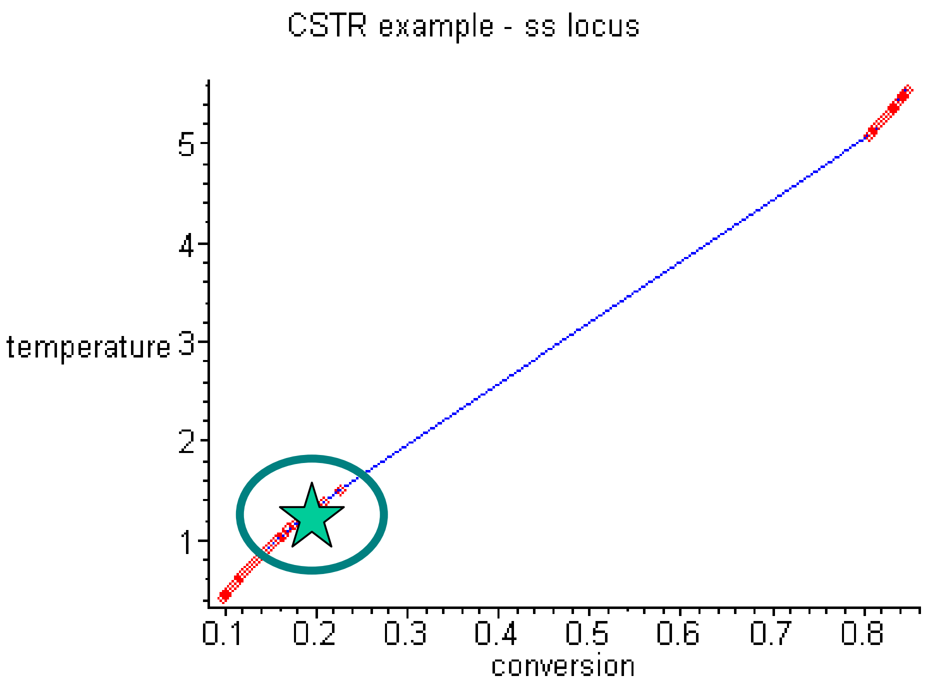

- dynamic case
  - » scaling achieved by “scaling operator” - filter

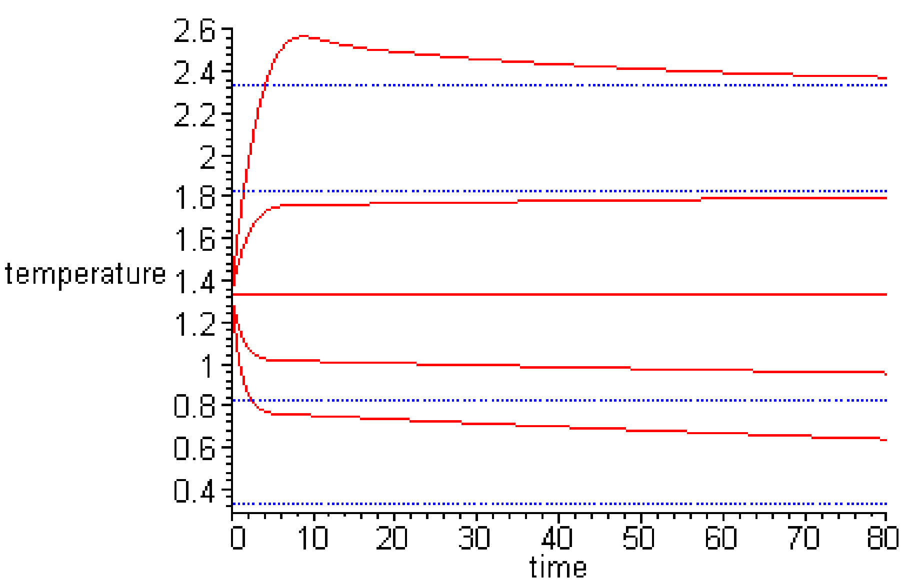
# Example - Stirred Tank Reactor

Steady-state RMS curvature = 1.74

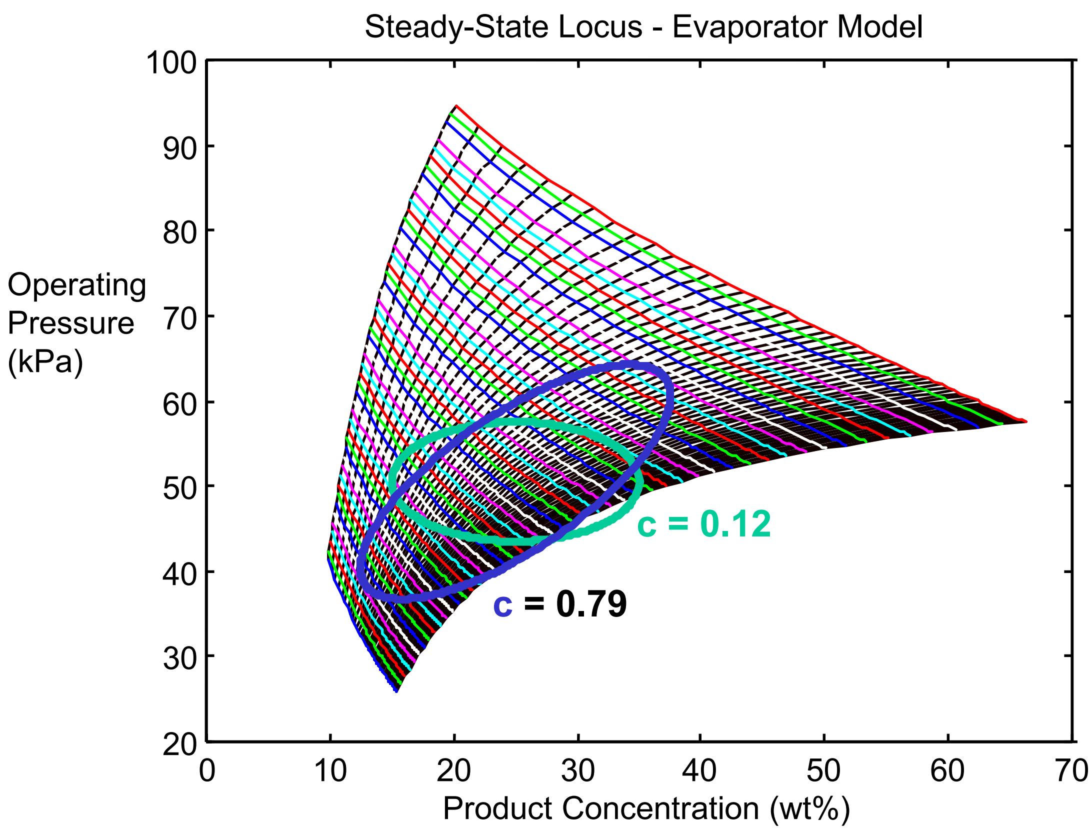
» tangential relative curvature = 1.73

» normal relative curvature =  0.12



