# Control and Statistical Mechanics

**Henrik Sandberg, Jean-Charles Delvenne, and John Doyle**

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**Topics:**

- **Statistical mechanics formalism using linear system theory**
- **How come real systems look dissipative when energy is conserved? Does this give limitations?**
- **Back action of measurements (without quantum effects)**
- **How do we convert heat into work using control theory?**

# Motivation and Background

• **Hard limits**: With ideal devices causality alone gives limitations (John). But what other limitations are there?

• **Uncertainty**: Relation information theory, control theory, statistical mechanics? Channel capacity, Bode-Shannon, Carnot cycles,… Entropy is everywhere!

• **Energy conservation**: Measurements are not unproblematic, even using classical physics

• How much of this can we understand with simple linear systems and some approximation theory?

# Outline

Focus here: Control theory and statistical mechanics. Connection to information theory not clear yet.

1. Energy and lossless/dissipative models (physical models)
2. Lossless approximations of dissipative models, emergence of noise and limitations
3. Back action of measurements
4. Examples: Conversion of heat into useful work (compare with Carnot heat engine)

# Physical Linear System: Lossless and Strictly Causal

We *assume* linear physical models have the structure:

$$\dot{x}(t) = Jx(t) + Bu(t), \quad x(t) \in \mathbb{R}^n,$$
$$y(t) = B^T x(t)$$

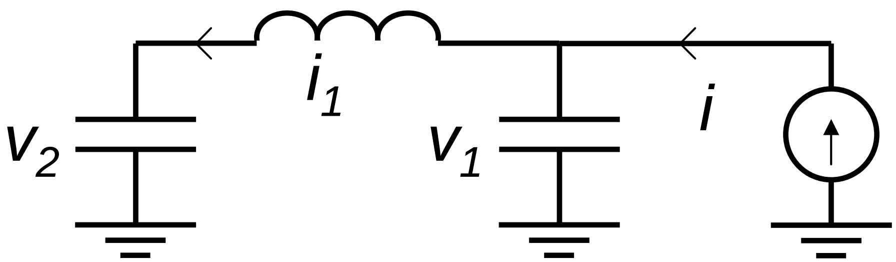
- **Internal energy**: $U(x(t)) = \frac{1}{2} x(t)^T x(t)$
- **Energy preserving**: $J = -J^T$ (anti-symmetric)
- **Work rate:** $w(t) = y(t)^T u(t)$
- **Lossless:**

$$\frac{dU(x(t))}{dt} = x(t)^T \dot{x}(t) = x(t)^T (Jx(t) + Bu(t)) = y(t)^T u(t)$$

- **Strictly causal and (*J*,*B*) controllable**

# Example: LC Circuit

Choice of inputs/outputs not always simple.
Assume choice is already made.




Input: current $i$
Output: voltage $v_1$

**Dynamics:**

$$\dot{x} = \begin{pmatrix} 0 & -1/\sqrt{C_1 L_1} & 0 \\ 1/\sqrt{C_1 L_1} & 0 & -1/\sqrt{L_1 C_2} \\ 0 & 1/\sqrt{L_1 C_2} & 0 \end{pmatrix} x + \begin{pmatrix} 1/\sqrt{C}_1 \\ 0 \\ 0 \end{pmatrix} u$$

**Output, state:**

$$y = \begin{pmatrix} 1/\sqrt{C}_1 & 0 & 0 \end{pmatrix} x, \quad x^T = \begin{pmatrix} \sqrt{C}_1 v_1 & \sqrt{L}_1 i_1 & \sqrt{C}_2 v_2 \end{pmatrix}$$

**Energy, work rate:**

$$U = \frac{1}{2} x^T x = \frac{1}{2}(C_1 v_1^2 + L_1 i_1^2 + C_2 v_2^2), \quad w = yu = v_1 i.$$

