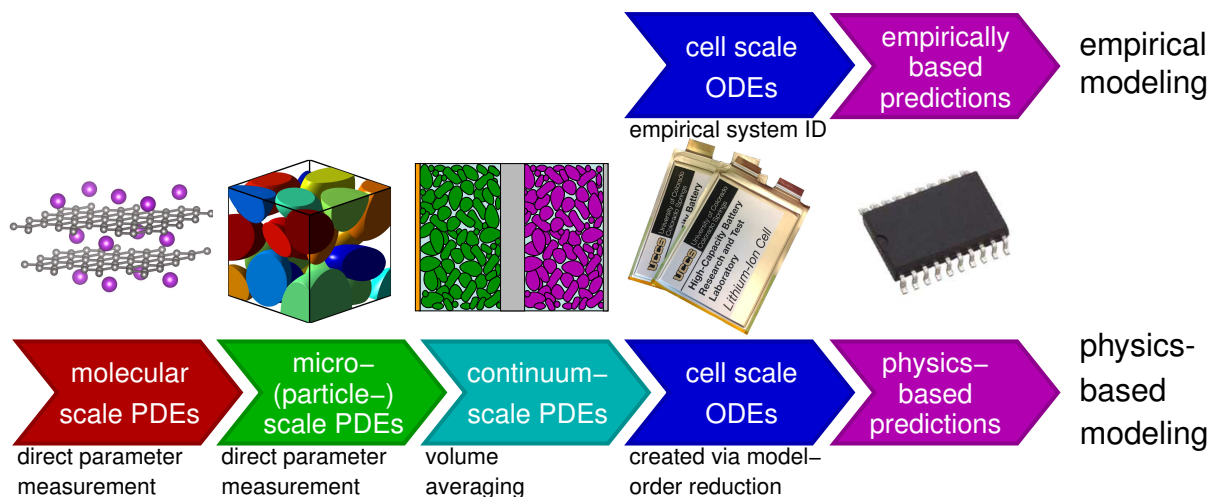


State-Space Models and the Discrete-Time Realization Algorithm

5.1: Introduction to state-space models

- The coupled PDEs derived in earlier chapters of notes are too complex to be used in real-time applications.
 - They are “infinite dimensional.” For every point in time t , there are an infinite number of x - and r - dimension variables to solve for.
 - *i.e.*, $c_s(x, r, t)$, $\bar{c}_e(x, t)$, $\bar{\phi}_s(x, t)$, $\bar{\phi}_e(x, t)$, for a pseudo-two dimensional model.



- We desire to create cell-scale ODEs that retain, as much as possible, the fidelity of the continuum-scale PDEs, but which reduce their order from infinite order to some (small) finite order.
 - The result is a small coupled set of ODEs, which can be simulated very easily and quickly.
- In this chapter, we introduce “state-space” models, which is the final form of the reduced-order models we will develop.

- We then preview the approach to generate the state-space models from the PDEs of the variables of interest:
 - We start by generating transfer functions for each PDE;
 - We then use the “discrete-time realization algorithm” to convert transfer functions to state-space form.

A quick introduction to state-space models

- Transfer functions provide a system’s input-output mapping only:

$$u[k] \rightarrow G(z) \rightarrow y[k].$$

- State-space models provide access to what is going on *inside* the system, in addition to the input-output mapping.
 - What’s going on inside the system is called the system’s “state”.

DEFINITION: The internal state of a system at time k_0 is the minimum amount of information at k_0 that, together with the input $u[k]$, $k \geq k_0$, uniquely determines the behavior of the system for all $k \geq k_0$.

- State-space models describe a system’s dynamics via two equations:
 - The “state equation” describes how the input influences the state;
 - The “output equation” describes how the state and the input both directly influence the output.
- Discrete-time LTI state-space models have the following form:

$$\mathbf{x}[k + 1] = \mathbf{A}\mathbf{x}[k] + \mathbf{B}\mathbf{u}[k]$$

$$\mathbf{y}[k] = \mathbf{C}\mathbf{x}[k] + \mathbf{D}\mathbf{u}[k],$$

where $\mathbf{u}[k] \in \mathbb{R}^m$ is the input, $\mathbf{y}[k] \in \mathbb{R}^p$ is the output, and $\mathbf{x}[k] \in \mathbb{R}^n$ is the state vector.

- Different systems have different n , A , B , C , and D .
- A block diagram can help visualize the signal flows:

EXAMPLE: Convert the following single-input single-output difference equation into a discrete-time state-space form,

$$y[k] + a_1 y[k-1] + a_2 y[k-2] + a_3 y[k-3] = b_1 u[k-1] + b_2 u[k-2] + b_3 u[k-3].$$

- We're going to do the conversion by first recognizing that the transfer function of this system is,

$$G(z) = \frac{b_1 z^2 + b_2 z + b_3}{z^3 + a_1 z^2 + a_2 z + a_3} = \frac{Y(z)}{U(z)}.$$

- Break up transfer function into two parts. $G_p(z) = V(z)/U(z)$ contains all of the poles:

$$G_p(z) = \frac{1}{z^3 + a_1 z^2 + a_2 z + a_3} = \frac{V(z)}{U(z)}$$

$$\Rightarrow v[k+3] + a_1 v[k+2] + a_2 v[k+1] + a_3 v[k] = u[k].$$

- Choose current and advanced versions of $v[k]$ as state (this is a choice: there are other equally valid choices, as we will see)

$$x[k] = \begin{bmatrix} v[k+2] & v[k+1] & v[k] \end{bmatrix}^T.$$

- Then

$$x[k+1] = \begin{bmatrix} v[k+3] \\ v[k+2] \\ v[k+1] \end{bmatrix} = \begin{bmatrix} -a_1 & -a_2 & -a_3 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} v[k+2] \\ v[k+1] \\ v[k] \end{bmatrix} + \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} u[k].$$

- We now add zeros, $G(z) = (b_1z^2 + b_2z + b_3) G_p(z)$. Equivalently,

$$Y(z) = [b_1z^2 + b_2z + b_3] V(z),$$

or, $y[k] = b_1v[k + 2] + b_2v[k + 1] + b_3v[k]$.

- In summary, we have the state-space model:

$$x[k + 1] = \begin{bmatrix} -a_1 & -a_2 & -a_3 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} x[k] + \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} u[k]$$

$$y[k] = [b_1 \ b_2 \ b_3] x[k] + [0] u[k].$$

- Note: There are many other equally valid state-space models of this particular transfer function. We will soon see how they are related.
- Many discrete-time transfer functions are not strictly proper. Solve by polynomial long division, and setting D equal to the quotient.
- MATLAB command `[A, B, C, D] = tf2ss(num, den, Ts)` converts a rational-polynomial transfer function form to state-space form.

5.2: Working with state-space systems

State-space to transfer function

- In the prior example, we saw it is possible to convert from a difference equation (or transfer function) to a state-space form quite easily.
- Now, we'll see that the opposite translation is also straightforward.
- Start with the state equations

$$\mathbf{x}[k + 1] = \mathbf{A}\mathbf{x}[k] + \mathbf{B}\mathbf{u}[k]$$

$$y[k] = \mathbf{C}\mathbf{x}[k] + \mathbf{D}\mathbf{u}[k].$$

- Take the z -transform of both sides of both equations

$$z\mathbf{X}(z) - z\mathbf{x}[0] = \mathbf{A}\mathbf{X}(z) + \mathbf{B}\mathbf{U}(z)$$

$$\mathbf{Y}(z) = \mathbf{C}\mathbf{X}(z) + \mathbf{D}\mathbf{U}(z),$$

or

$$(z\mathbf{I} - \mathbf{A})\mathbf{X}(z) = \mathbf{B}\mathbf{U}(z) + z\mathbf{x}[0]$$

$$\mathbf{X}(z) = (z\mathbf{I} - \mathbf{A})^{-1}\mathbf{B}\mathbf{U}(z) + (z\mathbf{I} - \mathbf{A})^{-1}z\mathbf{x}[0].$$

- This gives,

$$\mathbf{Y}(z) = \underbrace{[\mathbf{C}(z\mathbf{I} - \mathbf{A})^{-1}\mathbf{B} + \mathbf{D}]}_{\text{transfer function of system}} \mathbf{U}(z) + \underbrace{\mathbf{C}(z\mathbf{I} - \mathbf{A})^{-1}z\mathbf{x}[0]}_{\text{response to initial conditions}}.$$

- So,

$$\mathbf{G}(z) = \frac{\mathbf{Y}(z)}{\mathbf{U}(z)} = \mathbf{C}(z\mathbf{I} - \mathbf{A})^{-1}\mathbf{B} + \mathbf{D}.$$

- Note that $(z\mathbf{I} - \mathbf{A})^{-1} = \frac{\text{adj}(z\mathbf{I} - \mathbf{A})}{\det(z\mathbf{I} - \mathbf{A})}$, so we can write a system's transfer function as

$$\mathbf{G}(z) = \frac{\mathbf{C} \text{adj}(z\mathbf{I} - \mathbf{A})\mathbf{B} + \mathbf{D} \det(z\mathbf{I} - \mathbf{A})}{\det(z\mathbf{I} - \mathbf{A})}.$$

- Extremely important observation: The poles of the system are where $\det(z\mathbf{I} - \mathbf{A}) = 0$, which (by definition) are the eigenvalues of \mathbf{A} .

Transformation

- State-space representations of a particular system's dynamics are not unique. Selection of state $x[k]$ is somewhat arbitrary.
- To see this, analyze the transformation of

$$\mathbf{x}[k + 1] = \mathbf{A}\mathbf{x}[k] + \mathbf{B}\mathbf{u}[k]$$

$$\mathbf{y}[k] = \mathbf{C}\mathbf{x}[k] + \mathbf{D}\mathbf{u}[k],$$

where we let $\mathbf{x}[k] = \mathbf{T}\mathbf{w}[k]$, where \mathbf{T} is an invertible (similarity) transformation matrix. Then,

$$(\mathbf{T}\mathbf{w}[k + 1]) = \mathbf{A}(\mathbf{T}\mathbf{w}[k]) + \mathbf{B}\mathbf{u}[k]$$

$$\mathbf{y}[k] = \mathbf{C}(\mathbf{T}\mathbf{w}[k]) + \mathbf{D}\mathbf{u}[k].$$

- Multiplying the first equation by \mathbf{T}^{-1} gives

$$\mathbf{w}[k + 1] = \underbrace{\mathbf{T}^{-1}\mathbf{A}\mathbf{T}}_{\bar{\mathbf{A}}}\mathbf{w}[k] + \underbrace{\mathbf{T}^{-1}\mathbf{B}}_{\bar{\mathbf{B}}}\mathbf{u}[k]$$

$$\mathbf{y}[k] = \underbrace{\mathbf{C}\mathbf{T}}_{\bar{\mathbf{C}}}\mathbf{w}[k] + \underbrace{\mathbf{D}}_{\bar{\mathbf{D}}}\mathbf{u}[k]$$

$$\text{so, } \mathbf{w}[k + 1] = \bar{\mathbf{A}}\mathbf{w}[k] + \bar{\mathbf{B}}\mathbf{u}[k]$$

$$\mathbf{y}[k] = \bar{\mathbf{C}}\mathbf{w}[k] + \bar{\mathbf{D}}\mathbf{u}[k].$$

- To show that $\mathbf{H}_1(z) = \mathbf{H}_2(z)$,

$$\mathbf{H}_1(z) = \mathbf{C}(z\mathbf{I} - \mathbf{A})^{-1}\mathbf{B} + \mathbf{D}$$

$$= \mathbf{C}\mathbf{T}\mathbf{T}^{-1}(z\mathbf{I} - \mathbf{A})^{-1}\mathbf{T}\mathbf{T}^{-1}\mathbf{B} + \mathbf{D}$$

$$\begin{aligned}
&= (\mathbf{C}\mathbf{T})[\mathbf{T}^{-1}(z\mathbf{I} - \mathbf{A})\mathbf{T}]^{-1}(\mathbf{T}^{-1}\mathbf{B}) + \mathbf{D} \\
&= \bar{\mathbf{C}}(z\mathbf{I} - \bar{\mathbf{A}})^{-1}\bar{\mathbf{B}} + \bar{\mathbf{D}} = \mathbf{H}_2(z).
\end{aligned}$$

- Transfer function not changed by similarity transform

CONCLUSION: Can arrive at state-space representations having identical input-output relationship but different $(\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{D})$ matrices.

EXAMPLE: Consider transforming the system

$$\begin{aligned}
\mathbf{A} &= \begin{bmatrix} -a_1 & -a_2 & -a_3 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, & \mathbf{B} &= \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, & \text{with } \mathbf{T} &= \mathbf{T}^{-1} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}. \\
\mathbf{C} &= \begin{bmatrix} b_1 & b_2 & b_3 \end{bmatrix}, & \mathbf{D} &= \begin{bmatrix} 0 \end{bmatrix}
\end{aligned}$$

- Note that multiplying on the right by \mathbf{T} flips the original entries left-to-right; multiplying on the left flips the original entries top-to-bottom.
- So, for this transformation matrix, we get:

$$\begin{aligned}
\bar{\mathbf{A}} &= \mathbf{T}^{-1}\mathbf{A}\mathbf{T} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} -a_1 & -a_2 & -a_3 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} \\
&= \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -a_3 & -a_2 & -a_1 \end{bmatrix}
\end{aligned}$$

$$\bar{\mathbf{B}} = \mathbf{T}^{-1}\mathbf{B} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

$$\bar{\mathbf{C}} = \mathbf{C}\mathbf{T} = \begin{bmatrix} b_1 & b_2 & b_3 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} = \begin{bmatrix} b_3 & b_2 & b_1 \end{bmatrix}$$

$$\bar{\mathbf{D}} = \mathbf{D} = 0.$$

- We can find the transfer function of this new form as

$$\mathbf{G}(z) = \bar{\mathbf{C}}(z\mathbf{I} - \bar{\mathbf{A}})^{-1}\bar{\mathbf{B}} + \bar{\mathbf{D}}$$

$$\begin{aligned} &= \begin{bmatrix} b_3 & b_2 & b_1 \end{bmatrix} \left(\begin{bmatrix} z & 0 & 0 \\ 0 & z & 0 \\ 0 & 0 & z \end{bmatrix} - \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -a_3 & -a_2 & -a_1 \end{bmatrix} \right)^{-1} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} + 0 \\ &= \begin{bmatrix} b_3 & b_2 & b_1 \end{bmatrix} \left(\begin{bmatrix} z & -1 & 0 \\ 0 & z & -1 \\ a_3 & a_2 & z + a_1 \end{bmatrix} \right)^{-1} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \\ &= \frac{\begin{bmatrix} b_3 & b_2 & b_1 \end{bmatrix} \begin{bmatrix} z^2 + a_1z + a_2 & a_1 + z & 1 \\ -a_3 & z^2 + a_1z & z \\ -a_3z & -a_2z - a_3 & z^2 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}}{z^3 + a_1z^2 + a_2z + a_3} \\ &= \frac{\begin{bmatrix} b_3 & b_2 & b_1 \end{bmatrix} \begin{bmatrix} 1 \\ z \\ z^2 \end{bmatrix}}{z^3 + a_1z^2 + a_2z + a_3} = \frac{b_1z^2 + b_2z + b_3}{z^3 + a_1z^2 + a_2z + a_3}, \end{aligned}$$

which was the transfer function we started with before transformation.

