Hybrid Dynamic Modeling and Identification

Daniel M. Webb, W. Fred Ramirez advising

Department of Chemical and Biological Engineering
University of Colorado, Boulder

May 8, 2007

Problem Introduction

ODE models:

- $\dot{\mathbf{X}} = f(\mathbf{X}, \nu(\mathbf{X}, \omega))$

Problem Introduction

ODE models:

- $\dot{\mathbf{X}} = f(\mathbf{X}, \nu(\mathbf{X}, \omega))$
- $X(t = 0) = X_0$

Problem Introduction

ODE models:

- $\dot{\mathbf{X}} = f(\mathbf{X}, \nu(\mathbf{X}, \omega))$
- $X(t = 0) = X_0$

Model uses (especially batch systems):

- Optimize yield

Problem Introduction

ODE models:

- $\dot{\mathbf{X}} = f(\mathbf{X}, \nu(\mathbf{X}, \omega))$
- $X(t = 0) = X_0$

Model uses (especially batch systems):

- Optimize yield
- Minimize unwanted products

Problem Introduction

ODE models:

- $\dot{\mathbf{X}} = f(\mathbf{X}, \nu(\mathbf{X}, \omega))$
- $X(t = 0) = X_0$

Model uses (especially batch systems):

- Optimize yield
- Minimize unwanted products
- Reduce run-to-run variation

Problem Introduction

ODE models:

- $\dot{\mathbf{X}} = f(\mathbf{X}, \nu(\mathbf{X}, \omega))$
- $X(t = 0) = X_0$

Model uses (especially batch systems):

- Optimize yield
- Minimize unwanted products
- Reduce run-to-run variation
- Real-time optimal control

Problem Introduction

ODE models:

- $\dot{\mathbf{X}} = f(\mathbf{X}, \nu(\mathbf{X}, \omega))$
- $X(t = 0) = X_0$

Model uses (especially batch systems):

- Optimize yield
- Minimize unwanted products
- Reduce run-to-run variation
- Real-time optimal control

Some basic modeling steps:

- Formulate

Problem Introduction

ODE models:

- $\dot{\mathbf{X}} = f(\mathbf{X}, \nu(\mathbf{X}, \omega))$
- $X(t = 0) = X_0$

Model uses (especially batch systems):

- Optimize yield
- Minimize unwanted products
- Reduce run-to-run variation
- Real-time optimal control

Some basic modeling steps:

- Formulate
- Train (identify model parameters)

Problem Introduction

ODE models:

- $\dot{\mathbf{X}} = f(\mathbf{X}, \nu(\mathbf{X}, \omega))$
- $X(t = 0) = X_0$

Model uses (especially batch systems):

- Optimize yield
- Minimize unwanted products
- Reduce run-to-run variation
- Real-time optimal control

Some basic modeling steps:

- Formulate
- Train (identify model parameters)
- Offline optimization

Problem Introduction

ODE models:

- $\dot{\mathbf{X}} = f(\mathbf{X}, \nu(\mathbf{X}, \omega))$
- $X(t = 0) = X_0$

Model uses (especially batch systems):

- Optimize yield
- Minimize unwanted products
- Reduce run-to-run variation
- Real-time optimal control

Some basic modeling steps:

- Formulate
- Train (identify model parameters)
- Offline optimization
- Online optimization (real-time optimal control)

Problem Introduction

ODE models:

- $\dot{\mathbf{X}} = f(\mathbf{X}, \nu(\mathbf{X}, \omega))$
- $X(t = 0) = X_0$

Model uses (especially batch systems):

- Optimize yield
- Minimize unwanted products
- Reduce run-to-run variation
- Real-time optimal control

Some basic modeling steps:

- Formulate
- **Train (identify model parameters)**
- Offline optimization
- Online optimization (real-time optimal control)

Park-Ramirez Bioreactor Model

For genetically modified yeast in a fed-batch reactor, predict:

Accumulation		Generation	Input	Dilution
$\dot{V}$	=			
$\dot{X}$	=			
$\dot{S}$	=			
$\dot{P}_T$	=			
$\dot{P}_M$	=			