# Macroscopic Dissipative Systems (Example: Resistor)

- Consider a linear static input-output device

$$y(t) = ku(t)$$

- If *k>0,* the device is dissipative

$$w(t) = y(t)u(t) = ku(t)^2 \geq 0$$

- Can also be modeled by the convolution

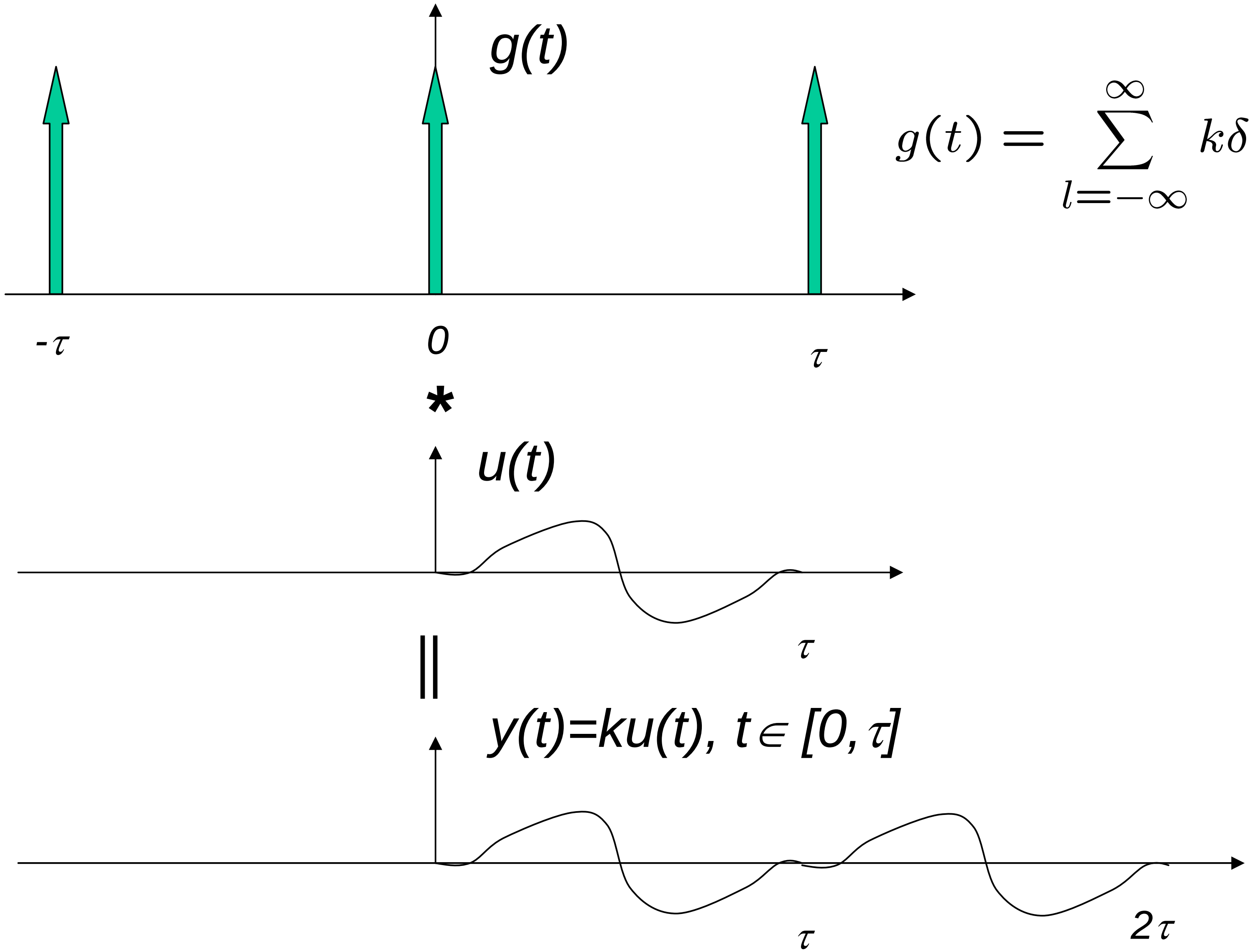
$$y(t) = \int_0^\infty k\delta(t-s)u(s)ds$$