5.3: Discrete-time Markov parameters

- It turns out that the discrete unit-pulse response of a state-space system has a special form that is important to us later.
- For example, let's look at the unit-pulse response of a single-input state-space system. (Note that, by definition, $x[0] = 0$ when finding a unit-pulse response).

- We find that

$$\begin{aligned}
 y[0] &= \mathbf{C}\mathbf{x}[0] + \mathbf{D}u[0] = \mathbf{D}, & \mathbf{x}[1] &= \mathbf{B} \\
 y[1] &= \mathbf{C}\mathbf{x}[1] + \mathbf{D}u[1] = \mathbf{C}\mathbf{B}, & \mathbf{x}[2] &= \mathbf{A}\mathbf{B} \\
 y[2] &= \mathbf{C}\mathbf{x}[2] + \mathbf{D}u[2] = \mathbf{C}\mathbf{A}\mathbf{B}, & \mathbf{x}[3] &= \mathbf{A}^2\mathbf{B} \\
 &\vdots & &\vdots \\
 y[k] &= \mathbf{C}\mathbf{A}^{k-1}\mathbf{B}, & k &\geq 1.
 \end{aligned}$$

- These unit-pulse-response values, $\{\mathbf{D}, \mathbf{C}\mathbf{B}, \mathbf{C}\mathbf{A}\mathbf{B}, \mathbf{C}\mathbf{A}^2\mathbf{B}, \mathbf{C}\mathbf{A}^3\mathbf{B}, \dots\}$ are called the Markov parameters of the system.
 - This turns out to be of critical importance to realizing our transfer functions, as we will see.
- Specifically, we define the Markov parameters to be:

$$\mathbf{g}_k = \begin{cases} \mathbf{D}, & k = 0; \\ \mathbf{C}\mathbf{A}^{k-1}\mathbf{B}, & k > 0. \end{cases}$$

CLARITY ISSUE: ■ For SISO systems, the Markov parameters are scalars.

- For a single-input multi-output (SIMO) system the Markov parameters are (column) vectors.

- The i th entry (row) of each Markov parameter is computed as the unit-pulse response from the input to the i th output.
- Equivalently, the entire vector Markov parameter is the unit-pulse response from the input to the vector output.
- For multi-input single-output (MISO) systems, the Markov parameters are row vectors.
 - The j th entry (column) of each Markov parameter is computed via the unit-pulse response from the j th input to the output.
- For multi-input multi output (MIMO) systems, the Markov parameters are matrices.
 - The (i, j) th entries yield the the unit-pulse response from the j th input to the i th output.
 - Equivalently, the j th column of each Markov parameter is vector (as in the SIMO case) which is computed via the unit-pulse response from the j th input to the vector output.

EXAMPLE: Given the following discrete-time system, with zero initial condition, find the unit-pulse response:

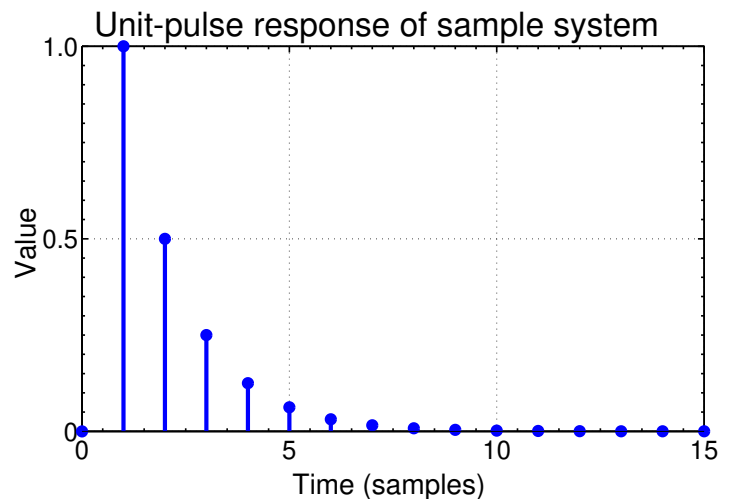
$$\mathbf{A} = \begin{bmatrix} 0.5 & 0 \\ 0 & 1 \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \mathbf{C} = \begin{bmatrix} 1 & -1 \end{bmatrix}, \quad \mathbf{D} = 0.$$

- The Markov parameters are given by

$$\begin{aligned} \mathbf{g}_k &= \{\mathbf{D}, \mathbf{C}\mathbf{B}, \mathbf{C}\mathbf{A}\mathbf{B}, \mathbf{C}\mathbf{A}^2\mathbf{B}, \dots\} \\ &= \{0, 1, 0.5, 0.25, \dots\}. \end{aligned}$$

- MATLAB's `impulse.m` command confirms this result:

```
A = [0.5 0; 0 1];
B = [1 ; 0];
C = [1 -1]; D = 0;
sys = ss(A,B,C,D,-1);
y = impulse(sys,0:15);
stem(0:15,y,'filled');
```



Before proceeding...

- We have now quickly previewed state-space models, with the claim that there will be a method to represent our battery models in that particular form.
- We now begin to investigate that claim—the first step is to create transfer-function models for the variables of interest.
- In this chapter, we look at representing c_s as a transfer function; in the next chapter we look at the remainder of the model equations.
 - Note that in chapter 3 we used symbols without an over-line to indicate point-wise values for variables of interest: *i.e.*, c_s , c_e , ϕ_s , ϕ_e .
 - In chapter 4 we used symbols with an over-line to indicate volume average versions of these point-wise variables: *i.e.*, \bar{c}_e , $\bar{\phi}_s$, and $\bar{\phi}_e$.
 - We now drop the over-line notation, because otherwise the equations get so highly decorated that they are impossible to parse. We are still talking about the volume-average quantities of chapter 4.

5.4: Equations describing the solid dynamics

Finding the transfer function $\tilde{C}_{s,e}(s)/J(s)$

- To find the transfer function for c_s , we follow the approach by Jacobsen and West¹
- We start with the underlying partial-differential equation,

$$\frac{\partial c_s(r, t)}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(D_s r^2 \frac{\partial c_s(r, t)}{\partial r} \right),$$

with standard boundary conditions,

$$D_s \frac{\partial c_s(0, t)}{\partial r} = 0, \quad \text{and} \quad D_s \frac{\partial c_s(R_s, t)}{\partial r} = -j(t), \quad t \geq 0,$$

and with initial equilibrium concentration,

$$c_s(r, 0) = c_{s,0}, \quad 0 \leq r \leq R_s.$$

- Note that we run into problems solving this PDE directly if $c_{s,0} \neq 0$.
- So, to enforce a homogeneous PDE in later steps, we define $\tilde{c}_s(r, t) = c_s(r, t) - c_{s,0}$. The “tilde” notation denotes the difference between an absolute quantity and its equilibrium set-point.
- If we assume constant D_s , the differential equations become:

$$\frac{\partial \tilde{c}_s(r, t)}{\partial t} = \frac{D_s}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \tilde{c}_s(r, t)}{\partial r} \right),$$

with boundary conditions,

$$D_s \frac{\partial \tilde{c}_s(0, t)}{\partial r} = 0, \quad \text{and} \quad D_s \frac{\partial \tilde{c}_s(R_s, t)}{\partial r} = -j(t), \quad t \geq 0,$$

and with initial equilibrium concentration,

$$\tilde{c}_s(r, 0) = 0, \quad 0 \leq r \leq R_s.$$

¹ Jacobsen, T., and West, K., “Diffusion Impedance in Planar, Cylindrical and Spherical Symmetry,” *Electrochimica Acta*, 40(2), 1995, pp. 255–62.

- We continue by taking the Laplace transform of the PDE:

$$s\tilde{C}_s(r, s) - \tilde{c}_0 = \frac{D_s}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \tilde{C}_s(r, s) \right)$$

$$s\tilde{C}_s(r, s) = \frac{D_s}{r^2} \left(2r \frac{\partial \tilde{C}_s(r, s)}{\partial r} + r^2 \frac{\partial^2 \tilde{C}_s(r, s)}{\partial r^2} \right).$$

- This is a 2nd-order ordinary differential equation in r , which may be written

$$\frac{\partial^2 \tilde{C}_s(r, s)}{\partial r^2} + \frac{2}{r} \frac{\partial \tilde{C}_s(r, s)}{\partial r} - \frac{s}{D_s} \tilde{C}_s(r, s) = 0.$$

- This homogeneous differential equation has a solution of the form

$$\tilde{C}_s(r, s) = \frac{A}{r} \exp\left(r \sqrt{\frac{s}{D_s}}\right) + \frac{B}{r} \exp\left(-r \sqrt{\frac{s}{D_s}}\right)$$

$$= \frac{A}{r} \exp(\beta(r)) + \frac{B}{r} \exp(-\beta(r)),$$

where we define $\beta(r) = r \sqrt{s/D_s}$. We note that $\beta(r)$ is also a function of s , but we omit this dependence in the notation for compactness.

- The constants A and B are chosen to satisfy the boundary conditions.
- Consider first the outer boundary condition at $r = R_s$, which is

$$D_s \frac{\partial \tilde{c}_s(r, t)}{\partial r} \Big|_{r=R_s} = -j(t).$$

- The equivalent Laplace-domain boundary condition is

$$D_s \frac{\partial \tilde{C}_s(r, s)}{\partial r} \Big|_{r=R_s} = -J(s).$$

- To substitute this in, we will need to compute $\partial \tilde{C}_s(r, s) / \partial r$

$$\frac{\partial \tilde{C}_s(r, s)}{\partial r} = \frac{A \sqrt{\frac{s}{D_s}} r \exp(\beta(r)) - B \exp(-\beta(r))}{r^2}$$

$$\begin{aligned} & - \frac{A \exp(\beta(r)) + B \sqrt{\frac{s}{D_s}} r \exp(-\beta(r))}{r^2} \\ & = \frac{A(\beta(r) - 1) \exp(\beta(r)) - B(1 + \beta(r)) \exp(-\beta(r))}{r^2}. \end{aligned}$$

- We substitute $r = R_s$ and the boundary condition

$$\begin{aligned} \left. \frac{\partial \tilde{C}_s(r, s)}{\partial r} \right|_{r=R_s} &= \frac{A(\beta(R_s) - 1) \exp(\beta(R_s)) - B(1 + \beta(R_s)) \exp(-\beta(R_s))}{R_s^2} \\ - \frac{J(s)}{D_s} &= \frac{A(\beta(R_s) - 1) \exp(\beta(R_s)) - B(1 + \beta(R_s)) \exp(-\beta(R_s))}{R_s^2}. \end{aligned}$$

- This gives us an expression for $J(s)$,

$$J(s) = - \frac{D_s}{R_s^2} (A(\beta(R_s) - 1) \exp(\beta(R_s)) - B(1 + \beta(R_s)) \exp(-\beta(R_s))).$$

- If we immediately substitute the second boundary condition at $r = 0$, we run into some divide-by-zero issues.

- So, instead, we substitute $r = r_\delta$, which we think of as a very small value. We will then later take the limit as $r_\delta \rightarrow 0$.

$$0 = \frac{A(\beta(r_\delta) - 1) \exp(\beta(r_\delta)) - B(1 + \beta(r_\delta)) \exp(-\beta(r_\delta))}{r_\delta^2}.$$

- This allows us to write

$$\begin{aligned} \frac{A(\beta(r_\delta) - 1) \exp(\beta(r_\delta))}{r_\delta^2} &= \frac{B(1 + \beta(r_\delta)) \exp(-\beta(r_\delta))}{r_\delta^2} \\ A &= B \frac{(1 + \beta(r_\delta)) \exp(-\beta(r_\delta))}{(\beta(r_\delta) - 1) \exp(\beta(r_\delta))}. \end{aligned}$$

- We now take the limit as $r_\delta \rightarrow 0$, and find that $A = -B$.