# Example - Evaporator




## Effect of Scaling

Size and Orientation

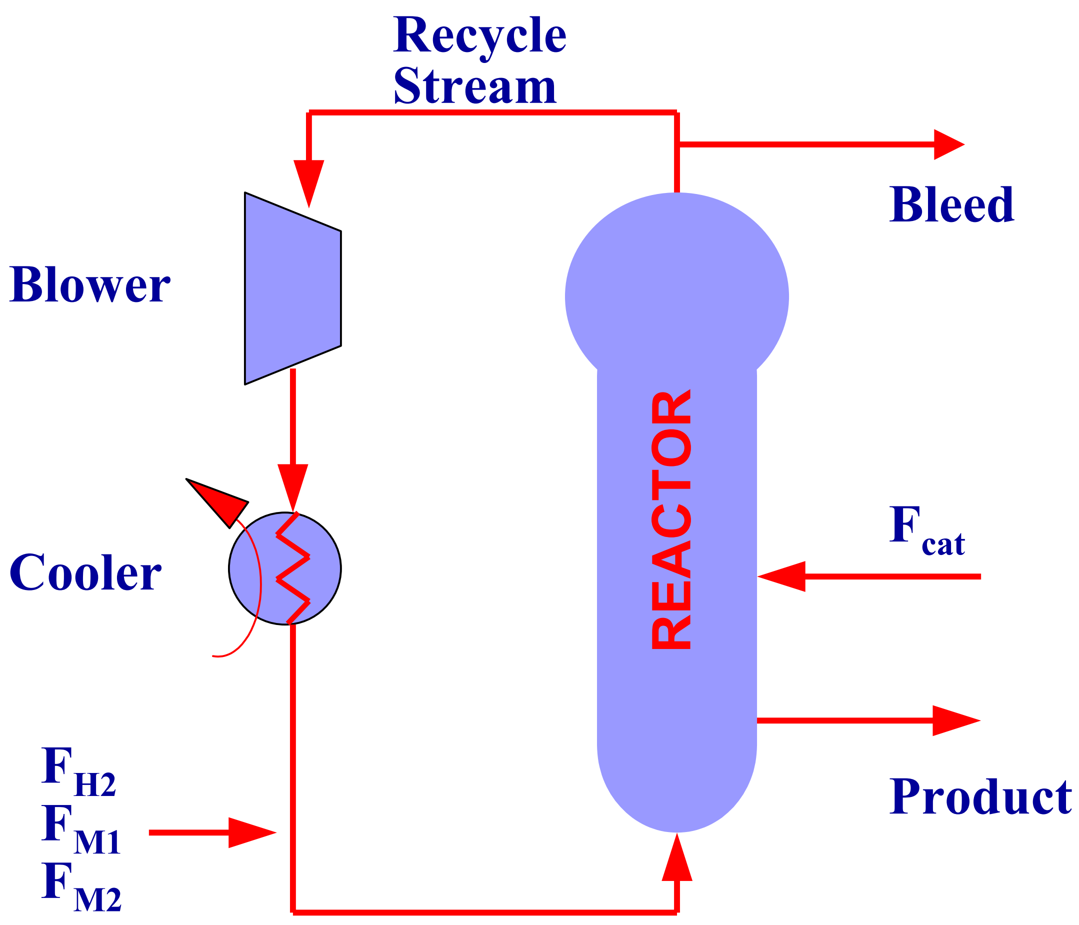
1. Diagonal Scaling Matrix c=0.12

2. Scaling matrix aligned with process gain c=0.79

from Guay et al. (1997)

*Care must be taken in specifying the magnitude and orientation of the region of interest. Poor specifications can lead to misleading indications of curvature.*