for smooth *u(t)*

- *Choose* a time interval [*0,* $\tau$] of interest

# Model with Recurrence Time $\tau$

$$g(t) = \sum_{l=-\infty}^{\infty} k\delta(t - l\tau)$$



# Fourier Expansion and Physical Realization

- Expansion of impulse response (in distribution sense)

$$g(t) \sim \frac{k}{2\tau} + \sum_{l=1}^{\infty} \frac{k}{\tau} \cos l\omega_0 t \triangleq g_+(t) + g_-(t), \qquad \omega_0 = \frac{2\pi}{\tau}$$

- $g_+(t)$ causal and $g_-(t)$ anti-causal

- Truncate and keep *N* terms and realize $2g_+(t)$ with *lossless* and *strictly causal* linear system $G_N$:

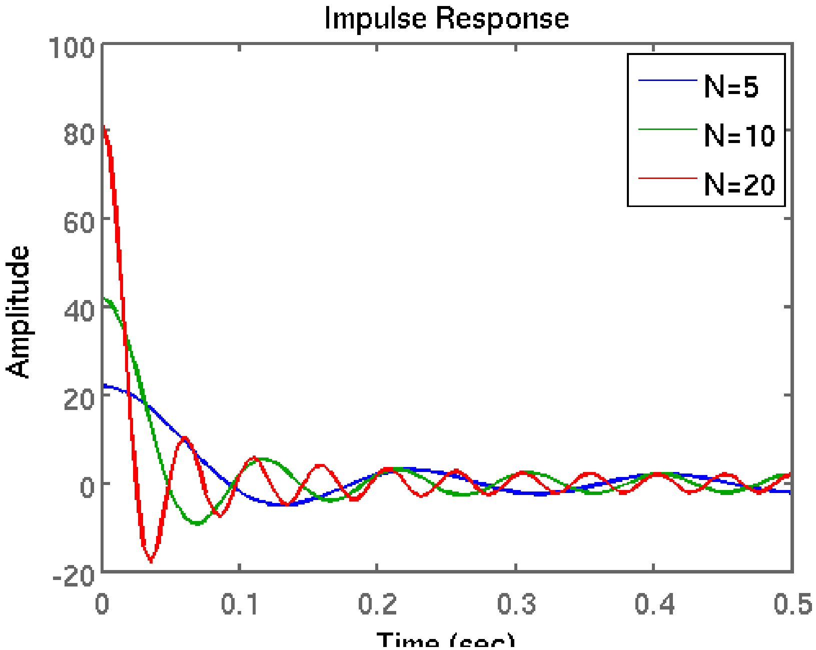
$$J = \begin{bmatrix} 0 & \Omega & 0 \\ -\Omega^T & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \qquad \Omega = \text{diag}\{\omega_0, 2\omega_0, \ldots, N\omega_0\}$$

$$C = 2\sqrt{\frac{k}{\tau}}\begin{pmatrix} 1 & \ldots & 1 & 0 & \ldots & 0 & \frac{1}{\sqrt{2}} \end{pmatrix}$$