- We are now ready to construct the transfer function $\tilde{C}_s(s, r)/J(s)$

$$\begin{aligned}
\frac{\tilde{C}_s(r, s)}{J(s)} &= \frac{-R_s^2}{D_s r} \left[\frac{A \exp(\beta(r)) + B \exp(-\beta(r))}{A(\beta(R_s) - 1) \exp(\beta(R_s)) - B(1 + \beta(R_s)) \exp(-\beta(R_s))} \right] \\
&= \frac{-R_s^2}{D_s r} \left[\frac{A}{-A} \right] \left[\frac{\exp(\beta(r)) - \exp(-\beta(r))}{(1 - \beta(R_s)) \exp(\beta(R_s)) - (1 + \beta(R_s)) \exp(-\beta(R_s))} \right] \\
&= \frac{R_s^2}{D_s r} \left[\frac{\exp(\beta(r)) - \exp(-\beta(r))}{(1 - \beta(R_s)) \exp(\beta(R_s)) - (1 + \beta(R_s)) \exp(-\beta(R_s))} \right].
\end{aligned}$$

- This expression can be used to determine the lithium concentration anywhere within the particle.
- However, we are most interested in determining the concentration at the *surface* of the particle, where $r = R_s$. So, we substitute $r = R_s$

$$\frac{\tilde{C}_{s,e}(s)}{J(s)} = \frac{R_s}{D_s} \left[\frac{\exp(\beta(R_s)) - \exp(-\beta(R_s))}{(1 - \beta(R_s)) \exp(\beta(R_s)) - (1 + \beta(R_s)) \exp(-\beta(R_s))} \right].$$

- To compact the notation yet again, write $\beta(R_s)$ as simply β ,

$$\begin{aligned}
\frac{\tilde{C}_{s,e}(s)}{J(s)} &= \frac{R_s}{D_s} \left[\frac{\exp(\beta) - \exp(-\beta)}{(1 - \beta) \exp(\beta) - (1 + \beta) \exp(-\beta)} \right] \\
&= \frac{R_s}{D_s} \left[\frac{\exp(\beta) - \exp(-\beta)}{\exp(\beta) - \exp(-\beta) - \beta [\exp(\beta) + \exp(-\beta)]} \right] \\
&= \frac{R_s}{D_s} \left[\frac{\frac{\exp(\beta) - \exp(-\beta)}{\exp(\beta) + \exp(-\beta)}}{\frac{\exp(\beta) - \exp(-\beta)}{\exp(\beta) + \exp(-\beta)} - \beta} \right] \\
&= \frac{R_s}{D_s} \left[\frac{\tanh(\beta)}{\tanh(\beta) - \beta} \right] = \frac{R_s}{D_s} \left[\frac{1}{1 - \beta \coth(\beta)} \right].
\end{aligned}$$

- To recap to this point, re-expanding notation, where $\beta(s, r) = r\sqrt{s/D_s}$,

$$\boxed{\tilde{C}_{s,e}(s) = \frac{R_s}{D_s} \left[\frac{1}{1 - \beta(s, R_s) \coth(\beta(s, R_s))} \right] J(s).}$$

5.5: Removing the integrator pole

- While not immediately obvious by looking at the transfer function, it turns out that $\tilde{C}_{s,e}(s)/J(s)$ is unstable: There is a pole at $s = 0$.
 - This is intuitively clear, however, because we know that a step input will result in ever-increasing concentration.
 - This will be important when we look at how to convert the transfer function to a state-space model.
- To make a stable transfer function, define $\Delta\tilde{C}_{s,e}(s) = \tilde{C}_{s,e}(s) - \tilde{C}_{s,\text{avg}}(s)$, where $\tilde{C}_{s,\text{avg}}(s)$ is the bulk (average) concentration in the solid, less $c_{s,0}$.
- Note that we can write $\tilde{c}_{s,\text{avg}}(t_1)$ for some arbitrary point in time t_1 as

$$\tilde{c}_{s,\text{avg}}(t_1) = \int_0^{t_1} \frac{\text{Influx of Li, [mol s}^{-1}\text{]}}{\text{Volume of particle [m}^3\text{]}} dt.$$

- Note two things:
 - The volume of a sphere of radius R_s is $\frac{4}{3}\pi R_s^3$ [m³];
 - The influx of lithium is $-j(t)$ [mol m⁻² s⁻¹], occurring over the surface area $4\pi R_s^2$ [m²].
- This gives

$$\begin{aligned}\tilde{c}_{s,\text{avg}}(t_1) &= \int_0^{t_1} \frac{-j(t) \cdot 4\pi R_s^2}{\frac{4}{3}\pi R_s^3} dt \\ &= -\frac{3}{R_s} \int_0^{t_1} j(t) dt \\ \frac{d}{dt}\tilde{c}_{s,\text{avg}}(t) &= -\frac{3}{R_s} j(t).\end{aligned}$$

- Note that this result is perfectly general. We made no assumptions on how the lithium concentration is distributed inside the particle.
- Taking Laplace transforms, we find:

$$\frac{\tilde{C}_{s,\text{avg}}(s)}{J(s)} = -\frac{3}{R_s} \frac{1}{s}.$$

- Therefore,

$$\begin{aligned} \frac{\Delta \tilde{C}_{s,e}(s)}{J(s)} &= \frac{\tilde{C}_{s,e}(s)}{J(s)} - \frac{\tilde{C}_{s,\text{avg}}(s)}{J(s)} \\ &= \frac{R_s}{D_s} \left[\frac{\tanh(\beta)}{\tanh(\beta) - \beta} \right] + \frac{3}{R_s s} \\ &= \frac{R_s}{D_s} \left[\frac{\tanh(\beta) + \frac{3D_s}{sR_s^2} (\tanh(\beta) - \beta)}{\tanh(\beta) - \beta} \right] \\ &= \frac{R_s}{D_s} \left[\frac{\tanh(\beta) + \frac{3}{\beta^2} (\tanh(\beta) - \beta)}{\tanh(\beta) - \beta} \right] \\ &= \frac{R_s}{D_s} \left[\frac{\beta^2 \tanh(\beta) + 3 (\tanh(\beta) - \beta)}{\beta^2 (\tanh(\beta) - \beta)} \right] \\ &= \frac{R_s}{D_s} \left[\frac{(\beta^2 + 3) \tanh(\beta) - 3\beta}{\beta^2 (\tanh(\beta) - \beta)} \right]. \end{aligned}$$

State-space realization problem

- It turns out that for this specific case, we can find all the poles and zeros using a simple numeric method, and use that information to make a discrete-time state-space model.
- For the transfer functions we develop in the next chapter, however, this cannot be done.
- So, we must turn to alternative implementation approaches.

- One method is to use nonlinear optimization to select poles and residues to attempt to match the frequency response of the transfer functions.
 - This is fraught with problems.
 - We next introduce another approach, which directly gives us a discrete-time state-space approximate model of our transfer functions.
- This system-identification problem for state-space systems is sometimes called the “realization problem.”
- That is, we wish to find a realization (a set of A , B , C , and D matrices) that describe a system’s dynamics.

5.6: State-space realization problem: Ho–Kalman method

- For now, we assume that we are able to find the Markov parameters of our transfer functions.

PROBLEM: Given a system's Markov parameters, find the system dimension n and (A, B, C, D) , up to similarity transforms.

- One of the first (maybe *the* first) state-space realization methods was introduced by Ho and Kalman.²
- It is key to the discrete-time realization algorithm we will develop.
- Notice that something curious happens when we multiply the following matrices together:

$$\underbrace{\begin{bmatrix} C \\ CA \\ CA^2 \\ \vdots \\ CA^{n-1} \end{bmatrix}}_{\mathcal{O}} \underbrace{\begin{bmatrix} B & AB & A^2B & \dots & A^{n-1}B \end{bmatrix}}_{\mathcal{C}} = \begin{bmatrix} CB & CAB & CA^2B & \dots & CA^{n-1}B \\ CAB & CA^2B & CA^3B & & \\ CA^2B & CA^3B & CA^4B & & \\ \vdots & & & \ddots & \vdots \\ CA^{n-1}B & & & \dots & CA^{2n-2}B \end{bmatrix}.$$

- For reasons beyond the scope of our discussion here, \mathcal{O} is called the “observability matrix” and \mathcal{C} is called the “controllability matrix.”

² B.L. Ho and R.E. Kalman, “Effective Construction of Linear State Variable Models from Input/Output Functions,” *Regelungstechnik*, vol. 14, no. 12, pp. 545–8, 1966.

- Notice that we get a Hankel matrix—a matrix having constant skew diagonals (an upside-down Toeplitz matrix).
- Note also that the values on the skew diagonals are the Markov parameters of the system (excluding g_0 and g_k for $k > 2n - 1$)

$$\mathcal{H} = \mathcal{O}\mathcal{C} = \begin{bmatrix} \mathbf{g}_1 & \mathbf{g}_2 & \cdots & \mathbf{g}_n \\ \mathbf{g}_2 & \mathbf{g}_3 & & \\ \vdots & & \ddots & \vdots \\ \mathbf{g}_n & & \cdots & \mathbf{g}_{2n-1} \end{bmatrix}.$$

- Ho–Kalman assumes that we know the Markov parameters.
 - Knowledge of g_0 gives us D directly.
 - Knowledge of the rest of the Markov parameters will ultimately result in A , B , and C .
- To use Ho–Kalman, we must first form the Hankel matrix \mathcal{H} .
- The next step is to factor $\mathcal{H} = \mathcal{O}\mathcal{C}$ into its \mathcal{O} and \mathcal{C} components.
- The third step is to use \mathcal{O} and \mathcal{C} to find A , B , and C .

ISSUE I: We don't know n . So, how do we form \mathcal{H} in the first place? That is, when do we stop adding unit-pulse-response values to \mathcal{H} ?

PRELIMINARY ANSWER: The rank of \mathcal{H} is equal to n . Keep adding data until the rank doesn't increase.

ISSUE II: How do we compute A , B , and C from \mathcal{O} and \mathcal{C} ?

ANSWER: C is extracted as the first block row of \mathcal{O} ; B is extracted as the first block column of \mathcal{C} . We'll see how to get A shortly.

ISSUE III: How do we do the factoring of \mathcal{H} into \mathcal{O} and \mathcal{C} ?

ANSWER: It doesn't matter, at least in principle. Any matrices \mathcal{O} and \mathcal{C} such that $\mathcal{O}\mathcal{C} = \mathcal{H}$ are okay.

- To see this latter point, consider what happens to \mathcal{O} and \mathcal{C} when the state-space model undergoes a similarity transformation.
 - Recall that $\bar{A} = T^{-1}AT$, $\bar{B} = T^{-1}B$, and $\bar{C} = CT$.
 - The observability and controllability matrices of the new representation are

$$\bar{\mathcal{O}} = \begin{bmatrix} \bar{C} \\ \bar{C}\bar{A} \\ \vdots \\ \bar{C}\bar{A}^{n-1} \end{bmatrix} = \begin{bmatrix} CT \\ CTT^{-1}AT \\ \vdots \\ CT(T^{-1}AT)^{n-1} \end{bmatrix} = \mathcal{O}T$$

$$\bar{\mathcal{C}} = \begin{bmatrix} \bar{B} & \bar{A}\bar{B} & \dots & \bar{A}^{n-1}\bar{B} \end{bmatrix}$$

$$= \begin{bmatrix} T^{-1}B & T^{-1}ATT^{-1}B & \dots & (T^{-1}AT)^{n-1}T^{-1}B \end{bmatrix} = T^{-1}\mathcal{C}.$$

- Therefore, $\bar{\mathcal{O}}\bar{\mathcal{C}} = (\mathcal{O}T)(T^{-1}\mathcal{C}) = \mathcal{O}\mathcal{C}$
 - If we factor \mathcal{H} one way, we end up with a representation that has one set of \mathcal{O} and \mathcal{C} .
 - If we factor \mathcal{H} any other way, we end up with a representation that has an alternate set of $\bar{\mathcal{O}}$ and $\bar{\mathcal{C}}$.
 - But, these representations are related via a similarity transformation T .
- That is, no matter how we factor \mathcal{H} , we end up with different A , B , and C matrices, but the same input-output relationship (same transfer function, same unit-pulse response, but different state descriptions).

- For example, we could choose to let $\mathcal{O} = \mathbf{I}$, and then $\mathcal{C} = \mathcal{H}$. This will result in an \mathbf{A} , \mathbf{B} , and \mathbf{C} that are in “observability canonical form.” (cf. ECE5520)
- Or, we could choose to let $\mathcal{C} = \mathbf{I}$, and then $\mathcal{O} = \mathcal{H}$. This will result in an \mathbf{A} , \mathbf{B} , and \mathbf{C} that are in “controllability canonical form.”

ISSUE IV: Is there a “best” way to factor \mathcal{H} ? Yes. . . enter the SVD.

5.7: Singular value decomposition

FACT: Any rectangular matrix $A \in \mathbb{R}^{m \times n}$, where $\text{rank}(A) = r$, can be factored into the form:

$$A = U \Sigma V^T.$$

- $U = [\mathbf{u}_1, \dots, \mathbf{u}_r] \in \mathbb{R}^{m \times r}$, and $U^T U = I$, and \mathbf{u}_i are the left or output singular vectors of A .
- $V = [\mathbf{v}_1, \dots, \mathbf{v}_r] \in \mathbb{R}^{n \times r}$, and $V^T V = I$, and \mathbf{v}_i are the right or input singular vectors of A .
- $\Sigma = \text{diag}(\sigma_1, \dots, \sigma_r)$ where $\sigma_1 \geq \dots \geq \sigma_r > 0$, and σ_i are the (nonzero) singular values of A .

▪ The above is called a compact SVD. Most often, we compute a full SVD, where

- $U = [\mathbf{u}_1, \dots, \mathbf{u}_m] \in \mathbb{R}^{m \times m}$, and $U^T U = I$,
- $V = [\mathbf{v}_1, \dots, \mathbf{v}_n] \in \mathbb{R}^{n \times n}$, and $V^T V = I$,
- The matrix $\Sigma \in \mathbb{R}^{m \times n}$ is “diagonal”

$$\Sigma = \begin{bmatrix} \sigma_1 & & 0 & 0 \\ & \ddots & & 0 \\ 0 & & \sigma_m & 0 \end{bmatrix} \text{ or } \Sigma = \begin{bmatrix} \sigma_1 & & 0 \\ & \ddots & \\ 0 & & \sigma_n \end{bmatrix} \text{ or } \Sigma = \begin{bmatrix} \sigma_1 & & 0 \\ & \ddots & \\ 0 & & \sigma_n \\ 0 & 0 & 0 \end{bmatrix}$$

when $m < n$, $m = n$ and $m > n$, respectively.