# Example - Polyethylene Reactor



# Polyethylene
# Gas Mass Balance Model

mv input

response

(McAuley, 1991)

$$\frac{d[H_2]}{dt} = \frac{1}{Vg}\left(F_{H2} - k_h Y [H_2] - \frac{[H_2]\cdot b}{C_t} - gl\cdot[H_2]\right)$$

$$\frac{d[M_2]}{dt} = \frac{1}{Vg+Vs}\left(F_{M2} - k_{p_2} Y [M_2] - \frac{[M_2] b}{C_t} - S[M_2] Y (k_{p1}[M_1] mw_1 + k_{p2}[M_2] mw_2)\right)$$

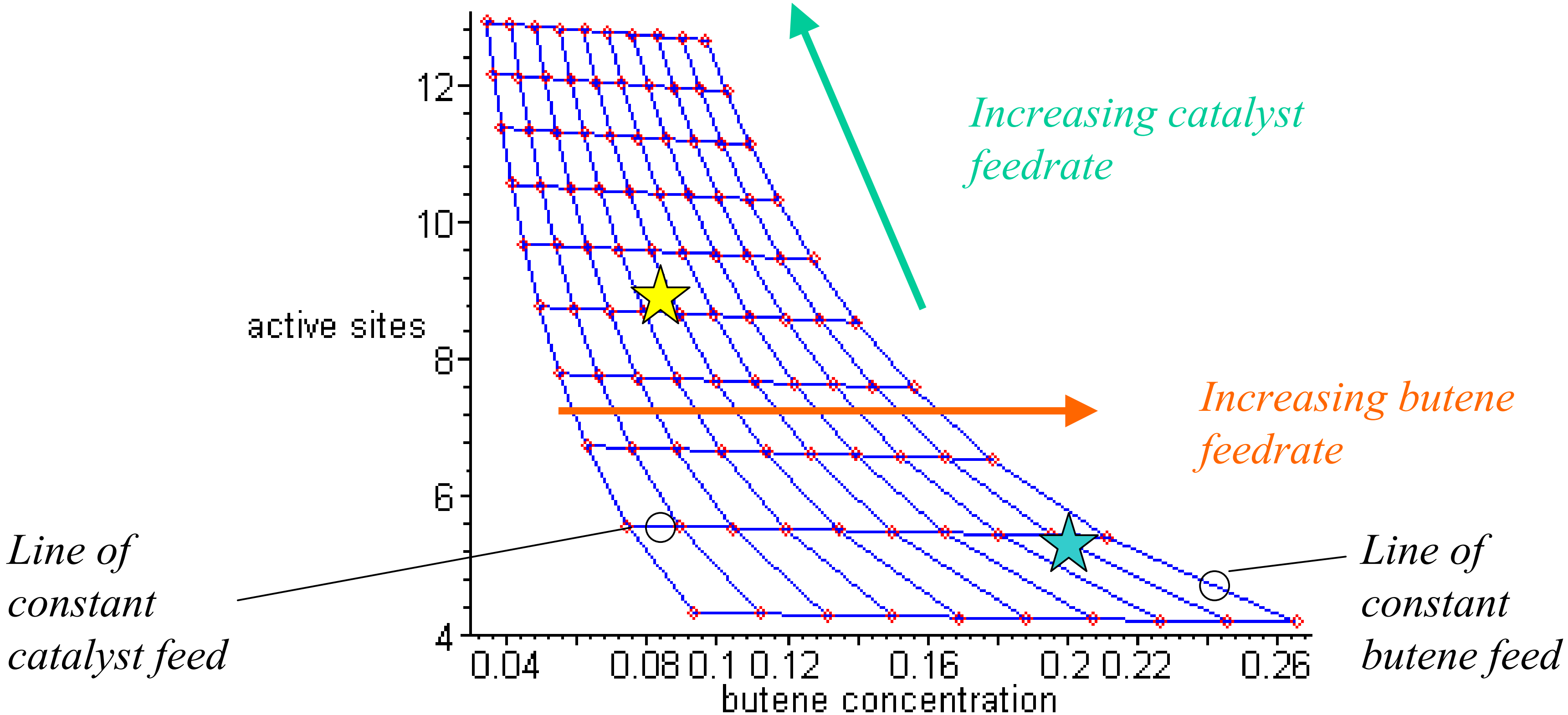
$$\frac{dY}{dt} = F_{cat}\, a_{cat} - \frac{(Y^2 (k_{p1}[M_1]\, mw_1 + k_{p2}\, [M2] mw_2)}{1000000\, B_w} - k_d Y$$

**Assumptions:**

- The total concentration $C_t$, and ethylene concentration $[M_1]$, are held constant by control
- The bleed flow is kept constant by a flow controller
- The reactor is operating under perfect bed weight control
- Temperature effects are negligible

# Case Study - Polyethlene Reactor

2D steady-state locus for active sites and butene concentration:



# Polyethylene Reactor

Relative curvature arrays for 3x3 problem

- » inputs: $F_{H2}$ , $F_{butene}$ , $F_{catalyst}$
- » states: $[H_2]$, [butene], #of active sites

$$\begin{bmatrix} 0 & .01433194630 & -.05528503012 \\ .01433194630 & -.0007519805158 & .0004090750200 \\ -.05528503013 & .0004090750202 & .003966788811 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 0 & 0 \\ 0 & .05031227979 & -.1780008491 \\ 0 & -.1780008492 & -.04312744855 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 0 & 0 \\ 0 & .04505144936 & -.06355706465 \\ 0 & -.06355706467 & -.1800296466 \end{bmatrix}$$