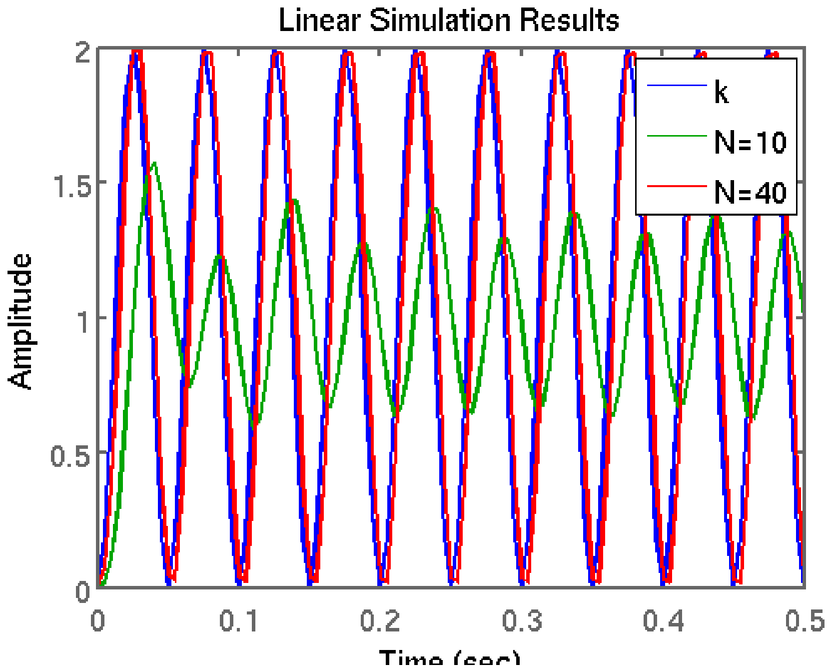
$$B = C^T.$$

# Simulations of *y(t)=ku(t)* and *$y_N(t)=G_N u(t)$* ($\tau$=1)

$g_N(t)$




$u(t) = 1 - \cos 40\pi t$




- Initial conditions zero
- $|y(t) - y_N(t)| \leq \frac{const.}{N}\left(|\dot{u}(t)| + \|\ddot{u}\|_{L_1[0,t]}\right), \quad t \in [0,\tau]$

# Input-Output Relation of Lossless Approximation

$$y_N(t) = B^T e^{Jt} x_N(0) + \int_0^t B^T e^{J(t-s)} Bu(s)ds$$

- Assume *u(t)=0*, then the covariance function of $y_N(t)$ is

$$R_{y_N}(t) = \mathbf{E} y_N(t) y_N(0)^T = B^T e^{Jt} (\mathbf{E} x_N(0) x_N(0)^T) B$$

- Stat. mech.: Assume thermal equilibrium, temperature *T*

$$\mathbf{E} x_N(0) x_N(0)^T = T \cdot I$$

- As *N* increases, we have (with *v(t)* white noise)

$$R_{y_N}(t) \to 2Tk\delta(t), \qquad t \in [0, \tau]$$

$$\boxed{y_\infty(t) = ku(t) + \sqrt{2Tk}\, v(t)}$$

# Implications and Discussion: Dissipation-Fluctuation

- We wanted to realize the dissipative model

$$y(t) = ku(t)$$

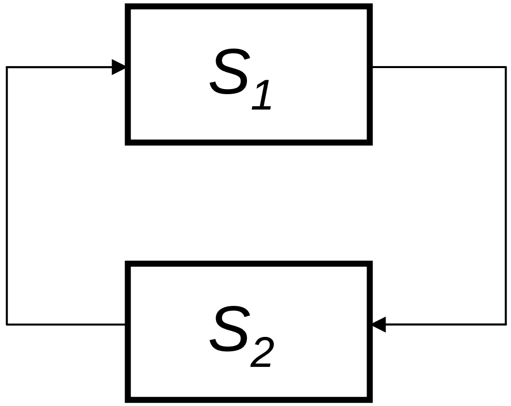
with lossless linear physical model

- Assumptions: $u(t)$ is smooth and finite-time interval $[0, \tau]$
- We needed "many" states *N*, and uncertainty in the initial state gave stochastic white noise:

$$y_\infty(t) = ku(t) + \sqrt{2Tk}v(t)$$

- Generalization of Johnson-Nyquist noise in resistors
- *N* $\sim$ number of atoms in a resistor. The recurrence time $\tau$ is *very* large

# Interconnections of Lossless Systems

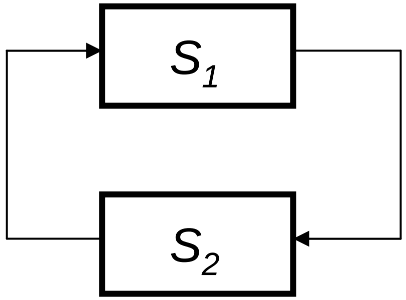



- Preserve the total energy
- Use feedback $u_1(t) = -y_2(t)$ and $u_2(t) = y_1(t)$
- Dynamics

$$\frac{d}{dt}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} J_1 & -B_1 B_2^T \\ B_2 B_1^T & J_2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