Park-Ramirez Bioreactor Model

For genetically modified yeast in a fed-batch reactor, predict:

Accumulation		Generation	Input	Dilution
$\dot{V}$	=		q	
$\dot{X}$	=			
$\dot{S}$	=			
$\dot{P}_T$	=			
$\dot{P}_M$	=			

Park-Ramirez Bioreactor Model

For genetically modified yeast in a fed-batch reactor, predict:

- cell growth,

		Accumulation	Generation	Input	Dilution
$\dot{V}$	=			q	
$\dot{X}$	=				
$\dot{S}$	=				
$\dot{P}_T$	=				
$\dot{P}_M$	=				

Park-Ramirez Bioreactor Model

For genetically modified yeast in a fed-batch reactor, predict:

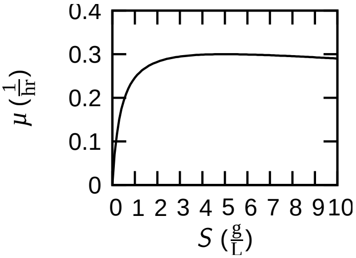
- cell growth,

	Accumulation		Generation	Input	Dilution
$\dot{V}$	=			q	
$\dot{X}$	=		μX		$- \frac{q}{V} X$
$\dot{S}$	=				
$\dot{P_T}$	=				
$\dot{P_M}$	=				

Park-Ramirez Bioreactor Model

For genetically modified yeast in a fed-batch reactor, predict:

- cell growth,

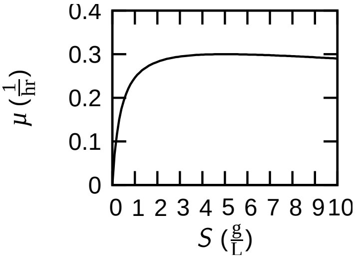


Accumulation		Generation	Input		Dilution
$\dot{V}$	=		q		
$\dot{X}$	=	μX		-	$\frac{q}{V} X$
$\dot{S}$	=				
$\dot{P}_T$	=				
$\dot{P}_M$	=				

Park-Ramirez Bioreactor Model

For genetically modified yeast in a fed-batch reactor, predict:

- cell growth,
- substrate consumption,

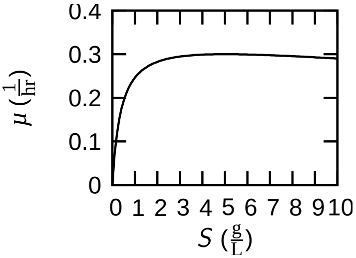


Accumulation		Generation	Input	Dilution
$\dot{V}$	=		q	
$\dot{X}$	=	μX		$-\ \frac{q}{V} X$
$\dot{S}$	=			
$\dot{P}_T$	=			
$\dot{P}_M$	=			

Park-Ramirez Bioreactor Model

For genetically modified yeast in a fed-batch reactor, predict:

- cell growth,
- substrate consumption,



Accumulation		Generation	Input	Dilution
$\dot{V}$	$=$		q	
$\dot{X}$	$=$	μX		$- \frac{q}{V} X$
$\dot{S}$	$=$	$-Y \mu X$	$+ \frac{q}{V} S_f$	$- \frac{q}{V} S$
$\dot{P}_T$	$=$			
$\dot{P}_M$	$=$			

Park-Ramirez Bioreactor Model

For genetically modified yeast in a fed-batch reactor, predict:

- cell growth,
- substrate consumption,
- foreign protein production,

Accumulation		Generation	Input	Dilution
$\dot{V}$	=		q	
$\dot{X}$	=	μX		$- \frac{q}{V} X$
$\dot{S}$	=	$-Y\mu X$	$+ \frac{q}{V} S_f$	$- \frac{q}{V} S$
$\dot{P}_T$	=			
$\dot{P}_M$	=			

Park-Ramirez Bioreactor Model

For genetically modified yeast in a fed-batch reactor, predict:

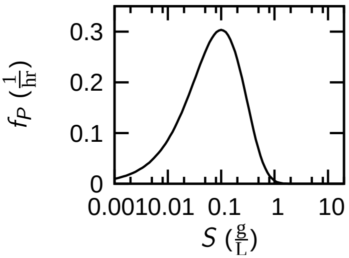
- cell growth,
- substrate consumption,
- foreign protein production,

Accumulation		Generation	Input	Dilution
$\dot{V}$	=		q	
$\dot{X}$	=	μX		$- \frac{q}{V} X$
$\dot{S}$	=	$-Y \mu X$	$+ \frac{q}{V} S_f$	$- \frac{q}{V} S$
$\dot{P_T}$	=	$f_P X$		$- \frac{q}{V} P_T$
$\dot{P_M}$	=			

Park-Ramirez Bioreactor Model

For genetically modified yeast in a fed-batch reactor, predict:

- cell growth,
- substrate consumption,
- foreign protein production,



Accumulation		Generation	Input	Dilution
$\dot{V}$	=		q	
$\dot{X}$	=	μX		$-\ \frac{q}{V}X$
$\dot{S}$	=	$-Y\mu X$	$+\ \frac{q}{V}S_f$	$-\ \frac{q}{V}S$
$\dot{P}_T$	=	$f_P X$		$-\ \frac{q}{V}P_T$
$\dot{P}_M$	=			

Park-Ramirez Bioreactor Model

For genetically modified yeast in a fed-batch reactor, predict:

- cell growth,
- substrate consumption,
- foreign protein production,
- and foreign protein secretion.

Accumulation		Generation	Input	Dilution
$\dot{V}$	$=$		q	
$\dot{X}$	$=$	μX		$- \frac{q}{V} X$
$\dot{S}$	$=$	$-Y\mu X$	$+ \frac{q}{V} S_f$	$- \frac{q}{V} S$
$\dot{P}_T$	$=$	$f_P X$		$- \frac{q}{V} P_T$
$\dot{P}_M$	$=$			

Park-Ramirez Bioreactor Model

For genetically modified yeast in a fed-batch reactor, predict:

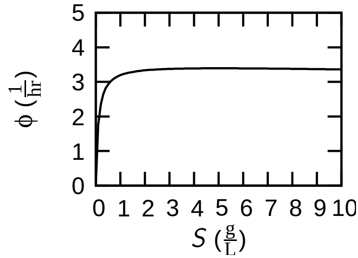
- cell growth,
- substrate consumption,
- foreign protein production,
- and foreign protein secretion.

	Accumulation		Generation	Input	Dilution
$\dot{V}$	=			q	
$\dot{X}$	=	μX			$- \frac{q}{V} X$
$\dot{S}$	=	$-Y\mu X$		$+ \frac{q}{V} S_f$	$- \frac{q}{V} S$
$\dot{P}_T$	=	$f_P X$			$- \frac{q}{V} P_T$
$\dot{P}_M$	=	$\phi(P_T - P_M)$			$- \frac{q}{V} P_M$

Park-Ramirez Bioreactor Model

For genetically modified yeast in a fed-batch reactor, predict:

- cell growth,
- substrate consumption,
- foreign protein production,
- and foreign protein secretion.



	Accumulation		Generation	Input		Dilution
	$\dot{V}$	=		q		
	$\dot{X}$	=	μX		-	$\frac{q}{V} X$
	$\dot{S}$	=	$-Y\mu X$	$+ \frac{q}{V} S_f$	-	$\frac{q}{V} S$
	$\dot{P_T}$	=	$f_P X$		-	$\frac{q}{V} P_T$
	$\dot{P_M}$	=	$\phi(P_T - P_M)$		-	$\frac{q}{V} P_M$

Park-Ramirez Bioreactor Model

For genetically modified yeast in a fed-batch reactor, predict:

- cell growth,
- substrate consumption,
- foreign protein production,
- and foreign protein secretion.