# Polyethylene Reactor

Relative curvature arrays for 3x3 problem

» inputs: $F_{H2}$ , $F_{butene}$ , $F_{catalyst}$

» states: $[H_2]$, [butene], #of active sites

$$\begin{bmatrix} 0 & .003970929239 & -.06316045948 \\ .003970929239 & -.0003382729455 & .001165085503 \\ -.06316045948 & .001165085503 & .01912352556 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 0 & 0 \\ 0 & .01864676171 & -.3080008442 \\ 0 & -.3080008442 & .1092919140 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 0 & 0 \\ 0 & .004769156421 & -.03175241269 \\ 0 & -.03175241268 & -.1964674629 \end{bmatrix}$$

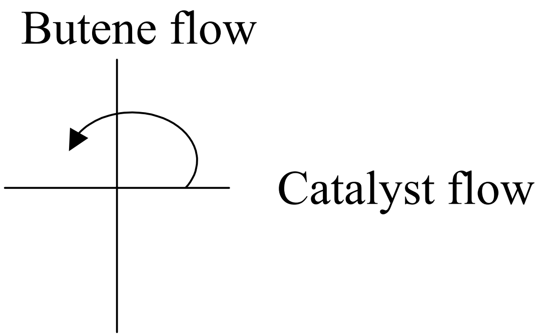
# Polyethylene Reactor

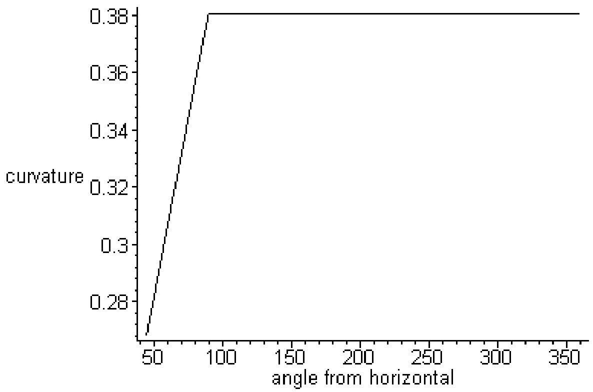
- application of Allgower measure to $F_{cat}$ - Y relationship
  - » ratio relative to input norm = 0.11
  - » ratio relative to output norm = 0.1
- application of Allgower measure to $F_{cat}$ - butene
  - » ratio relative to input norm = 0.005
  - » ratio relative to output norm = 0.5
    - significant curvature - indication of 50% error
- methodology
  - – step inputs
  - – basis of linear transfer function models
  - – least squares solution for model parameters

# Polyethylene Reactor

Dynamic Curvature

- Guay, McLellan and Bacon measure
- computed along process trajectory resulting from step change in catalyst flowrate
- overall dynamic curvature is 0.38 - changing $F_{cat}$
- consider over trajectories resulting from combinations of step changes in $F_{cat}$, $F_{butene}$



# Open-Loop Assessment

These tools apply to input-output (and input-state) system representations, and as such can be applied to closed-loop processes

- input is setpoint or disturbance
- output is process output, or performance index
- application to *steady-state closed-loop* relationships is typically of little benefit
  - setpoint tracking - identity map
  - disturbance rejection - zero map
  - exception - implications of perfect tracking for interaction within process - Guay et al. (1997)

# Closed-Loop Measures

Optimal Control Structure

» Doyle III and Stack (1997)

» using optimal control structure, measure nonlinearity of controller to assess extent to which nonlinearity is cancelled for optimal performance

» various open-loop measures can be used to assess degree of nonlinearity of optimal control structure

– e.g., coherence

# Open vs. Closed-Loop Approaches

Conceptually, these measures can be applied to any steady state or dynamic relationship -

- open-loop process
- closed-loop process - setpoint-output relationship
- control law - input is the measured response, output is the control action

Point of debate -

- significance of nonlinearity, and ultimately its impact on closed-loop stability (safety) and performance (economics)
- does significant open-loop nonlinearity translate into significant control performance degradation?

# Asking the relevant question

Control-relevant measures of nonlinearity

- Frank Doyle - optimal control structure approach
  - » complete elimination of nonlinearity is not necessarily optimal
  - » focus on control action required to obtain optimal performance, and investigate extent to which nonlinearity is compensated
    - – nonlinearity of optimal control law

# Asking the relevant question

Leung, Guay, Bacon and McLellan - examine performance measures

» focus on setpoint-output relationship, and assess nonlinearity in terms of performance measures

» performance measures

- integral time absolute error (itae)
- itae plots vs. setpoint changes
- curvature measurement on this relationship