- Overall system still lossless

# Interconnection to Heat Bath




- Assume the lossless system $S_2$ is "large" as before and can be modeled by $u_1(t) = ky_1(t) + \sqrt{2Tk}v(t)$
- Call $S_2$ a <u>heat bath</u> of temperature $T$
- Dynamics $\dot{x}_1 = (J_1 - kB_1B_1^T)x_1 - B_1\sqrt{2Tk}v$
- $S_1$ looks dissipative while connected to heat bath $S_2$!
- <u>Stochastic model</u> because of <u>unknown initial state in $S_2$</u>

# Heat Dynamics, Equilibrium, and Energy Equipartition

Mean evolution in $S_1$:

$$\frac{d}{dt}\mathbf{E}x_1 = (J_1 - kB_1B_1^T)\mathbf{E}x_1$$

Variance evolution $S_1$:

$$X_1 = \mathbf{E}(x_1 - \mathbf{E}x_1)(x_1 - \mathbf{E}x_1)^T$$

$$\dot{X}_1 = \underbrace{(J_1 - kB_1B_1^T)X_1 + X_1(J_1 - kB_1B_1^T)^T}_{\text{"heat flow out" from } S_1} + \underbrace{2TkB_1B_1^T}_{\text{"heat flow in"}}$$

Expected internal energy $S_1$:

$$\mathbf{E}U_1 = \tfrac{1}{2}(\mathbf{E}x_1)^T\mathbf{E}x_1 + \tfrac{1}{2}\mathrm{Tr}X_1$$

If $(J_1,B_1)$ controllable:

$$X_1(t) \to T \cdot I,$$
$$\mathbf{E}x_1(t) \to 0,$$
$$\mathbf{E}U_1(t) \to \frac{1}{2}nT, \qquad t \to \infty$$

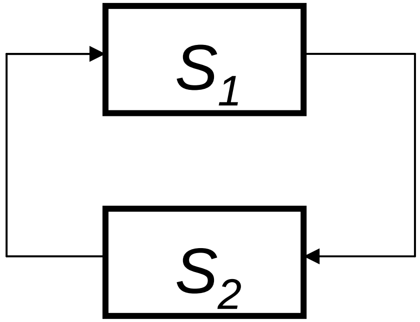
# Linear Measurements

- Measure the state $x_1$ (scalar) of lossless system $S_1$
- Choose a linear measurement device: $y(t) = kx_1(t)$
- A <u>lossless</u> implementation of $S_2$ gives

$$y_1(t) = kx_1(t) + \sqrt{2T_m k}v(t)$$

if measurement device has temperature $T_m$

- $S_1$ connected to measurement device $S_2$:



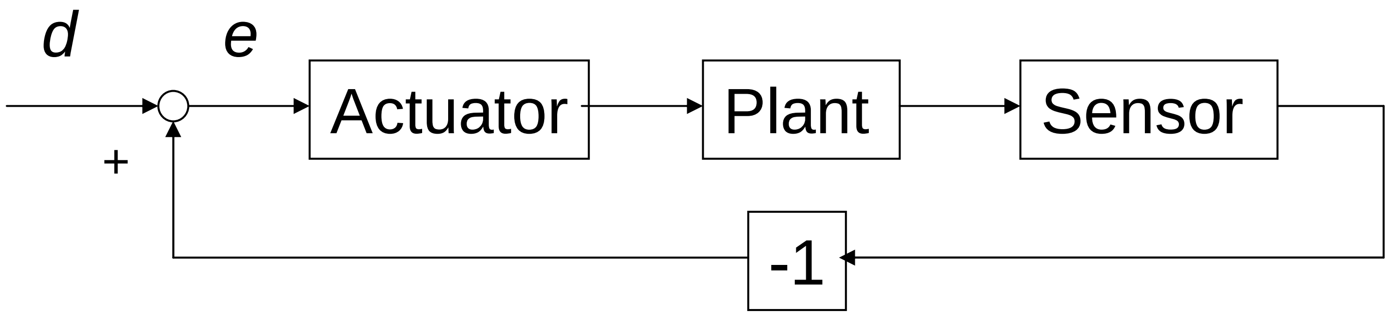

$$\dot{x}_1(t) = (J_1 - kB_1B_1^T)x_1(t) - B_1\sqrt{2kT_m}v(t)$$

$$\hat{x}_1(t) = x_1(t) + \sqrt{\frac{2T_m}{k}}v(t)$$

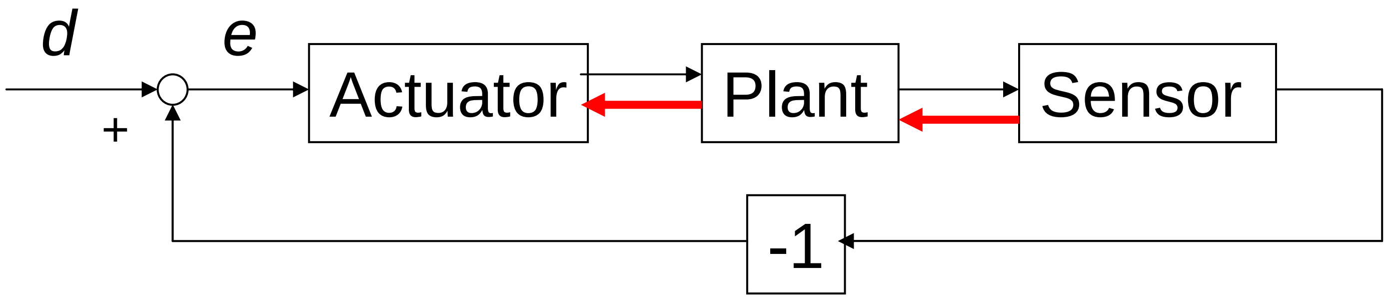
Back action: **E**(process noise x measurement noise) = $2T_m$

# Control Loops of Increasing Complexity and Realism

**Ideal devices**: Causality alone gives Bode integral limitations




**Lossless devices:** Energy conservation gives back action from sensor and actuator and additional limitations!



# Example: Conversion of Heat into Work I

- Classic thermodynamics problem. Here a controls version using increasingly realistic models with back action
- Assume $S_1$ is lossless and $\mathbf{E}x_1(0)=0$
- Extracted work: $W = -\int y_1(t)u_1(t)dt$
- With no extra information about the initial state of $S_1$:

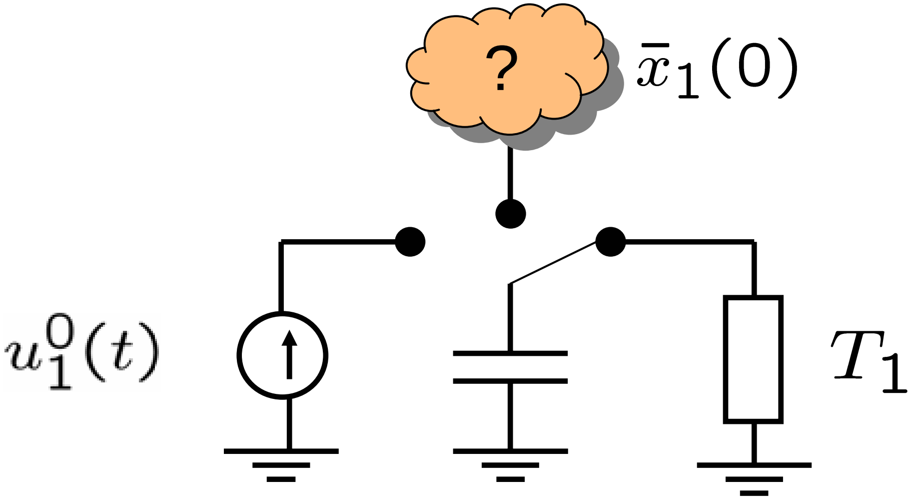
$$\mathbf{E}y_1(t) = \underbrace{B_1^T e^{J_1 t}\mathbf{E}x_1(0)}_{=0} + \int_0^t B_1^T e^{J_1(t-s)} B_1 u_1(s)ds$$

- Then $\mathbf{E}W = 0$, since on average we only get out what we put in
- With information about the initial state, we can do better!