- In this case, $\sigma_1 \geq \dots \geq \sigma_r > 0$, and $\sigma_i = 0$ for $i > r$.
- In MATLAB, `svd.m` and `svds.m`
- We often write the full SVD as partitioned:

$$A = \begin{bmatrix} U_1 & \vdots & U_2 \end{bmatrix} \begin{bmatrix} \Sigma_1 & \vdots & \mathbf{0}_{r \times (n-r)} \\ \hline \mathbf{0}_{(m-r) \times r} & \vdots & \mathbf{0}_{(m-r) \times (n-r)} \end{bmatrix} \begin{bmatrix} V_1^T \\ \hline V_2^T \end{bmatrix},$$

where $A = U_1 \Sigma_1 V_1^T$ is the compact SVD.

- Note that the singular values are related to matrix norm. In particular, $\|A\| = \sigma_1$.
- Can view operation $y = Ax$ as $y = (U \Sigma V^T)x$, decomposing the operation into
 - Computing coefficients of x along the input directions v_1, \dots, v_r (rotating by V^T)
 - ◆ v_1 is the most sensitive (highest gain) input direction
 - Scaling the coefficients by σ_i (dilation)
 - Reconstituting along output directions u_1, \dots, u_r .
 - ◆ u_1 is the highest gain output direction. $Av_1 = \sigma_1 u_1$.
- SVD gives a picture of gain as a function of input/output directions.

EXAMPLE: Consider $A \in \mathbb{R}^{4 \times 4}$ with $\Sigma = \text{diag}(10, 7, 0.1, 0.05)$.

- Input components along directions v_1 and v_2 are amplified (by about 10) and come out mostly along the plane spanned by u_1 and u_2 .
- Input components along directions v_3, v_4 are attenuated (by about 10).
- $\|Ax\| / \|x\|$ can range between 10 and 0.05; A is nonsingular.
- For some applications you might say that A is *effectively* rank 2 (this will be important for us later).

Low-rank approximations

- Suppose that $A \in \mathbb{R}^{m \times n}$ and $\text{rank}(A) = r$, with SVD

$$A = U \Sigma V^T = \sum_{i=1}^r \sigma_i \mathbf{u}_i \mathbf{v}_i^T.$$

- We want to approximate A by \hat{A} , where $\text{rank}(\hat{A}) \leq p < r$ such that $\hat{A} \approx A$ in the sense that $\|A - \hat{A}\|$ is minimized.

- The optimal rank p approximator is $\hat{A} = \sum_{i=1}^p \sigma_i \mathbf{u}_i \mathbf{v}_i^T$ and hence

$$\|A - \hat{A}\| = \left\| \sum_{i=p+1}^r \sigma_i \mathbf{u}_i \mathbf{v}_i^T \right\| = \sigma_{p+1}$$

because σ_{p+1} is the maximum remaining singular value.

INTERPRETATION: SVD dyads $\mathbf{u}_i \mathbf{v}_i^T$ are ranked in order of ‘importance’; take p of them to get a rank p approximant.

APPLICATION: We can use this idea to simplify models (very useful).

Suppose that

- $\mathbf{y} = A\mathbf{x} + \mathbf{v}$ where $A \in \mathbb{R}^{100 \times 30}$ has SVs 10, 7, 2, 0.5, 0.01, \dots , 0.0001.
- $\|\mathbf{x}\|$ is on the order of 1, and unknown error or noise \mathbf{v} has norm on the order of 0.1.
- Then, the terms $\sigma_i \mathbf{u}_i \mathbf{v}_i^T \mathbf{x}$ for $i = 5, \dots, 30$ are substantially smaller than the noise term \mathbf{v} .
- So, we can approximate $\mathbf{y} = A\mathbf{x} + \mathbf{v}$ by the much simplified model

$$\mathbf{y} = \sum_{i=1}^4 \sigma_i \mathbf{u}_i \mathbf{v}_i^T \mathbf{x} + \mathbf{v}.$$

5.8: Back to Ho–Kalman

- Recall Ho–Kalman “ISSUE 1,” how do we form the Hankel matrix \mathcal{H} if we don’t know the dimension of the system state n ?
- To address this issue, consider the infinite, skew-diagonal matrix \mathcal{H}_∞ :

$$\mathcal{H}_\infty = \begin{bmatrix} \mathbf{g}_1 & \mathbf{g}_2 & \mathbf{g}_3 & \mathbf{g}_4 & \cdots \\ \mathbf{g}_2 & \mathbf{g}_3 & \mathbf{g}_4 & \mathbf{g}_5 & \cdots \\ \mathbf{g}_3 & \mathbf{g}_4 & \mathbf{g}_5 & \mathbf{g}_6 & \cdots \\ \mathbf{g}_4 & \mathbf{g}_5 & \mathbf{g}_6 & \mathbf{g}_7 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

where the entries \mathbf{g}_k correspond to the Markov parameters for the given system.

- This form is called an infinite Hankel matrix, or Hankel operator.
- We can also define a finite Hankel matrix, formed by the first k rows and l columns of \mathcal{H}

$$\mathcal{H}_{k,l} = \begin{bmatrix} \mathbf{g}_1 & \mathbf{g}_2 & \mathbf{g}_3 & \cdots & \mathbf{g}_l \\ \mathbf{g}_2 & \mathbf{g}_3 & \mathbf{g}_4 & \cdots & \mathbf{g}_{l+1} \\ \mathbf{g}_3 & \mathbf{g}_4 & \mathbf{g}_5 & \cdots & \mathbf{g}_{l+2} \\ \vdots & \vdots & \vdots & & \vdots \\ \mathbf{g}_k & \mathbf{g}_{k+1} & \mathbf{g}_{k+2} & \cdots & \mathbf{g}_{k+l-1} \end{bmatrix}.$$

- This finite Hankel matrix factors into $\mathcal{H}_{k,l} = \mathcal{O}_k \mathcal{C}_l$ where:

$$\mathcal{O}_k = \begin{bmatrix} \mathbf{C} \\ \mathbf{C}\mathbf{A} \\ \vdots \\ \mathbf{C}\mathbf{A}^{k-1} \end{bmatrix}, \quad \mathcal{C}_l = \begin{bmatrix} \mathbf{B} & \mathbf{A}\mathbf{B} & \mathbf{A}^2\mathbf{B} & \cdots & \mathbf{A}^{l-1}\mathbf{B} \end{bmatrix}.$$

- The approach we will take is to make a $\mathcal{H}_{k,l}$ of larger size than we expect for a hypothesized value of n . That is, $k > n$ and $l > n$.

- Therefore $\mathcal{O}_k \neq \mathcal{O}$ and $\mathcal{C}_l \neq \mathcal{C}$ even though the matrices have the same general form. We call \mathcal{O}_k the extended observability matrix and \mathcal{C}_l the extended controllability matrix.
- We then apply the SVD to $\mathcal{H}_{k,l}$

$$\begin{aligned}\mathcal{H}_{k,l} &= U \Sigma V^T = U \Sigma^{1/2} \Sigma^{1/2} V^T \\ &= U \Sigma^{1/2} T T^{-1} \Sigma^{1/2} V^T \\ &= \underbrace{(U \Sigma^{1/2} T)}_{\mathcal{O}_k} \underbrace{(T^{-1} \Sigma^{1/2} V^T)}_{\mathcal{C}_l}.\end{aligned}$$
- The first n non-zero singular values provide insight into model order.
 - Problem: Noisy data yields more than n non-zero singular values.
 - Need to look at a few and determine when there is a “significant” drop off in the magnitude of the SVDs.
- Note that this approach also gives us \mathcal{O}_k and \mathcal{C}_l automatically in a “balanced realization”. Solves “ISSUE III” and “ISSUE IV”.
 - T must be invertible, but selection of T is otherwise arbitrary. Usually use $T = I$.
- How to decompose further into (A, B, C) to solve “ISSUE II”?
- Note the shift property of a Hankel matrix. If we shift \mathcal{H} up by one block row, we get $\mathcal{H}_{k+1,l}^\uparrow = \mathcal{O}_k A \mathcal{C}_l$.

$$\mathcal{H}_{k+1,l}^\uparrow = \begin{bmatrix} \mathbf{g}_2 & \mathbf{g}_3 & \mathbf{g}_4 & \cdots & \mathbf{g}_{l+1} \\ \mathbf{g}_3 & \mathbf{g}_4 & \mathbf{g}_5 & \cdots & \mathbf{g}_{l+2} \\ \vdots & \vdots & \vdots & & \vdots \\ \mathbf{g}_k & \mathbf{g}_{k+1} & \mathbf{g}_{k+2} & \cdots & \mathbf{g}_{k+l-1} \\ \mathbf{g}_{k+1} & \mathbf{g}_{k+2} & \mathbf{g}_{k+3} & \cdots & \mathbf{g}_{k+l} \end{bmatrix}$$

$$\begin{aligned}
&= \begin{bmatrix} \mathbf{CAB} & \mathbf{CA}^2\mathbf{B} & \mathbf{CA}^3\mathbf{B} & \dots & \mathbf{CA}^l\mathbf{B} \\ \mathbf{CA}^2\mathbf{B} & \mathbf{CA}^3\mathbf{B} & \mathbf{CA}^4\mathbf{B} & & \mathbf{CA}^{l+1}\mathbf{B} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{CA}^{k-1}\mathbf{B} & \mathbf{CA}^k\mathbf{B} & \mathbf{CA}^{k+1}\mathbf{B} & \dots & \mathbf{CA}^{k+l-2}\mathbf{B} \\ \mathbf{CA}^k\mathbf{B} & \mathbf{CA}^{k+1}\mathbf{B} & \mathbf{CA}^{k+2}\mathbf{B} & \dots & \mathbf{CA}^{k+l-1}\mathbf{B} \end{bmatrix} \\
&= \mathcal{O}_{k+1}^\uparrow \mathbf{C}_l = \mathcal{O}_k \mathbf{C}_{l+1}^\leftarrow = \mathcal{O}_k \mathbf{A} \mathbf{C}_l.
\end{aligned}$$

- Using the pseudo-inverse to solve for \mathbf{A} gives $\mathbf{A} = \mathcal{O}_k^\dagger \mathcal{H}_{k+1,l}^\uparrow \mathbf{C}_l^\dagger$.
- In MATLAB, we can compute either

```
Ahat = pinv(Ok)*HankelUp*pinv(Cl);
```

or

```
Ahat = (Ok\HankelUp)/Cl;
```

- As before, we extract \mathbf{B} from the first block column of the controllability matrix we derived via SVD.
- Also, extract \mathbf{C} from the first block row of the observability matrix we derived via SVD, and set $\mathbf{D} = \mathbf{g}_0$.

5.9: Ho–Kalman summary and example

STEP I: Collect the unit-pulse response values into two Hankel matrices

1. An original finite Hankel matrix
2. A shifted version matrix of the original Hankel matrix (same size)

STEP II: Compute the SVD of the (unshifted) Hankel matrix

- Identify system order from the singular values
- May need to iterate on choice of Hankel matrix (discussed later)

STEP III: Compute the extended observability and controllability matrices

- Use appropriately dimensioned SVD components
- Typically use $T = I_n$

STEP IV: Identify the system matrices (A, B, C). $D = g_0$.

EXAMPLE: Suppose that a unit pulse yields the following response:

$$y = (0, 1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, \dots).$$

- We recognize this output as the Fibonacci sequence generated by $g_k = g_{k-1} + g_{k-2}$ with initial conditions $g_0 = 0$ and $g_1 = 1$.
- A typical realization for this sequence is given by the state-space system:

$$\mathbf{A} = \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \mathbf{C} = \begin{bmatrix} 1 & 0 \end{bmatrix}, \quad \mathbf{D} = 0.$$

- We'll try to come up with an equivalent realization based on only the unit-pulse response.

```
% Define true system, compute the Markov parameters as "y"
A = [0 1; 1 1]; B = [1; 1]; C = [1 0]; D = 0; dt = 1;
sysTrue = ss(A,B,C,D,dt); % "typical" Fibonacci ss model
y = dt*impulse(sysTrue); % scale by dt to get unit-pulse response
```

- The Hankel matrices that we will require are:

$$\mathcal{H}_{4,4} = \begin{bmatrix} 1 & 1 & 2 & 3 \\ 1 & 2 & 3 & 5 \\ 2 & 3 & 5 & 8 \\ 3 & 5 & 8 & 13 \end{bmatrix}, \quad \mathcal{H}_{5,4}^{\uparrow} = \begin{bmatrix} 1 & 2 & 3 & 5 \\ 2 & 3 & 5 & 8 \\ 3 & 5 & 8 & 13 \\ 5 & 8 & 13 & 21 \end{bmatrix}.$$

```
% Form H{4,4} and shifted H{5,4}. Note: Do not include "zero-th"
% parameter (first element of y), which corresponds to the matrix D.
bigHankel = hankel(y(2:end)); % don't forget to omit h(0) term = y(1)
H = bigHankel(1:4,1:4); % for this example, keep only 4x4 portion
Hup = bigHankel(2:5,1:4); % shifted H{5,4}
```

- The SVD yields

$$\sigma_1 = 54.56 \quad \sigma_2 = 0.43988 \quad \sigma_i = 0, \quad i \geq 3$$

which indicates that $n = 2$.

```
% Compute singular values of Hankel matrix
[U,S,V] = svd(H);

% Identify system order off-line as n = 2 based on values of S
n = 2;
```

- We now extract the two left columns of U and V

$$U = V = \begin{bmatrix} -0.1876 & 0.7947 \\ -0.3035 & -0.4911 \\ -0.4911 & 0.3035 \\ -0.7947 & -0.1876 \end{bmatrix}.$$

- Compute the extended observability and controllability matrices

$$\mathbf{C}_l = \mathbf{\Sigma}^{1/2} \mathbf{V}^T = \begin{bmatrix} -0.8507 & -1.3764 & -2.2270 & -3.6034 \\ 0.5257 & -0.3249 & 0.2008 & -0.1241 \end{bmatrix}$$

$$\mathbf{O}_k = \mathbf{U} \mathbf{\Sigma}^{1/2} = \mathbf{C}_l^T.$$

```
% Compute extended observability and controllability matrices, sized to
% the order for the system inferred by the singular values.
```

```
Us = U(:,1:n); Ss = S(1:n,1:n); Vs = V(:,1:n);
```

```
Ok = Us*sqrtm(Ss); Cl = sqrtm(Ss)*Vs';
```