# Curvature of Performance Measure

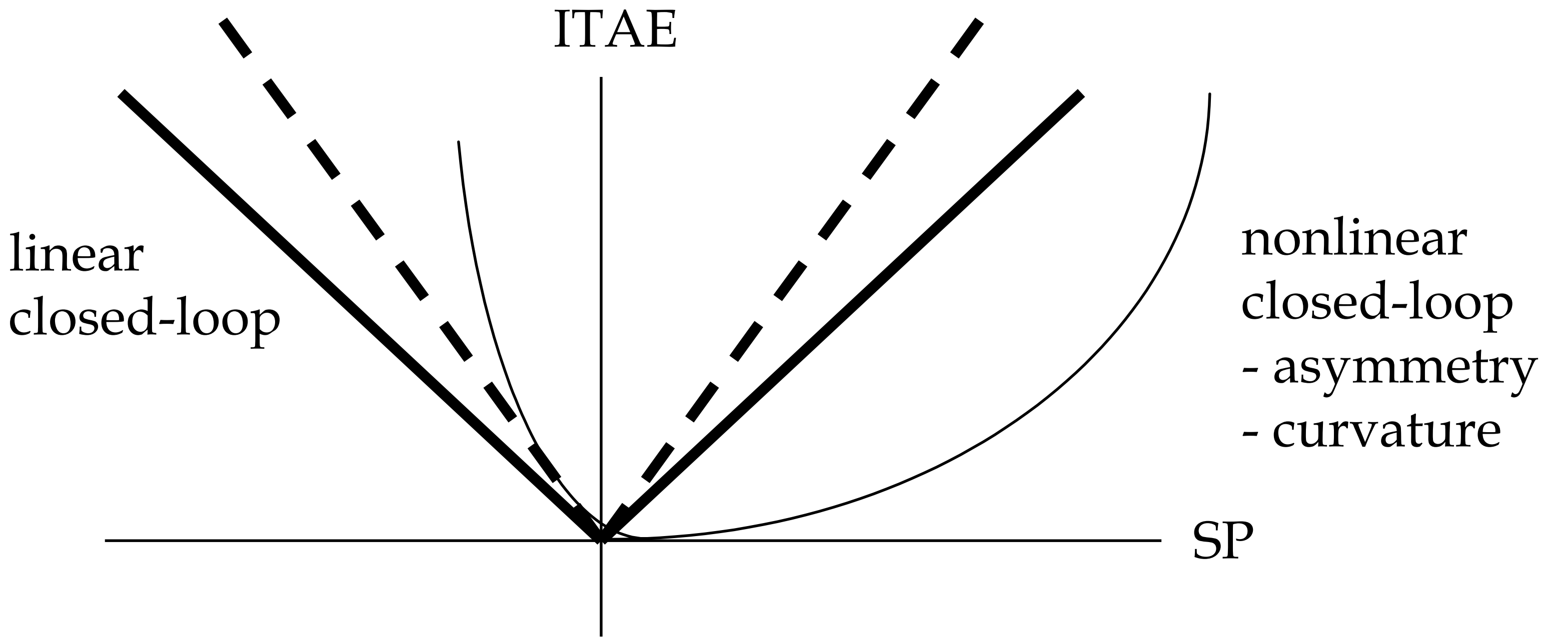
Motivation -

- pointwise comparisons of linear vs. nonlinear control performance, in terms of a given index, do not provide a complete assessment
  - "I can tune my controller to match" argument
- major benefit of nonlinear control is improved control over a *range* of operation
- examine growth of performance measure over a family of external input changes

# Curvature of Performance Measure

Graphically:

$$ITAE = \int_0^T t\left|SP - y_{cl}\right| dt = \int_0^T t\left|SP - G_{cl}(SP)\right| dt$$



# Curvature of Performance Measure

Interpretation

- linear profiles - closed-loop linear process
- differences in slope
  - different controller structures
  - different controller tunings - e.g., different pole placements for input-output linearization
- nonlinear profiles
  - linear controller on nonlinear plant
  - partial compensation of nonlinearity
- quantitative assessment can be obtained by applying curvature measures to setpoint-performance measure relationship
- cf., profile plots in nonlinear regression

# Curvature of Performance Measure

Servo problem:

$$ITAE = \int_0^T t\left|SP - y_{cl}\right| dt = \int_0^T t\left|SP - G_{cl}(SP)\right| dt$$

- $G_{cl}$ is closed-loop process
- if closed-loop process is linear,
  $G_{cl}$ ($k$ SP) = $k$ $G_{cl}$(SP)
  and the ITAE grows linearly with size of step change
- choose SP(t) to be unit step function
- similar results apply for Integral Absolute Error (IAE)

# Our Current Work -

- Benda, McAuley and McLellan (2000)
  - » assessment of nonlinearity of a gas-phase polyethylene reactor and its impact on controller performance
    - over range of grade transitions
    - comparison between nonlinear and linear state feedback control designs
  - » observed lack of systematic relationship between steady-state nonlinearity and controller performance
  - » wide range of nonlinearity exhibited

# Our Current Work

- Dier, Guay and McLellan (2001- in progress)
  - » development of performance sensitivity array
    - examine third derivative of performance objective with respect to manipulated variable inputs
    - apply to performance function associated with linearized optimal controller design
    - examine deviation in performance as we perturb control action from that computed using linearized controller
  - » application - chemostat bioreactor model
    - – some consistency in nonlinearity as a function of aggressiveness of controller

# Objectives

Dier, Guay and McLellan (2001)

- Relate design decisions to non-linearity
- Optimal linear regulator cost function

$$\eta = \int_0^\infty \left( x(t)^T Q x(t) + \nu(t)^T R \nu(t) \right) dt$$

- Optimal cost
  - long-time, or sustained, performance where $K_\infty$ is optimal gain

$$J = x^T(\infty) K_\infty x(\infty)$$

# Performance Sensitivity

Dier, Guay and McLellan (2001)

- Third derivative of J w.r.t. perturbation, u

$$\frac{\partial^3 J}{\partial u^3} = 6 \frac{\partial^2 x(t)}{\partial u^2} K_\infty \frac{\partial x(t)}{\partial u}$$

- "Performance Sensitivity Array" (pXpXp)

$$\frac{\partial^3 J}{\partial \mu^3} = 6 \frac{\partial^2 z(t)}{\partial \mu^2} \frac{\partial z(t)}{\partial \mu}$$

  - z, μ are scaled states and inputs - scaling by ...