Accumulation		Generation	Input	Dilution
$\dot{V}$	=		q	
$\dot{X}$	=	μX		$- \frac{q}{V} X$
$\dot{S}$	=	$-Y \mu X$	$+ \frac{q}{V} S_f$	$- \frac{q}{V} S$
$\dot{P}_T$	=	$f_P X$		$- \frac{q}{V} P_T$
$\dot{P}_M$	=	$\phi (P_T - P_M)$		$- \frac{q}{V} P_M$

The optimal control problem:

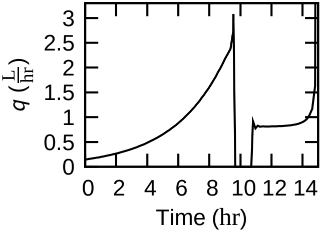
$$MAX(\Phi)$$

$$\Phi = P_M(t_f) \cdot V(t_f)$$

Park-Ramirez Bioreactor Model

For genetically modified yeast in a fed-batch reactor, predict:

- cell growth,
- substrate consumption,
- foreign protein production,
- and foreign protein secretion.



	Accumulation		Generation	Input	Dilution
	$\dot{V}$	=		q	
	$\dot{X}$	=	μX		$- \frac{q}{V} X$
	$\dot{S}$	=	$-Y \mu X$	$+ \frac{q}{V} S_f$	$- \frac{q}{V} S$
	$\dot{P}_T$	=	$f_P X$		$- \frac{q}{V} P_T$
	$\dot{P}_M$	=	$\phi (P_T - P_M)$		$- \frac{q}{V} P_M$

Hybrid Dynamic Park-Ramirez Model

$$
\begin{aligned}
\dot{X} &= \mu X - \frac{q}{V} X \\
\dot{S} &= -Y\mu X + \frac{q}{V}(S_f - S) \\
\dot{P_T} &= f_P X - \frac{q}{V} P_T \\
\dot{P_M} &= \phi(P_T - P_M) - \frac{q}{V} P_M \\
\dot{V} &= q
\end{aligned}
$$

Hybrid Dynamic Park-Ramirez Model

$$
\begin{aligned}
\dot{X} &= \mu X - \tfrac{q}{V} X \\
\dot{S} &= -Y \mu X + \tfrac{q}{V} (S_f - S) \\
\dot{P}_T &= f_P X - \tfrac{q}{V} P_T \\
\dot{P}_M &= \phi (P_T - P_M) - \tfrac{q}{V} P_M \\
\dot{V} &= q
\end{aligned}
$$

Replace μ, f_P, and ϕ with neural networks: $\mu(S, \omega_1)$, $f_P(S, \omega_2)$, and $\phi(S, \omega_3)$.

Hybrid Dynamic Park-Ramirez Model

$$
\begin{aligned}
\dot{X} &= \mu X - \frac{q}{V} X \\
\dot{S} &= -Y \mu X + \frac{q}{V}(S_f - S) \\
\dot{P}_T &= f_P X - \frac{q}{V} P_T \\
\dot{P}_M &= \phi(P_T - P_M) - \frac{q}{V} P_M \\
\dot{V} &= q
\end{aligned}
$$

Replace μ, f_P, and ϕ with neural networks:
$\mu(S, \omega_1)$, $f_P(S, \omega_2)$, and $\phi(S, \omega_3)$.

How to find $\omega_1, \omega_2, \omega_3$?

Derivative Method

$$
\begin{aligned}
\dot{X} &= \mu X - \frac{q}{V} X \\
\dot{S} &= -Y\mu X + \frac{q}{V}(S_f - S) \\
\dot{P_T} &= f_P X - \frac{q}{V} P_T \\
\dot{P_M} &= \phi(P_T - P_M) - \frac{q}{V} P_M \\
\dot{V} &= q
\end{aligned}
$$