# Heat into Work I

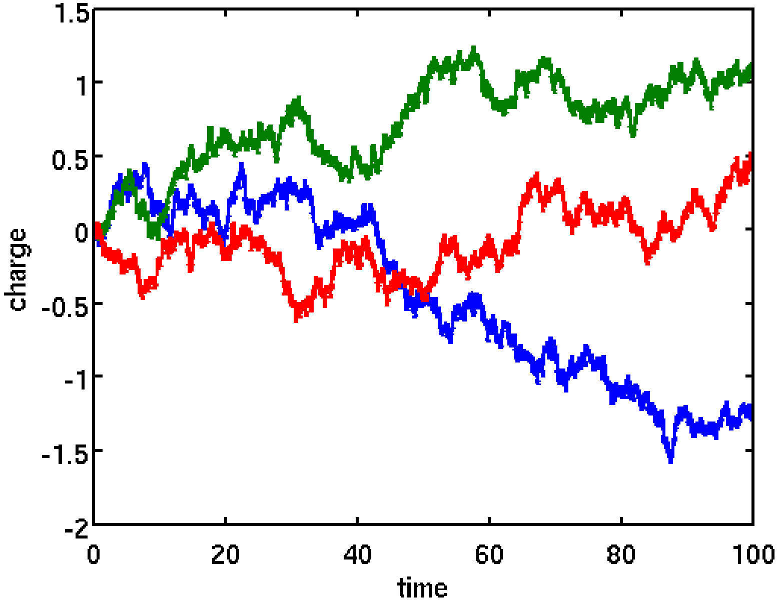
**Idea** (assuming we have correct model of *$S_1$*):

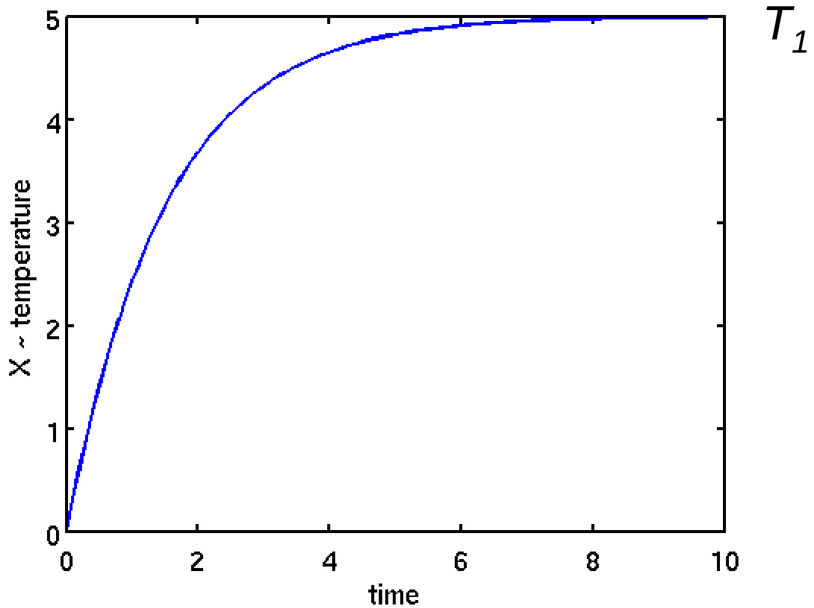
1. First heat (lossless) capacitor (*$S_1$*) to temperature $T_1$
2. Disconnect it, and *somehow* estimate its state: $\bar{x}_1(0)$
3. Use estimate to pull out energy to ideal current source, using open loop signal $u_1^0(t)$




How efficiently can we do this?