# Chemostat Bioreactor

Dier, Guay and McLellan (2001)

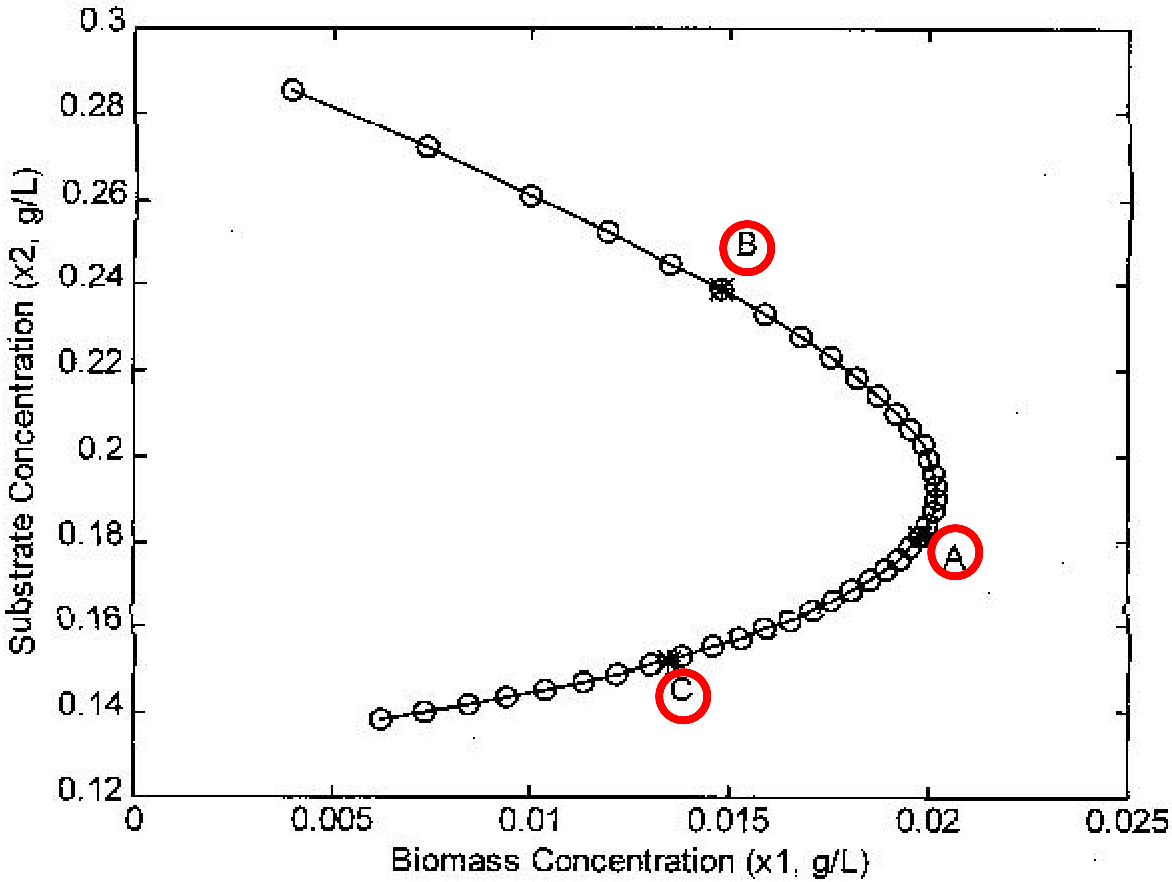
- Governing equations

$$\begin{bmatrix} \dfrac{dx_1}{dt} \\ \dfrac{dx_2}{dt} \end{bmatrix} = \begin{bmatrix} \dfrac{\mu x_1 x_2}{1 + x_2 + K_I x_2^{\;2}} - k_d x_1 - \nu_1 x_1 \\ -\dfrac{\mu x_1 x_2}{1 + x_2 + K_I x_2^{\;2}} + (S_0 - x_2)\nu_1 \end{bmatrix}$$

Guay, 1996

# Chemostat Bioreactor

Dier, Guay and McLellan (2001)