Derivative Method

$$\begin{aligned}
\dot{X} &= \mu X - \frac{q}{V} X \\
\dot{S} &= -Y\mu X + \frac{q}{V}(S_f - S) \\
\dot{P_T} &= f_P X - \frac{q}{V} P_T \\
\dot{P_M} &= \phi(P_T - P_M) - \frac{q}{V} P_M \\
\dot{V} &= q
\end{aligned}$$

Get input-output data to train neural networks:

Derivative Method

$$
\begin{aligned}
\dot{X} &= \mu X - \frac{q}{V} X \\
\dot{S} &= -Y \mu X + \frac{q}{V}(S_f - S) \\
\dot{P_T} &= f_P X - \frac{q}{V} P_T \\
\dot{P_M} &= \phi(P_T - P_M) - \frac{q}{V} P_M \\
\dot{V} &= q
\end{aligned}
$$

Get input-output data to train neural networks:

$$
\dot{X} = (\mu - \frac{q}{V}) X \quad \Longrightarrow \quad \mu = \frac{\dot{X}}{X} + \frac{q}{V}
$$

Derivative Method

$$
\begin{aligned}
\dot{X} &= \mu X - \tfrac{q}{V} X \\
\dot{S} &= -Y\mu X + \tfrac{q}{V}(S_f - S) \\
\dot{P_T} &= f_P X - \tfrac{q}{V} P_T \\
\dot{P_M} &= \phi(P_T - P_M) - \tfrac{q}{V} P_M \\
\dot{V} &= q
\end{aligned}
$$

Get input-output data to train neural networks:

$$\dot{X} = (\mu - \tfrac{q}{V})X \quad \Longrightarrow \quad \mu = \frac{\dot{X}}{X} + \frac{q}{V}$$

What if not much data available for a state?

Optimal Control Identification

Optimal control identification process:

Optimal Control Identification

Optimal control identification process:

Optimal Control Identification

Optimal control identification process:

1. For each run, treat identification problem as optimal control problem:

Optimal Control Identification

Optimal control identification process:

1. For each run, treat identification problem as optimal control problem:
   - $\mu(t)$, $f_P(t)$, and $\phi(t)$ are controls.

Optimal Control Identification

Optimal control identification process:

1. For each run, treat identification problem as optimal control problem:
   - $\mu(t)$, $f_P(t)$, and $\phi(t)$ are controls.
   - $\Phi = E = \sum(\mathbf{X}_m - \mathbf{X})^2$

Optimal Control Identification

Optimal control identification process:

1. For each run, treat identification problem as optimal control problem:
   - $\mu(t)$, $f_P(t)$, and $\phi(t)$ are controls.
   - $\Phi = E = \sum(\mathbf{X}_m - \mathbf{X})^2$
2. Neural networks are trained using a set of input-output pairs.
   - $\mu(t)$, $f_P(t)$, and $\phi(t)$ from step 1 are outputs.

Optimal Control Identification

Optimal control identification process:

1. For each run, treat identification problem as optimal control problem:
   - $\mu(t)$, $f_P(t)$, and $\phi(t)$ are controls.
   - $\Phi = E = \sum(\mathbf{X}_m - \mathbf{X})^2$
2. Neural networks are trained using a set of input-output pairs.
   - $\mu(t)$, $f_P(t)$, and $\phi(t)$ from step 1 are outputs.
   - States corresponding to each output are the inputs.

Optimal Control Identification

Optimal control identification process:

1. For each run, treat identification problem as optimal control problem:
   - $\mu(t)$, $f_P(t)$, and $\phi(t)$ are controls.
   - $\Phi = E = \sum(\mathbf{X}_m - \mathbf{X})^2$
2. Neural networks are trained using a set of input-output pairs.
   - $\mu(t)$, $f_P(t)$, and $\phi(t)$ from step 1 are outputs.
   - States corresponding to each output are the inputs.
   - Normal neural network training identifies weights ω.

Optimal Control Identification

Optimal control identification process:

1. For each run, treat identification problem as optimal control problem:
   - $\mu(t)$, $f_P(t)$, and $\phi(t)$ are controls.
   - $\Phi = E = \sum(\mathbf{X}_m - \mathbf{X})^2$
2. Neural networks are trained using a set of input-output pairs.
   - $\mu(t)$, $f_P(t)$, and $\phi(t)$ from step 1 are outputs.
   - States corresponding to each output are the inputs.
   - Normal neural network training identifies weights ω.