- Identify the system matrices $(\hat{\mathbf{A}}, \hat{\mathbf{B}}, \hat{\mathbf{C}})$ up to similarity transform

$$\hat{\mathbf{A}} = \mathbf{O}_k^\dagger \mathcal{H}_{k+1,l}^\dagger \mathbf{C}_l^\dagger = \begin{bmatrix} 1.6180 & 0 \\ 0 & -0.6180 \end{bmatrix}$$

$$\hat{\mathbf{B}} = \mathbf{C}_l(1:n, 1:m) = \mathbf{C}_l(1:2, 1) = \begin{bmatrix} -0.8057 \\ 0.5257 \end{bmatrix}$$

$$\hat{\mathbf{C}} = \mathbf{O}_k(1:p, 1:n) = \mathbf{O}_k(1, 1:2) = \begin{bmatrix} -0.8057 & 0.5257 \end{bmatrix}$$

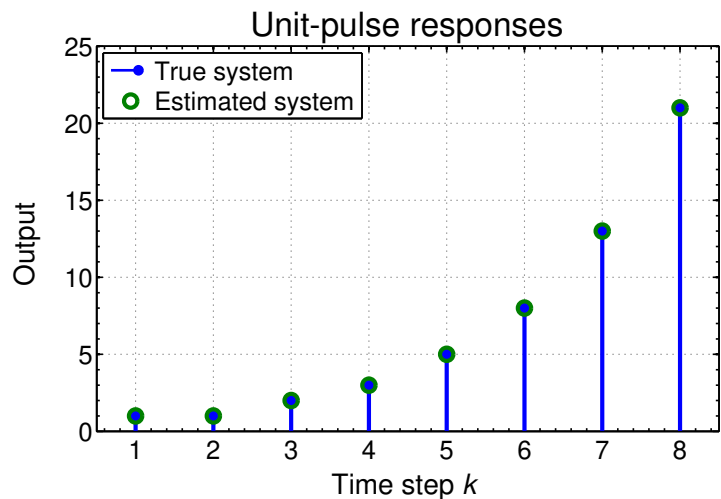
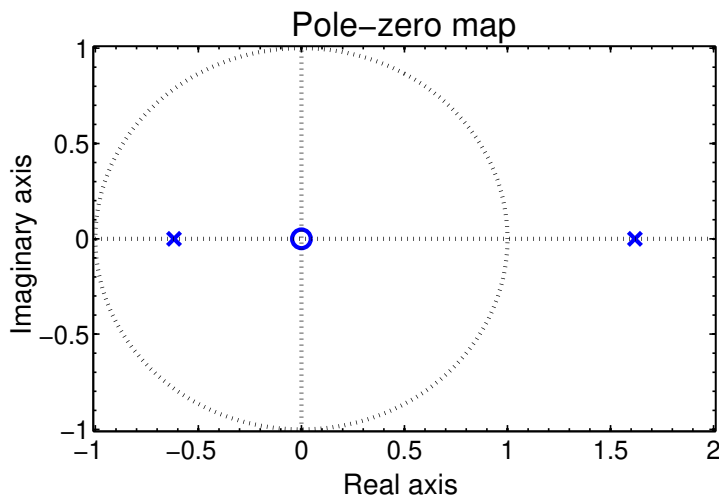
$$\hat{\mathbf{D}} = g_0 = 0.$$

```
% Identify system assuming p = m = 1 (SISO), using shifted Hankel matrix
```

```
Ahat = (Ok\Hup)/Cl; Bhat = Cl(:,1); Chat = Ok(1,:); Dhat = y(1);
```

```
sysEst = ss(Ahat, Bhat, Chat, Dhat, dt);
```

- Now, let's compare the true and identified (“estimated”) systems
 - Same pole-zero mapping (eigenvalues...transfer function)
 - Same unit-pulse responses



COMMENTS: Selecting an appropriate amount of output data to store may require iteration (“how big an \mathcal{H} do I need?”)

- Until $\text{rank}(\mathcal{H}_{k,l}) = \text{rank}(\mathcal{H}_{k-1,l-1})$, or
- Until the next singular value is “insignificant.”
- Interesting to note that $\mathbf{A} = \mathbf{A}^T$ and that $\mathbf{B} = \mathbf{C}^T$ for the identified system in the example.
 - This property holds for square Hankel matrices
 - The identification process will work so long as the Hankel matrix dimensions exceed the system order (\mathcal{H} need not be square)

REMAINING QUESTION: From whence come the \mathbf{g}_k ?

- This is key to making the DRA work.

5.10: Discrete-Time Realization Algorithm (DRA)

- Given a continuous-time transfer function in the Laplace domain, $H(s) = Y(s)/U(s)$, and a sampling period, T_s , we want to derive a reduced-order discrete-time state-space realization of the form

$$\mathbf{x}[k + 1] = \mathbf{A}\mathbf{x}[k] + \mathbf{B}\mathbf{u}[k]$$

$$\mathbf{y}[k] = \mathbf{C}\mathbf{x}[k] + \mathbf{D}\mathbf{u}[k],$$

- A *sufficient* condition for the DRA to operate is that $H(s)$ be an element of the Hardy space \mathcal{H}_∞ , which implies that it is a strictly stable and proper system.
- This is not a *necessary* condition, however, as we will later generalize the method to work with systems having isolated pole(s) on the imaginary axis.
- Note that we do not restrict $H(s)$ to be formulated as a quotient of polynomials in the Laplace variable “ s ” (for which well-known methods exist to find the discrete-time system).
- We describe the algorithm in four steps, which we preview here, and discuss in more detail in the following subsections.

STEP 1: Sample the continuous-time transfer function $H(s)$ in the frequency domain at a high rate, and take the inverse discrete Fourier transform (IDFT) of the samples to get an approximation to the continuous-time impulse response $h(t)$.

STEP 2: Use $h(t)$ to approximate the continuous-time step response $h_{\text{step}}(t)$, also sampled at the high rate.

STEP 3: Compute discrete-time unit-pulse response g_k with inter-sample period T_s from continuous-time step response $h_{\text{step}}(t)$, assuming a sample and hold circuit connected to system input.

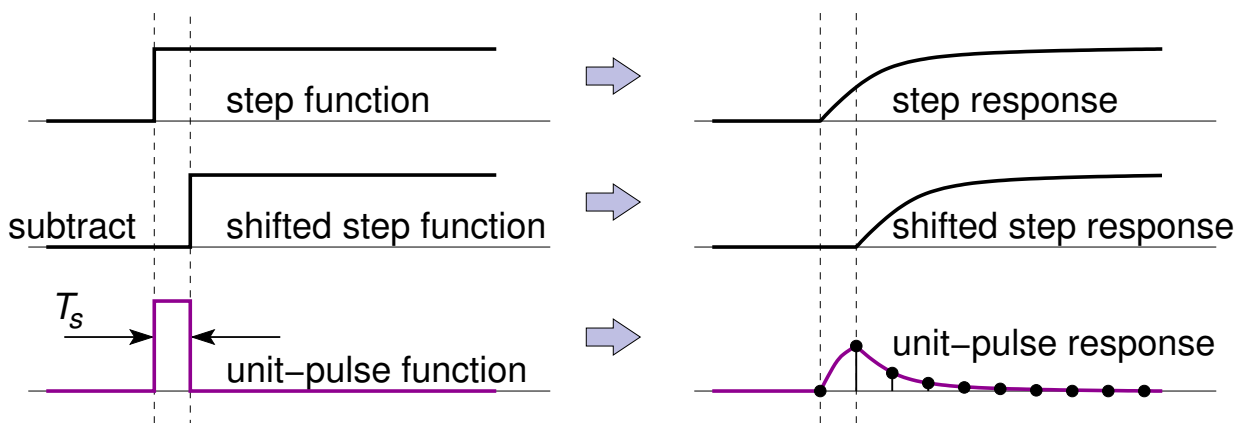
STEP 4: Generate a discrete-time state-space realization using the deterministic Ho–Kalman algorithm.

- We note that a system having a pole at the origin does not meet the strictly-stable requirement. However, we also show that this pole can be automatically accounted for.

Building the DRA from the end to the beginning

STEP 3: If we have the system's unit-pulse response, we can use Ho–Kalman to find a state-space representation.

- But, how to find the unit pulse response? Let's assume that we know the continuous-time step response $h_{\text{step}}(t)$:



- The continuous-time response to a unit pulse of length T_s seconds is $h_{\text{pulse}}(t) = h_{\text{step}}(t) - h_{\text{step}}(t - T_s)$.
- The discrete-time response is found by sampling: $g_k = h_{\text{pulse}}(kT_s)$.

STEP 2: If we have the system's continuous-time step response, we can find a state-space representation.

- But, how to find the step response? Let's assume that we know the continuous-time impulse response $h(t)$. Then,

$$h_{\text{step}}(t) = \int_0^t h(\tau) d\tau.$$

- In fact, since the DRA is a numeric algorithm, we can't deal with continuous time directly. Instead, we select a fast sample frequency F_1 such that $T_1 = \frac{1}{F_1} \ll T_s$.
- Then, the finely sampled continuous-time step response is:

$$h_{\text{step}}(kT_1) = T_1 \sum_{i=0}^{k-1} h(iT_1).$$

STEP 1: Given the system's finely sampled continuous-time impulse response, we can find a state-space representation.

- How to find the finely sampled continuous-time impulse response?
- We approximate the continuous-time impulse response via a “discrete equivalent” approach (frequency-domain emulation).
- We use the bilinear transform to write a high-sample-rate discrete-time approximation to the original continuous-time transfer function

$$H(z) \approx H(s) \Big|_{s=\frac{2}{T_1} \frac{z-1}{z+1}},$$

where T_1 is the same emulation sampling period as before.³

³ In order to arrive at an accurate estimation of the continuous time transfer function, the sampling frequency, $F_1 = 1/T_1$, must be high enough to capture the system dynamics. As a rule of thumb, the sampling frequency must be at least 20 times the as great as the bandwidth of the system to get an rough approximation in the frequency domain. A higher emulation sampling frequency gives more accurate results.

- We now recognize that the discrete Fourier transform (DFT) of a sequence is related to its z -transform via the relationship

$$\begin{aligned} H[f] &= H(z) \Big|_{z=\exp(j2\pi f/N)} = H(s) \Big|_{s=\frac{2}{T_1} \left[\frac{e^{j2\pi f/N-1}}{e^{j2\pi f/N+1}} \right]} \\ &= H(s) \Big|_{s=\frac{2j}{T_1} \tan(\pi f/N)}, \quad 0 \leq f < N, \end{aligned}$$

where N is the number of points chosen for the underlying sequence, and is usually chosen to be a power of 2 for efficient computations.

- The inverse DFT of $H[f]$ gives $h(nT_1)$, which is the approximation of the continuous-time impulse response at the emulation sampling period, T_1

$$h(nT_1) = \frac{1}{N} \sum_{f=0}^{N-1} H[f] e^{j2\pi f n/N},$$

which is indexed from $n = 0$ to $n = N - 1$.

Examples of the DRA

- We will ultimately look at three examples to illustrate the DRA.
- The first two are rational-polynomial transfer functions, which we use because we can calculate the exact solution using other methods.
 - We can then compare the exact solutions to the approximate solutions obtained by the DRA.
- The third does not have a closed-form solution, but we can use a 1-D parabolic-elliptic partial differential equation solver to find an accurate near-exact solution against which to compare the DRA solution.
- We find excellent agreement between the exact solutions and DRA solutions in all cases.

5.11: Example 1: Rational polynomial transfer function

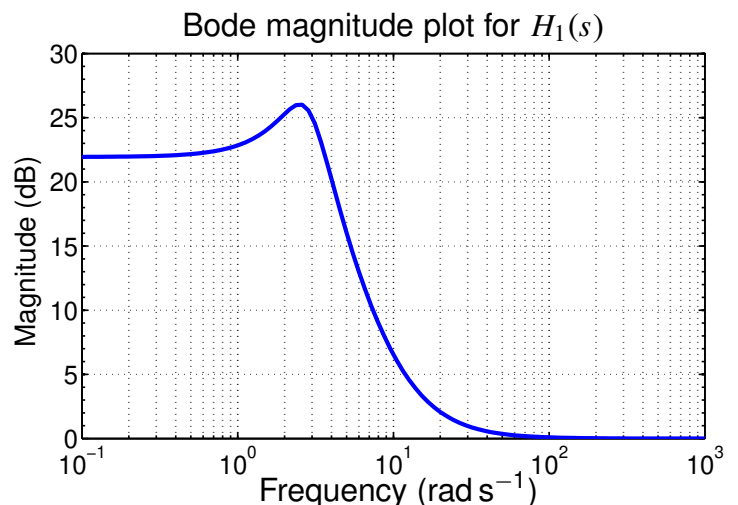
- The DRA method is first applied to a simple second-order system.
- We require a discrete-time realization with the a sampling period of $T_s = 0.1$ seconds from the continuous-time transfer function

$$H_1(s) = \frac{s^2 + 20s + 100}{s^2 + 2s + 8}.$$

- We compute the Bode plot to estimate the system bandwidth.

```
omega = logspace(-1,3,100);           % create freq. axis in rad/sec
s = 1j*omega;                         % create s = j*omega
H = (s.^2+20*s+100)./(s.^2+2*s+8);    % compute cplx. freq. response
semilogx(omega,20*log10(abs(H)));      % display the magnitude response
```

- Poles at $-1 \pm j2.65 \text{ rad s}^{-1}$, two zeros at 10 rad s^{-1} .
- The magnitude response of $H_1(s)$ is shown in the figure.
- The system bandwidth is on the order of 3 rad s^{-1} (about 0.5 Hz).



STEP 1: The sampling frequency is selected as 256 Hz which is (much) greater than 20 times the system bandwidth.