Guay, 1996

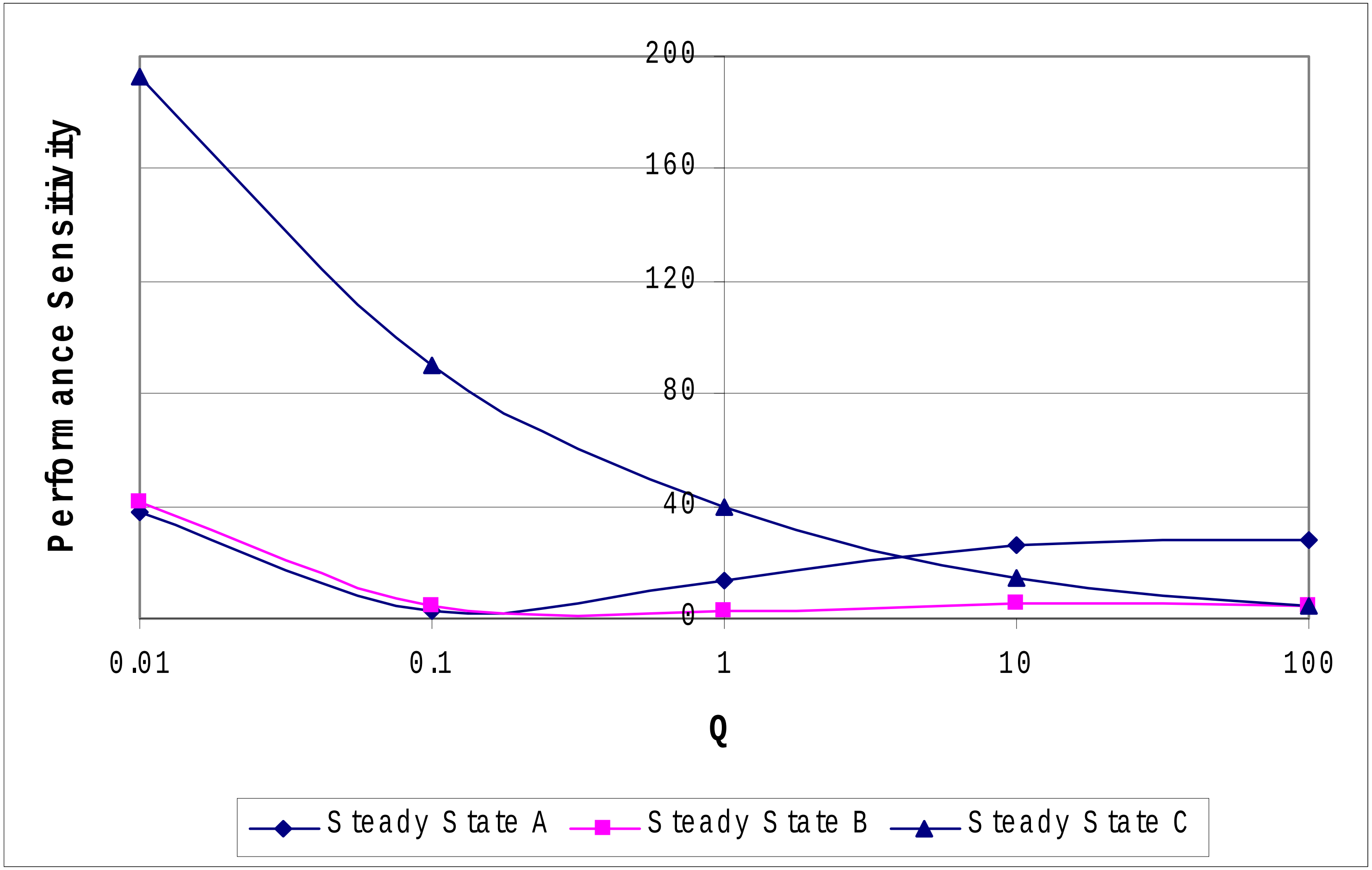
# Chemostat Bioreactor

Dier, Guay and McLellan (2001)

- Find optimal linear controller
- Compute performance sensitivities of closed-loop system
  - Performance Sensitivity Array (PSA)
- Simulate the system
- Conclude appropriate controller design