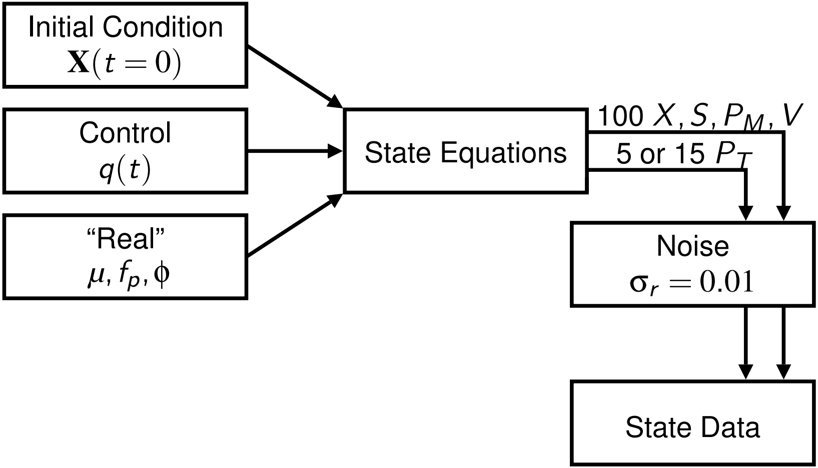
No limitations: if a system can be moved forward in time, this method can be used.

Testing Optimal Control Identification

How to test this new identification method?

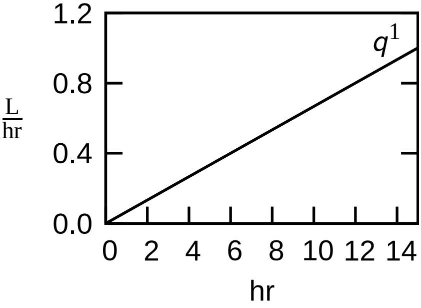
Testing Optimal Control Identification

How to test this new identification method?



Control: $q(t)$

Control ($q(t)$) for first set of examples.



Identification Problem Using IDP Optimal Control Algorithm

- Animation: Two-step IDP with 25 stages

Neural Network Training

Now we have $\mu(t)$, $f_P(t)$, and $\phi(t)$.

Neural Network Training

Now we have $\mu(t)$, $f_P(t)$, and $\phi(t)$.

How do we get the neural network input-output training data from that?

Neural Network Training

Now we have $\mu(t)$, $f_P(t)$, and $\phi(t)$.
How do we get the neural network input-output training data from that?

(Back to Animation)

Testing Optimal Control Identification

Identify Park-Ramirez hybrid model with 8 artificial data runs:

Testing Optimal Control Identification

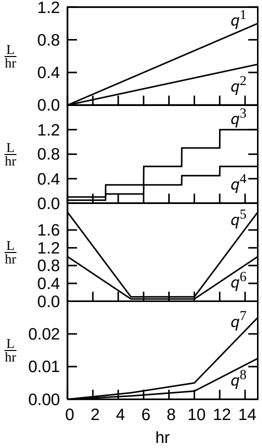
Identify Park-Ramirez hybrid model with 8 artificial data runs:

1. Create 8 data runs using 8 controls.

Testing Optimal Control Identification

Identify Park-Ramirez hybrid model with 8 artificial data runs:

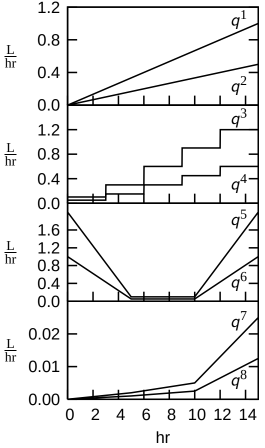
1. Create 8 data runs using 8 controls.