- Transfer function is sampled at discrete frequencies; inverse DFT yields an approximate continuous-time impulse response.

```
F1 = 256; T1 = 1/F1;                 % Interp. freq. of 256 Hz
minTlen = 6.5;                       % min. h(t) length in sec.
N = 2^(ceil(log2(minTlen*F1)));       % # of samples at rate F1
f = 0:N-1;                           % normalized freq. vector
s = (2j/T1)*tan(pi*f/N);             % substitute to get Hd[f]
```

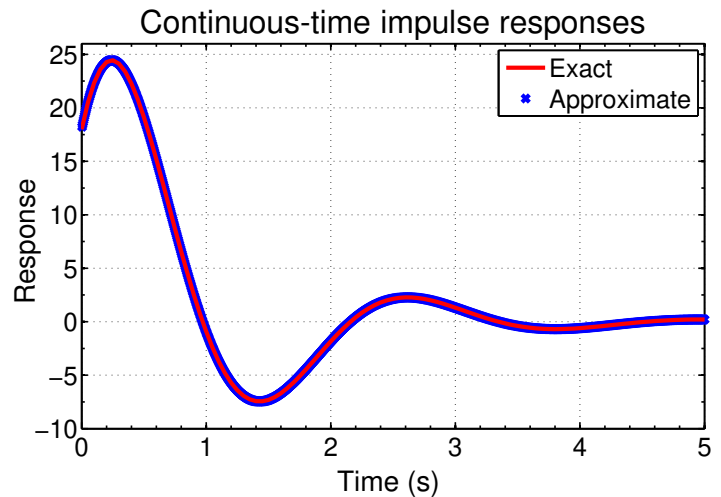
```

Hd = (s.^2+20*s+100) ./ (s.^2+2*s+8);           % Hd[f]
hd = real(iff(Hd)) * T1;                       % approximation to h(t)
td = T1*(0:N-1);                              % time vector for h(t)
plot(td,hd,'bx','markersize',8); hold on     % plot h(t)

H1 = tf([1 20 100],[1 2 8]);                  % true transfer function
[himpTrue,timpTrue] = impulse(H1,5);          % true impulse response
plot(timpTrue,himpTrue,'r'); axis([0 5 -10 26]); % plot on top

```

- The figure compares the approximate continuous-time impulse response computed via the inverse DFT to the exact continuous-time impulse response of $H_1(s)$.
- The solutions are coincident.



STEP 2: The approximation to the continuous-time step response is found by doing a cumulative summation of the impulse response.

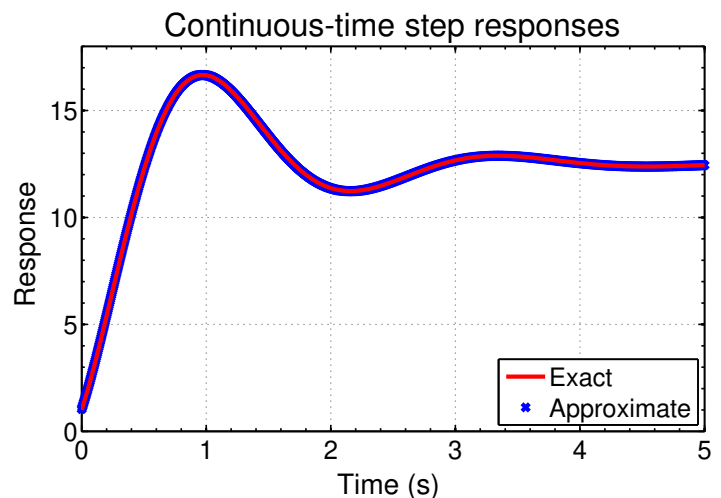
```

hstep = T1*cumsum(hd);                        % h_s(t)
plot(td,hstep,'bx','markersize',8); hold on % plot h_s(t)

[hstepTrue,tstepTrue] = step(H1,5);          % true step resp.
plot(tstepTrue,hstepTrue,'r'); axis([0 5 0 18]); % plot on top

```

- The results are shown in the figure and show excellent agreement with the exact step response of the continuous time system.



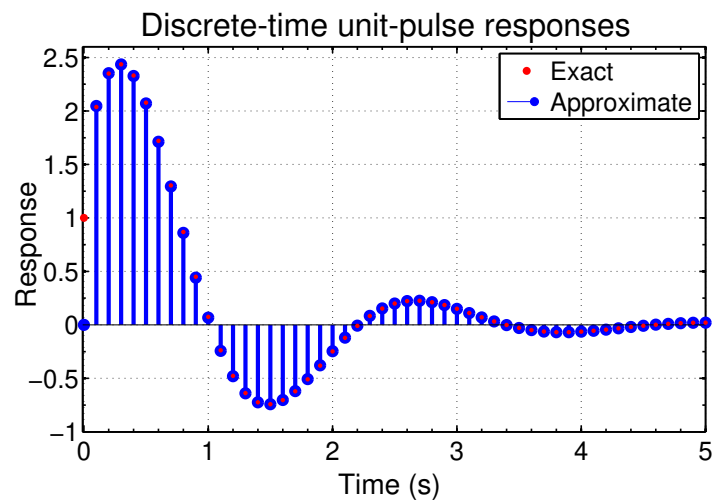
STEP 3: We now resample the continuous-time approximate step response at the final sample rate T_s , and compute the discrete-time unit-pulse response as $h_{\text{step}}[k] - h_{\text{step}}[k - 1]$

```
Ts = 0.1; tdisc = 0:Ts:6.5; % final time vector
hdisc = [0 diff(interp1(td,hstep,tdisc))]; % h[k]
stem(tdisc,hdisc,'filled'); hold on

[himpDiscTrue,timpDiscTrue] = impulse(c2d(H1,Ts),5);
% next line scales IMPULSE in new MATLAB to give unit-pulse resp.
himpDiscTrue = Ts*himpDiscTrue;
plot(timpDiscTrue,himpDiscTrue,'r.','markersize',8);
axis([-0.01 5 -1 2.6]);
```

- Note that in new versions of MATLAB, the “impulse” command works differently from old versions for discrete-time systems.
- We need to scale MATLAB’s output by T_s to compute the unit-pulse response that we desire.
- Again, there is excellent agreement between the approximate unit-pulse response and the exact solution, except at single point $t = 0$.
- This is often the case because of some properties of the inverse DFT.
- But it causes no problems since the unit-pulse response value at $t = 0$ is computed differently, using

$$D = g_0 = \lim_{s \rightarrow \infty} H(s).$$

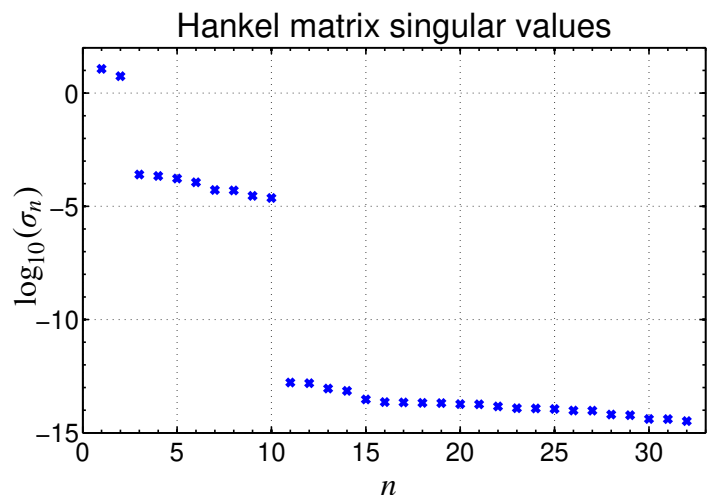


STEP 4: The Ho–Kalman algorithm is used to find state-space realization from approximate discrete-time unit-pulse response of Step 3.

- 64 points from the discrete-time unit-pulse response are used, which allows a maximum Hankel matrix of 32×32 .
- We first compute and plot the singular values of the Hankel matrix.

```
bigHankel = hankel(hdisc(2:66)); % don't forget to omit h(0) term!
% for this example, keep only 32x32 portion
Hankel = bigHankel(1:32,1:32);
HankelUp = bigHankel(2:33,1:32); % shifted Hankel matrix
[U, S, V] = svd(Hankel); % compute singular values
plot(log10(diag(S)), 'bx', 'markersize', 8); axis([0 33 -20 5]);
```

- Hankel-matrix SVD gives insight into the system's order.
- A log plot of the singular values is shown in the figure.
- The first two are almost three orders of magnitude greater than the third, so we select a reduced-order model dimension $p = 2$.



```
n = 2; % select via singular values
Us = U(:, 1:n); % Compute extended observability, controlability
Ss = S(1:n, 1:n); % matrices, sized to the order for the system
Vs = V(:, 1:n); % inferred by the singular values.
Ok = Us*sqrtm(Ss); Cl = sqrtm(Ss)*Vs';

Ahat = (Ok\HankelUp)/Cl; % calculate A from Ok, Cl
Bhat = Cl(1:n, 1); Chat = Ok(1, 1:n); % calculate B and C
Dhat = 1; % calculated manually
sysDRA = ss(Ahat, Bhat, Chat, Dhat, Ts); % final DRA ss model
```

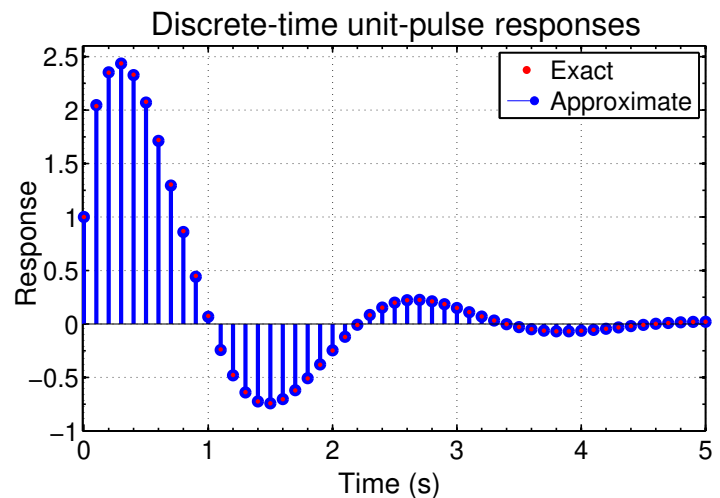

- Truncating to the first two states only, the Ho–Kalman algorithm gives a state-space realization with the following A , B , and C matrices

$$\hat{\mathbf{A}} = \begin{bmatrix} 0.8656 & -0.2367 \\ 0.2367 & 0.8811 \end{bmatrix}, \hat{\mathbf{B}} = \begin{bmatrix} -1.624 \\ 0.7692 \end{bmatrix}, \hat{\mathbf{C}} = \begin{bmatrix} -1.624 & -0.7692 \end{bmatrix}.$$

- The $\hat{\mathbf{D}}$ matrix is found from the initial value theorem and, for this example, is $\hat{\mathbf{D}} = [1]$.
- We compare the true discrete-time unit-pulse response and the final DRA model unit-pulse response:

```
% next line scales IMPULSE in new MATLAB to give unit-pulse resp.
[himpDRA,timpDRA] = impulse(sysDRA,5); himpDRA = Ts*himpDRA;
stem(timpDRA,himpDRA,'filled'); hold on
plot(timpDiscTrue,himpDiscTrue,'r.','markersize',8);
axis([-0.01 5 -1 2.6]);
```

- The results agree very well (note that $h[0]$ has been corrected by the correct calculation of the $\hat{\mathbf{D}}$ matrix in Step 4).



- Because the unit-pulse responses agree very well, the response of the reduced-order model will also agree well with the exact response for any input signal $u[k]$.

5.12: Example 2: Dealing with a pole in $H(s)$ at the origin

- This example has a pole in $H(s)$ at $s = 0$, so is not strictly stable, and violates the necessary conditions that make the DRA work.
- However, it is quite simple to deal with this case.
 - We first subtract the pole at the origin from the transfer function,
 - Then execute the DRA on the residual system,
 - Then compute a final discrete-time state-space model that augments the DRA result with additional dynamics to implement the function of the s -domain pole at the origin.

- A pole at the origin is removed by first calculating the residue of this pole and then subtracting it from the original transfer function.

$$H^*(s) = H(s) - \frac{\text{res}_0}{s} \quad \text{where} \quad \text{res}_0 = \lim_{s \rightarrow 0} sH(s).$$

- The remainder of the DRA is executed using $H^*(s)$ instead of $H(s)$.
- To re-incorporate the effect of the pole at $s = 0$ into the final reduced-order model, recall that this pole corresponds to an integrator. The discrete-time equivalent can be implemented as

$$x_i[k + 1] = x_i[k] + T_s u[k].$$

- We combine this with the DRA-produced state-space form

$$\underbrace{\begin{bmatrix} \mathbf{x}[k + 1] \\ x_i[k + 1] \end{bmatrix}}_{\mathbf{x}_{\text{aug}}[k+1]} = \underbrace{\begin{bmatrix} \widehat{\mathbf{A}} & \mathbf{0} \\ \mathbf{0} & 1 \end{bmatrix}}_{\widehat{\mathbf{A}}_{\text{aug}}} \underbrace{\begin{bmatrix} \mathbf{x}[k] \\ x_i[k] \end{bmatrix}}_{\mathbf{x}_{\text{aug}}[k]} + \underbrace{\begin{bmatrix} \widehat{\mathbf{B}} \\ T_s \end{bmatrix}}_{\widehat{\mathbf{B}}_{\text{aug}}} \mathbf{u}[k]$$

$$\mathbf{y}[k] = \underbrace{\begin{bmatrix} \widehat{\mathbf{C}} & \text{res}_0 \end{bmatrix}}_{\widehat{\mathbf{C}}_{\text{aug}}} \begin{bmatrix} \mathbf{x}[k] \\ x_i[k] \end{bmatrix} + \mathbf{D}\mathbf{u}[k]$$

where dotted lines delineate boundaries between block sub-matrices of the overall augmented state-space matrices $\hat{\mathbf{A}}_{\text{aug}}$, $\hat{\mathbf{B}}_{\text{aug}}$, and $\hat{\mathbf{C}}_{\text{aug}}$.