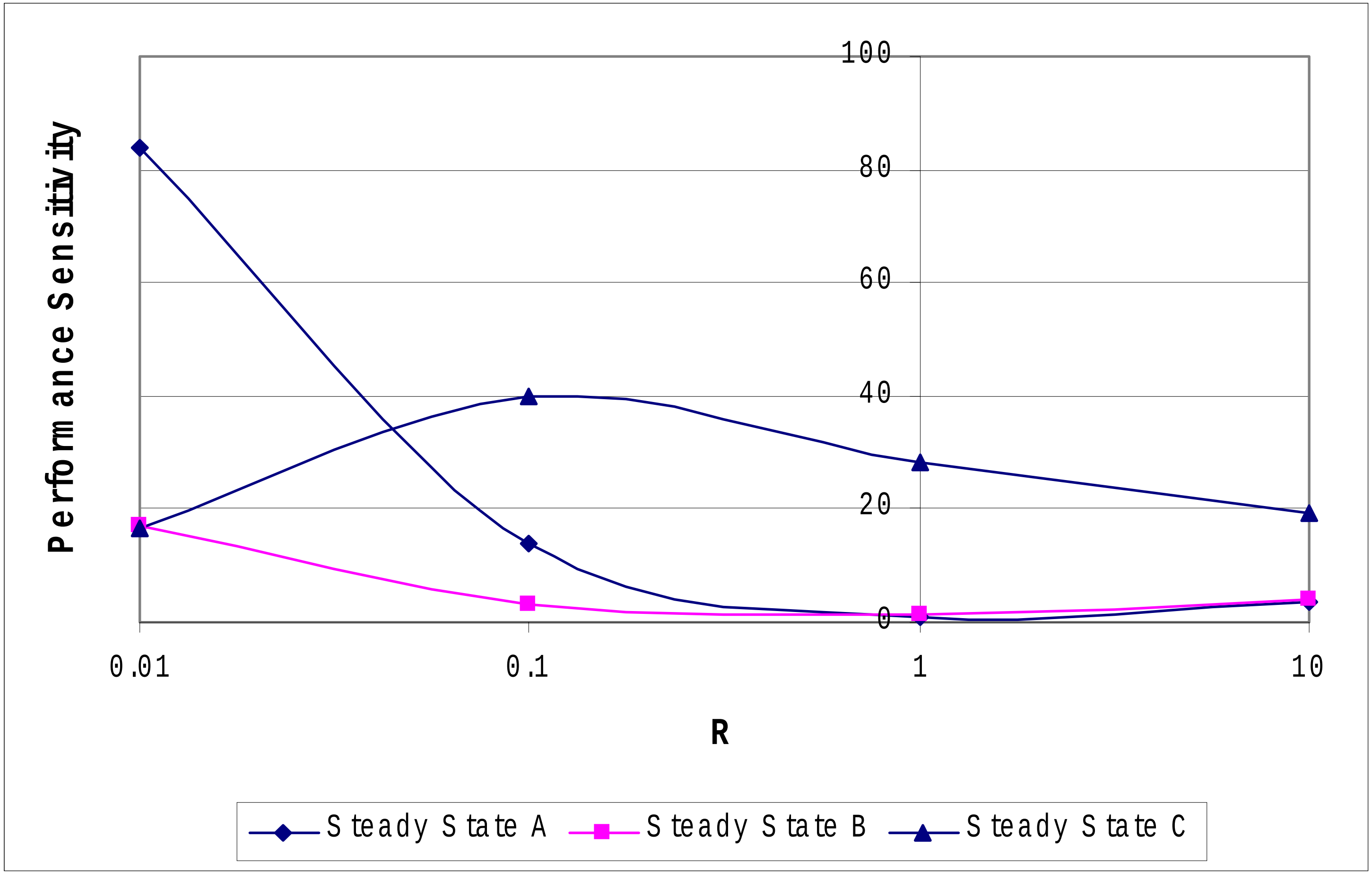
# PSA, R=0.1

Dier, Guay and McLellan (2001)



# PSA, Q=1

Dier, Guay and McLellan (2001)



# Dealing with nonlinearity in estimation and control

## Estimation

- » reparameterize model
  - » to address parameter-effects curvature
- » modify inherent structure of model
  - » to address intrinsic curvature
- » modify experimental design points
- » response transformations - error distribution?

## Control

- » reparameterize input-output relationship
  - • using transformation of mv inputs
  - • using feedback - function of inputs and responses
- » transform responses (outputs/states)

# An interpretation of feedback control

…feedback represents a re-parameterization of the process input-output model

Heater example

» open-loop model $$\frac{dT}{dt} = \theta_1 T + \theta_2 u$$

» feedback - set valve position to equal a (linear) function of temperature and the setpoint

» $u = f_1(T) + f_2(SP)$

» closed-loop model

$$\frac{dT}{dt} = (\theta_1 T + \theta_2 f_1(T)) + \theta_2 f_2(SP)$$

# An interpretation of feedback control

But dynamically and at steady state, T is a function of u

» $u = f_1(T(u)) + f_2(SP) = f_1(T(u)) + f_2(SP)$

» implies that $u = g(SP)$

» reparameterization

» setpoint tracking

- the feedback "reparameterization" takes the steady state process model and transforms it to $T = SP$

# Feedback Linearization as Reparameterization

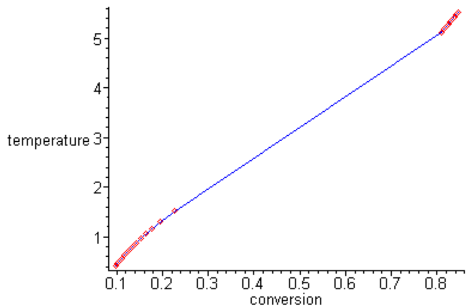
- State transformation - transformation of responses
- input reparameterization - immediate transformation of input variables
- feedback component - is ultimately an input reparameterization as well

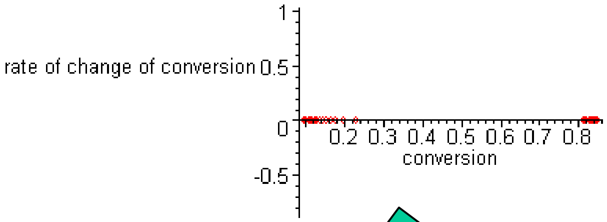
  - steady state - we have $u = \alpha(x(u), v)$
    - reparameterization via steady state functional dependence of states on inputs
  - dynamic $u(t) = \alpha(x(u(t)), x(0), v)$
    - feedback law is reparameterization based on state response and initial conditions, plus new reference input

# Example

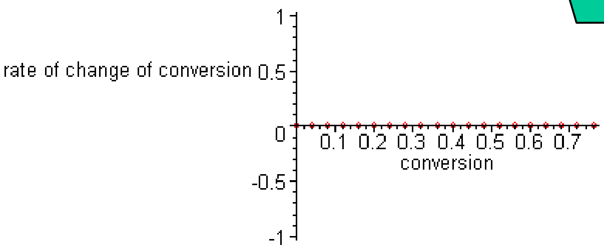
Calvet and Arkun CSTR - sequence

- state transformation -
  - » straight locus (elimination of intrinsic nonlinearity), with non-uniform parameter increments




- input reparameterization
  - » feedback reparameterization - elimination of non-uniformity on locus (parameter-effects nonlinearity)
  - » reparameterization of input also with introduction of setpoint



# Summary

- Why is nonlinearity a problem?
  - » in statistical model-building
  - » in process control
- How can the degree of nonlinearity be assessed?
  - » in statistical model-building
  - » in process control
- Duality - nonlinearity in estimation and control
  - » feedback as a reparameterization
- Application - stirred tank reactor example

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