Testing Optimal Control Identification

Identify Park-Ramirez hybrid model with 8 artificial data runs:

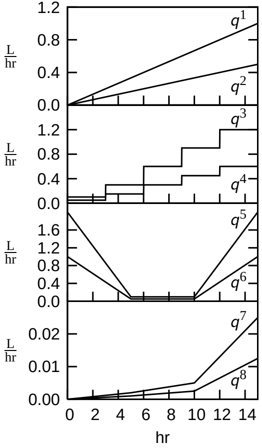
1. Create 8 data runs using 8 controls.
2. Identify $\mu(t)$, $f_P(t)$, and $\phi(t)$ for each run.



Testing Optimal Control Identification

Identify Park-Ramirez hybrid model with 8 artificial data runs:

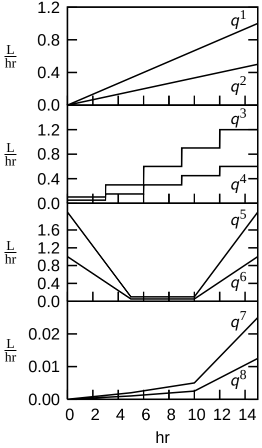
1. Create 8 data runs using 8 controls.
2. Identify $\mu(t)$, $f_P(t)$, and $\phi(t)$ for each run.
3. Convert $\mu(t)$, $f_P(t)$, and $\phi(t)$ data to input-output pairs.



Testing Optimal Control Identification

Identify Park-Ramirez hybrid model with 8 artificial data runs:

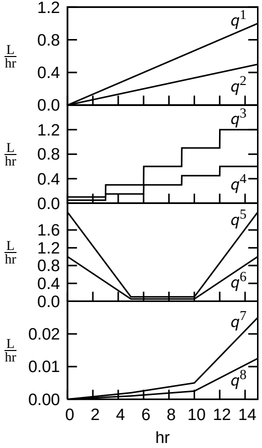
1. Create 8 data runs using 8 controls.
2. Identify $\mu(t)$, $f_P(t)$, and $\phi(t)$ for each run.
3. Convert $\mu(t)$, $f_P(t)$, and $\phi(t)$ data to input-output pairs.
4. Combine input-output pairs from all runs into a single set for each parameter function.



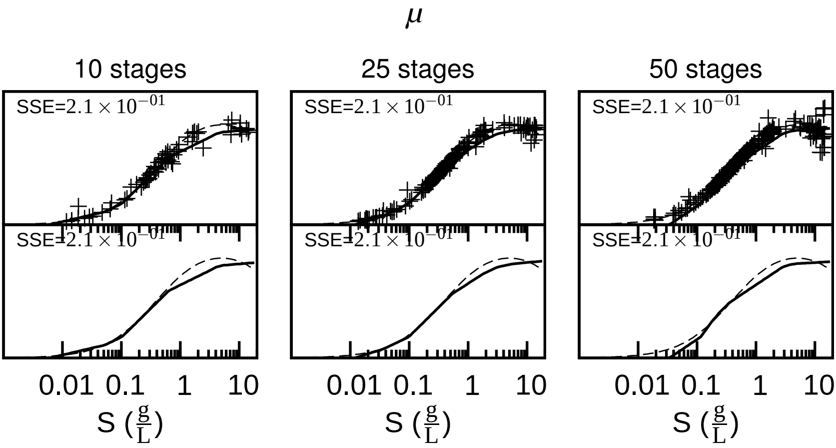
Testing Optimal Control Identification

Identify Park-Ramirez hybrid model with 8 artificial data runs:

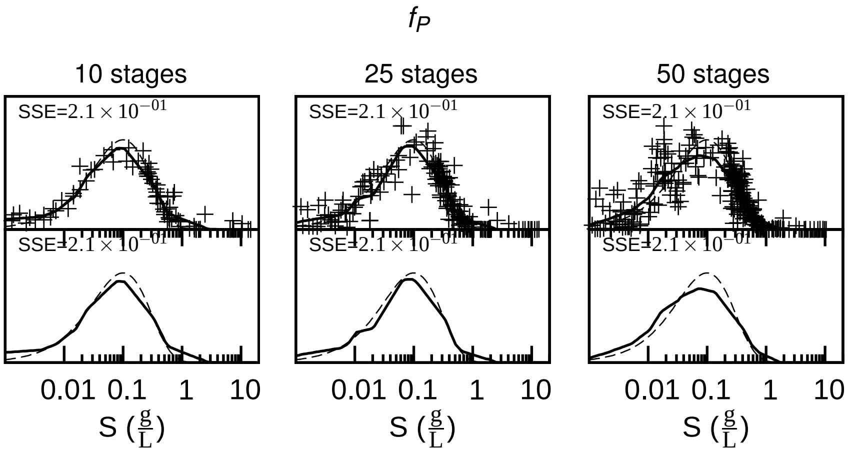
1. Create 8 data runs using 8 controls.
2. Identify $\mu(t)$, $f_P(t)$, and $\phi(t)$ for each run.
3. Convert $\mu(t)$, $f_P(t)$, and $\phi(t)$ data to input-output pairs.
4. Combine input-output pairs from all runs into a single set for each parameter function.
5. Train neural networks on combined input-output set.



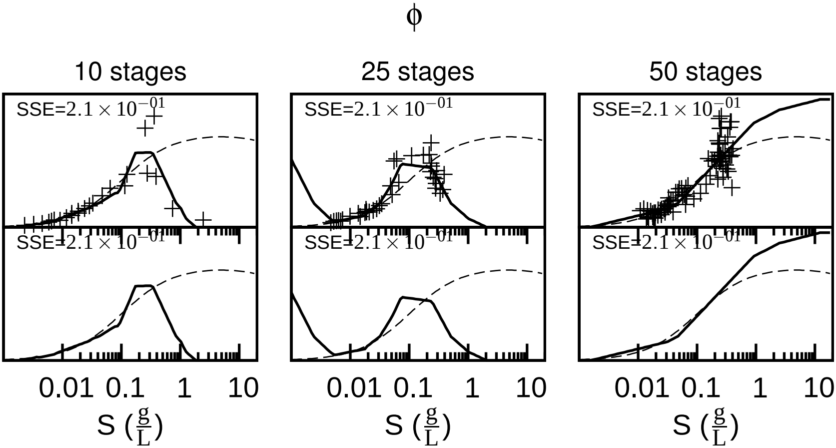
Growth Function



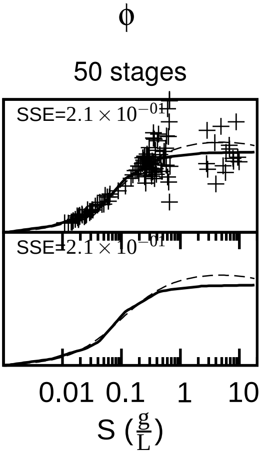
Protein Production Function



Protein Secretion Function



Protein Secretion Function (glucose bump)



Conclusions

- A new identification method for hybrid dynamic models was demonstrated.

Conclusions

- A new identification method for hybrid dynamic models was demonstrated.
    - No sensitivity derivatives needed.

Conclusions

- A new identification method for hybrid dynamic models was demonstrated.
  - No sensitivity derivatives needed.
  - Any function estimator can be used (RBF neural nets seem especially promising).

Acknowledgments

- Dr. W. Fred Ramirez

Acknowledgments

- Dr. W. Fred Ramirez
- National Science Foundation (funding)

Acknowledgments

- Dr. W. Fred Ramirez
- National Science Foundation (funding)
- The Free software community for the software tools.

Acknowledgments

- Dr. W. Fred Ramirez
- National Science Foundation (funding)
- The Free software community for the software tools.
- My wife Janet and daughter Ani for being patient with me.

Acknowledgments

- Dr. W. Fred Ramirez
- National Science Foundation (funding)
- The Free software community for the software tools.
- My wife Janet and daughter Ani for being patient with me.