Example 2: Rational polynomial transfer function with pole at origin

- In this example, we demonstrate how to handle a single pole at the origin. The continuous-time transfer function is given by

$$H_2(s) = \frac{1}{s} \left(\frac{1}{s^2 + 6s + 8} \right).$$

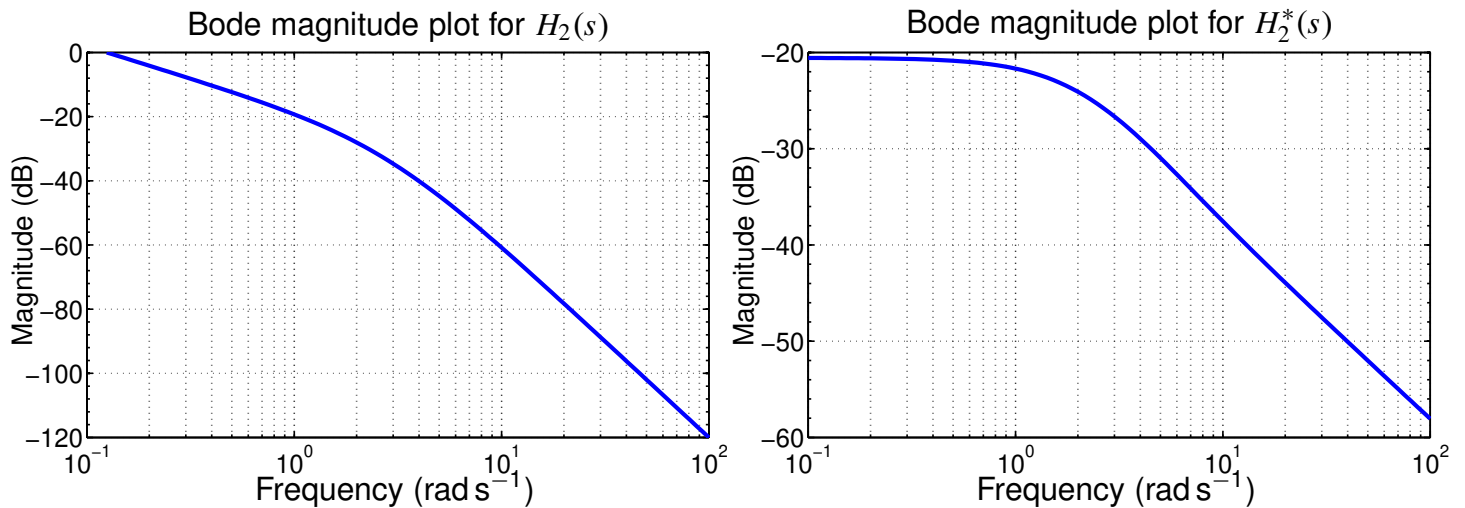
- This system has real poles at 0, 2 and 4 rad s⁻¹.
- Desire a discrete-time transfer function with sample period $T_s = 0.1$ s.
- Prior to Step 1 we remove the pole at the origin.
- This is accomplished by first calculating the residue for this pole.
- In this example, the residue can be computed analytically as

$$\text{res}_0 = \lim_{s \rightarrow 0} s H(s) = 0.125.$$

- In general, we find this residue by selecting a very small value for s and numerically computing res_0 , or by using a software tool like Mathematica to compute the limit.
- The reduced transfer function, $H_2^*(s)$ with the pole at the origin removed is

$$H_2^*(s) = \frac{1}{s} \left(\frac{1}{s^2 + 6s + 8} \right) - \frac{0.125}{s}.$$

- The figures below shows the magnitude plot of the original system and the system with the pole at the origin removed.



STEP 1. $H_2^*(s)$ is sampled at 256 Hz which is (much) more than 50 times greater than the system bandwidth. We could implement either

```
Hd = 1./(s.^3+6*s.^2+8*s) - 0.125./s;      % Hd[f]
Hd(1) = -6/64;                               % analytic solution
```

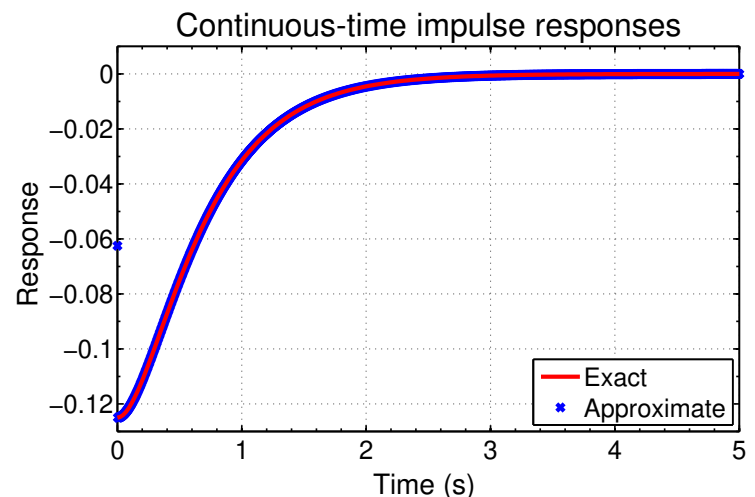
where $\lim_{s \rightarrow 0} H_2^*(s) = -6/64$, or compute by hand

$$\begin{aligned} H_2^*(s) &= \frac{1}{s} \left(\frac{1}{s^2 + 6s + 8} \right) - \frac{0.125}{s} \left(\frac{s^2 + 6s + 8}{s^2 + 6s + 8} \right) \\ &= -\frac{0.125}{s} \left(\frac{s^2 + 6s}{s^2 + 6s + 8} \right) = -0.125 \left(\frac{s + 6}{s^2 + 6s + 8} \right), \end{aligned}$$

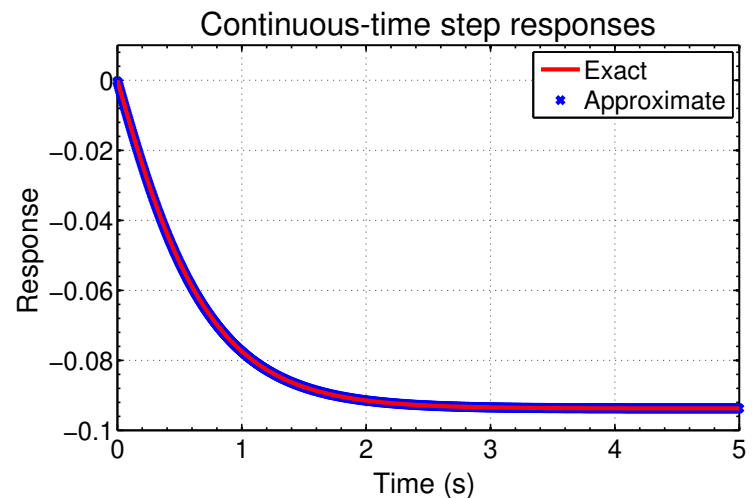
and implement

```
Hd = -0.125*(s+6) ./ (s.^2+6*s+8);
```

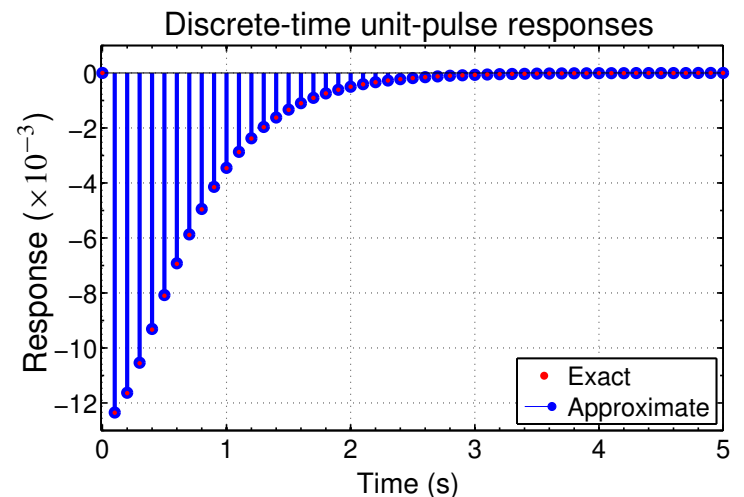
- The approximate continuous-time impulse response is computed and plotted.



STEP 2: The approximation to the continuous-time step response of $H_2^*(s)$ is calculated as in the first example and plotted.

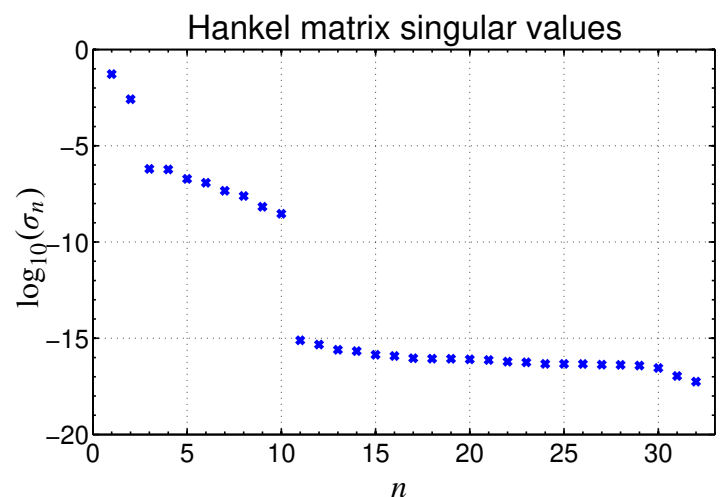


STEP 3: This step response is sampled at $T_s = 0.1$ seconds, and differenced to yield the discrete-time unit-pulse response, plotted in the figure.



STEP 4. The system Hankel matrix is generated from the discrete-time unit-pulse response found in Step 3.

- 64 discrete time points are used, resulting in a 32×32 Hankel matrix.
- The figure depicts the 32 singular values of the system Hankel matrix.
- The first two singular values are two orders of magnitude greater than the third, indicating that $H_2^*(s)$ is a second order system.



- The Ho–Kalman algorithm generates the $\hat{\mathbf{A}}$, $\hat{\mathbf{B}}$, and $\hat{\mathbf{C}}$ matrices after truncating all but the first two states. We find that

$$\hat{\mathbf{A}} = \begin{bmatrix} 0.8617 & -0.0906 \\ 0.0906 & 0.6274 \end{bmatrix}, \quad \hat{\mathbf{B}} = \begin{bmatrix} 0.1162 \\ -0.0340 \end{bmatrix}$$

$$\hat{\mathbf{C}} = \begin{bmatrix} -0.1162 & -0.0340 \end{bmatrix}.$$

In this example, we also compute $\hat{\mathbf{D}} = \lim_{s \rightarrow \infty} H_2^*(s) = 0$, which can also be quite easily seen in the high-frequency response of $H_2^*(s)$.

- The state-space representation for $H_2^*(s)$ is augmented to include the pole at the origin to create a representation for $H_s(s)$.

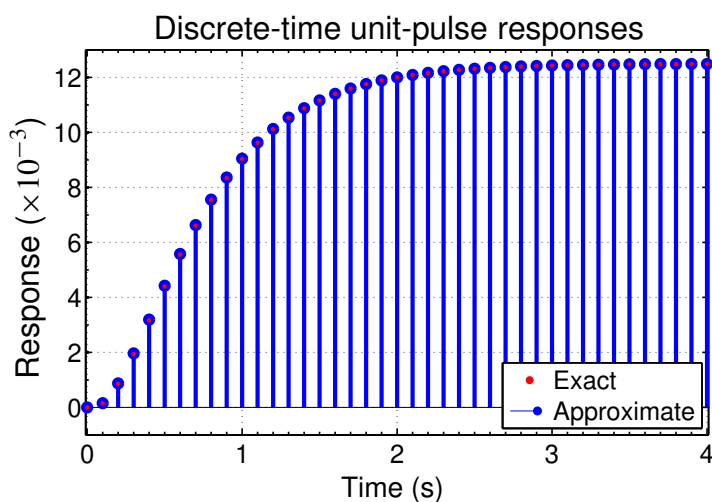
```
Aaug = [Ahat, zeros(n,1); zeros(1,n), 1];
Baug = [Bhat; Ts];
Caug = [Chat, res0];
sysDRA = ss(Aaug, Baug, Caug, Dhat, Ts) % final DRA state-space sys.
```

- The discrete-time realization of $H_2(s)$ is

$$\hat{\mathbf{A}}_{\text{aug}} = \left[\begin{array}{cc|c} 0.8617 & -0.0906 & 0 \\ 0.0906 & 0.6274 & 0 \\ \hline 0 & 0 & 1 \end{array} \right], \quad \hat{\mathbf{B}}_{\text{aug}} = \left[\begin{array}{c} 0.1162 \\ -0.0340 \\ \hline 0.1 \end{array} \right]$$

$$\hat{\mathbf{C}}_{\text{aug}} = \left[\begin{array}{cc|c} -0.1162 & -0.0340 & 0.125 \end{array} \right], \quad \hat{\mathbf{D}} = [0].$$

- The figure shows close comparison of the unit-pulse response found from the DRA and the exact solution.



5.13: Example 3: Transcendental transfer function

- In the first two examples, we used rational polynomials to illustrate the DRA method where order of the system is known *a priori*, and the exact answer could be calculated analytically.
- We now demonstrate the DRA with an infinite-order distributed-parameter system: Specifically the Jacobsen–West transfer function of lithium diffusion in a single particle, where

$$H_3(s) = \frac{\tilde{C}_{s,e}(s)}{J(s)} = \frac{R_s}{D_s} \left[\frac{1}{1 - R_s \sqrt{s/D_s} \coth(R_s \sqrt{s/D_s})} \right],$$

and where the integrator-removed transfer function is

$$\begin{aligned} H_3^*(s) &= \frac{\Delta \tilde{C}_{s,e}(s)}{J(s)} = \frac{\tilde{C}_{s,e}(s)}{J(s)} - \frac{\tilde{C}_{s,\text{avg}}(s)}{J(s)} \\ &= \frac{\frac{sR_s^2}{D_s} + 3 - 3R_s \sqrt{\frac{s}{D_s}} \coth\left(R_s \sqrt{\frac{s}{D_s}}\right)}{sR_s \left(1 - R_s \sqrt{\frac{s}{D_s}} \coth\left(R_s \sqrt{\frac{s}{D_s}}\right)\right)}, \end{aligned}$$

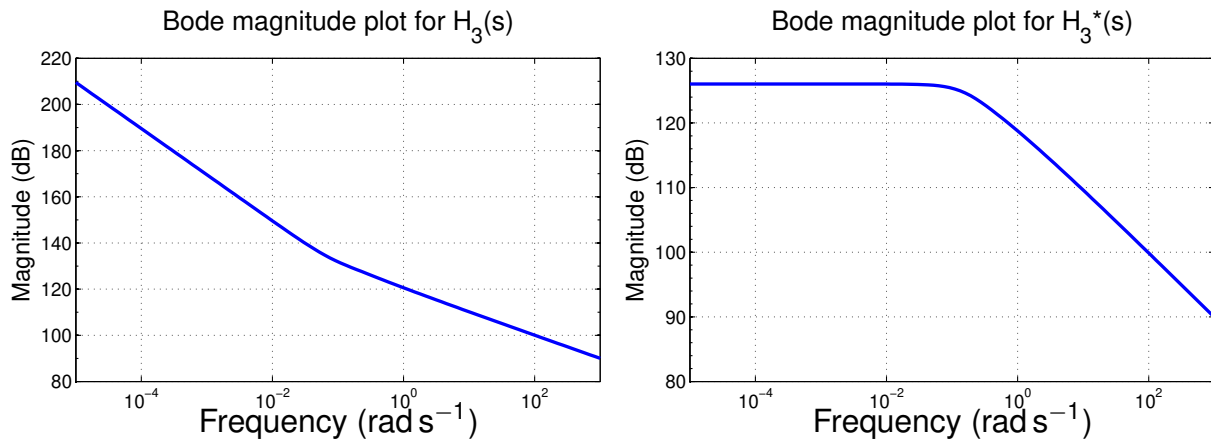
where we have used the relationship

$$\frac{\tilde{C}_{s,\text{avg}}(s)}{J(s)} = \frac{\text{res}_0}{s} = \frac{-3/R_s}{s}.$$

- Parameter values for the transfer functions used in this example are listed in the table, from which we can compute that $\text{res}_0 = -3 \times 10^5$.

Parameter name	Interpretation	Value
T_s	Sampling period	1 s
R_s	Particle radius	10^{-5} m
D_s	Diffusivity	10^{-12} m ² s ⁻¹
$c(r, 0)$	Initial lithium concentration	10 000 mol m ⁻³

STEP 1. The magnitude responses of $H_3(s)$ and $H_3^*(s)$ are shown below:



- $H_3^*(s)$ is sampled at 256 Hz for a total of 256 seconds.
- The frequency vector for $H_3^*(s)$ can be calculated as

```
beta = Rs*sqrt(s/Ds);
Hd = (Rs/Ds)*(1./(1-beta.*coth(beta))) + (3/Rs)./s;
Hd(1) = -Rs/(5*Ds); % analytic solution
```

where MATLAB numerically removes the integrator pole, or as

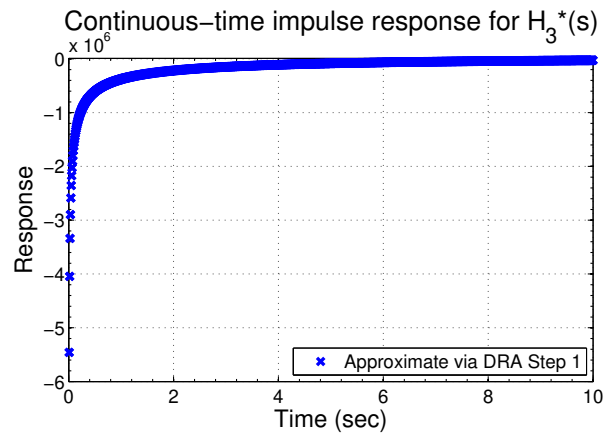
```
beta = Rs*sqrt(s/Ds);
Hd = (beta.^2+3-3*beta.*coth(beta))./(s.*Rs.*(1-beta.*coth(beta)));
Hd(1) = -Rs/(5*Ds); % analytic solution
```

- Note that both computations of Hd initially produce NaN for $s = 0$ due to numeric attempts to evaluate zero divided by zero.
- This entry must be manually replaced by a value computed analytically

$$\lim_{s \rightarrow 0} H_3^*(s) = \lim_{s \rightarrow 0} \frac{\frac{sR_s^2}{D_s} + 3 - 3R_s\sqrt{\frac{s}{D_s}} \coth\left(R_s\sqrt{\frac{s}{D_s}}\right)}{sR_s\left(1 - R_s\sqrt{\frac{s}{D_s}} \coth\left(R_s\sqrt{\frac{s}{D_s}}\right)\right)} = -\frac{R_s}{5D_s}.$$

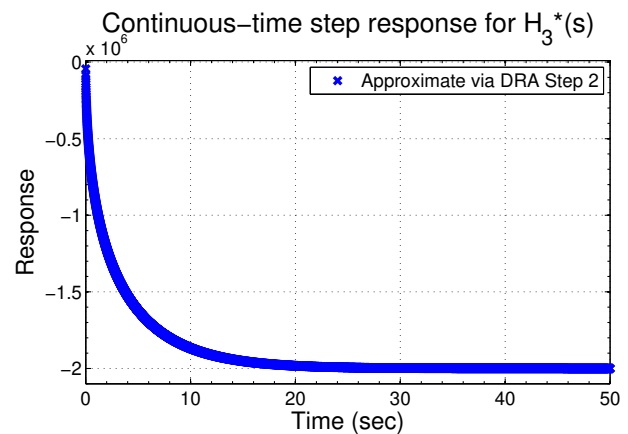
- Direct by-hand computation returns 0/0. We must use l'Hôpital's rule repeatedly until an answer is reached.
- When using transcendental transfer functions, we recommend computer tools such as Mathematica for symbolic manipulation.

- The approximate continuous-time impulse response is shown.
- There is no known exact solution against which to compare this result.

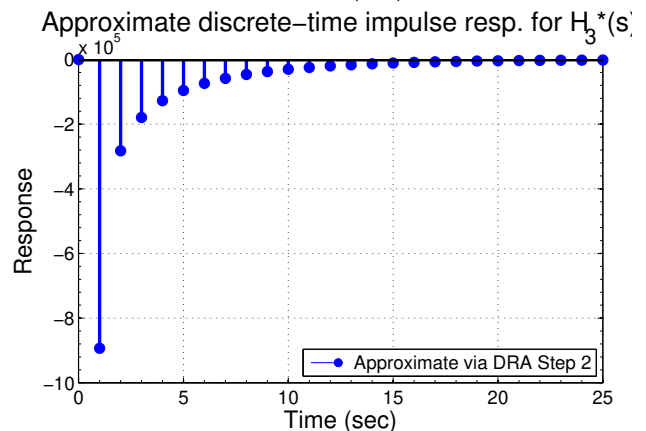


STEP 2. The approximate continuous-time step response is calculated by performing a cumulative sum of the impulse response of Step 1.

- The figure shows approximated continuous-time step response.
- Again, there is no known exact solution against which to compare this result.



STEP 3: The approximate continuous-time step response is sampled at $T_s = 1$ second, and differenced to produce the discrete-time unit-pulse response, shown here.



STEP 4. Hankel matrix is formed;
singular values are plotted.

- $H_3^*(s)$ represents a distributed-parameter system that actually has an infinite number of poles.
- However, only a few of them are significant to the solution.
- In particular, we choose to use a reduced-order model dimension $n = 2$ in the results we present here, imposing a tradeoff between the complexity and accuracy of the solution.
- The Ho–Kalman algorithm generates the $\hat{\mathbf{A}}$, $\hat{\mathbf{B}}$, and $\hat{\mathbf{C}}$ matrices to approximate $H_3^*(s)$ after truncating all but the first two states.

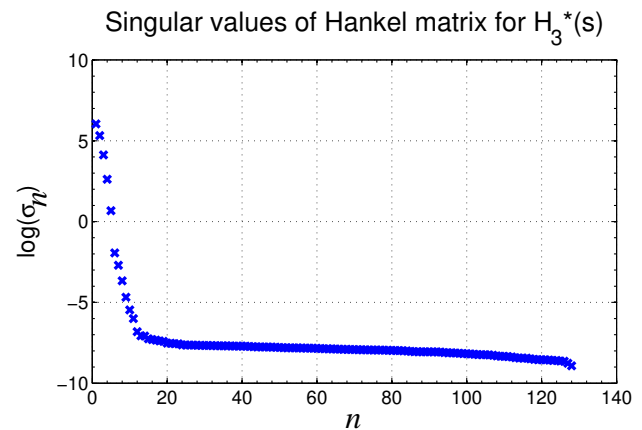
$$\hat{\mathbf{A}} = \begin{bmatrix} 0.4695 & 0.3296 \\ 0.3296 & 0.4355 \end{bmatrix}, \quad \hat{\mathbf{B}} = \begin{bmatrix} 919.1 \\ -220 \end{bmatrix}$$

$$\hat{\mathbf{C}} = \begin{bmatrix} -919.1 & 220 \end{bmatrix}.$$

- In this example, we also compute $\hat{\mathbf{D}} = \lim_{s \rightarrow \infty} H_3^*(s) = 0$, which can also be quite easily seen in the high-frequency response of $H_3^*(s)$.
- This state-space realization is augmented with the integrator state to give the final third-order model of the diffusion equation $H_3(s)$.

$$\hat{\mathbf{A}}_{\text{aug}} = \left[\begin{array}{cc|c} 0.4695 & 0.3296 & 0 \\ 0.3296 & 0.4355 & 0 \\ \hline 0 & 0 & 1 \end{array} \right], \quad \hat{\mathbf{B}}_{\text{aug}} = \left[\begin{array}{c|c} 919.1 \\ -220 \\ \hline 1 \end{array} \right]$$

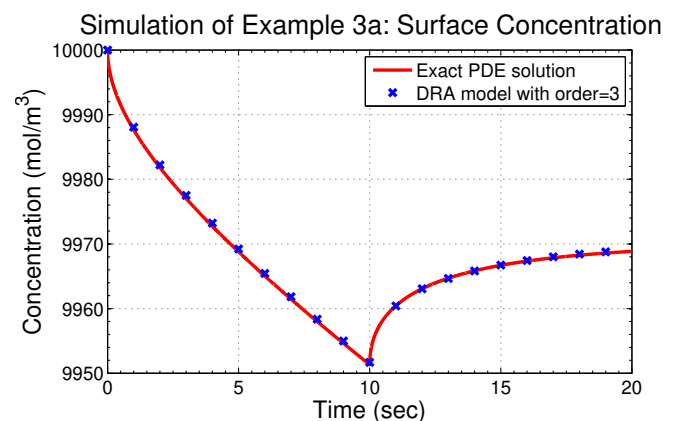
$$\hat{\mathbf{C}}_{\text{aug}} = \left[\begin{array}{cc|c} -919.1 & 220 & -3 \times 10^5 \end{array} \right], \quad \hat{\mathbf{D}} = [0].$$



- We demonstrate the the DRA-produced model by simulating a 10 s discharge pulse where the surface lithium flux (leaving the particle) was $j = 1 \times 10^{-5} \text{ mol m}^{-2} \text{ s}^{-1}$, followed by a 10 s rest.
- The augmented state-space model was simulated with this input to produce $\tilde{c}_{s,e}[k]$, and $c_{s,e}[k]$ was computed as $c_{s,e}[k] = \tilde{c}_{s,e}[k] + c_{s,0}$.

```
cs0 = 10000;
uk = 1e-5*[ones(1,10),zeros(1,10)];
[cseTilde,tk] = lsim(sysDRA,uk);
cse = cseTilde + cs0;
```

- All discrete-time model states are initialized to zero.
- The output of this discrete-time realization to a 10 second discharge followed by a 10 second rest is shown.
- We compare this result against the “truth” produced by simulating the PDE using MATLAB’s 1-D parabolic-elliptic PDE solver.



```
function [cse,t] = simCsePDE
    dr = 0.1e-6; % Radial resolution = 0.1 micro-meter
    dt = 0.001; % Time step in simulation, s
    Tfinal = 20; % Length of simulation, s
    Rp = 10e-6; % Radius of particle = 10 micro-meters
    Ds = 1e-12; % Solid diffusivity, m^2/s
    j = 1e-5; % mol/m^2/s

    x = 0:dr:Rp; % locations for solution
    t = 0:dt:Tfinal; % time steps for solution

    options = odeset('RelTol',1e-8,'AbsTol',1e-10);
    sol = pdepe(2,@csefun,@cseic,@csebc,x,t,options);
    cse = sol(:,end,1);

    function [c,f,s] = csefun(~,~,~,DuDx)
```

```
c = 1/Ds; f = DuDx; s = 0;
end

function u0 = cseic(~,~)
    c0 = 10000; u0 = c0;
end

function [pl,ql,pr,qr] = csebc(~,~,~,~,t)
    pl = 0; ql = 1; qr = Ds; pr = 0;
    if t<Tfinal/2, pr=j; end
end

end
```

- The code comprises nested functions, where the main function initializes variables and calls MATLAB's solver with pointers (function handles) to nested helper functions:
 - `csefun` implements the parameter values of the PDE;
 - `cseic` implements the initial conditions; and
 - `csebc` implements the boundary conditions.
- Note that we achieve good results with the PDE solver only if a fine time-step is used: here, we have used a 1 ms step size, which makes the PDE solver execute much more slowly than the DRA-produced model.

Where from here?

- We have now seen the form that the final model will take, and examples of the general methodology to go from the PDE continuum-scale model to the reduced-order model.
- We now proceed to develop transfer functions for all cell variables of interest, and see how well the overall cell model works.