# Heating of Capacitor – Step 1




- The charge in the capacitor fluctuates during heating

- The variance $\mathbf{E}x_1(t)^2$ (temperature) increases with time constant $1/RC$ towards equilibrium $T_1$

- $\mathbf{E}x_1(t)=0$, but it is unlikely that the charge is close to zero after long time of heating

# Heat into Work I: Ideal Sensor and Actuator

- Assume we have an optimal linear estimate $\bar{x}_1(0)$ of $x_1(0)$:

$$x_1(0) = \bar{x}_1(0) + \delta x_1(0), \; \mathbf{E}x_1(0) = \mathbf{E}\bar{x}_1(0),$$

$$\mathbf{E}\bar{x}_1(0)^T \delta x_1(0) = 0,$$

$$\underbrace{\mathbf{E}x_1(0)^T x_1(0)}_{\text{"available energy"}} = \mathbf{E}Q = nT_1, \quad \underbrace{\mathbf{E}\delta x_1(0)^T \delta x_1(0)}_{\text{"remaining uncertainty"}} = nT_2, \; T_2 \leq T_1$$

- Based on $\bar{x}_1(0)$, we can compute an input $u_1^0(t)$ so that $\bar{x}_1(t) \to 0$ in the model

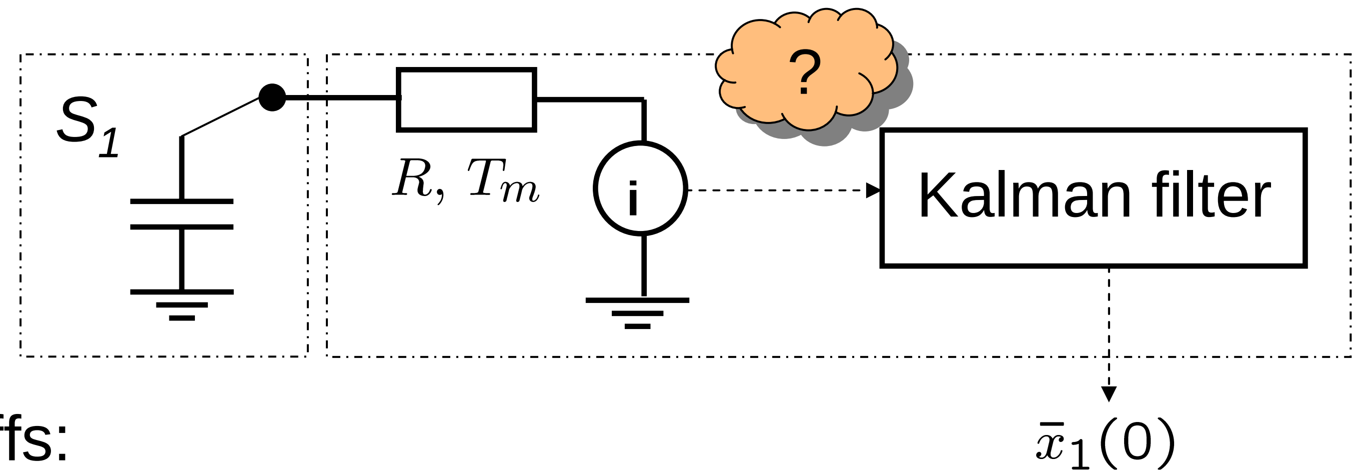
$$\dot{\bar{x}}_1(t) = J_1 \bar{x}_1(t) + B_1 u_1(t)$$
$$\bar{y}_1(t) = B_1^T \bar{x}_1(t)$$

- Expected extracted work to input heat ratio (compare Carnot):

$$\frac{\mathbf{E}W}{\mathbf{E}Q} = \frac{-\mathbf{E}\int y_1(t) u_1^0(t)dt}{nT_1} = \frac{T_1 - T_2}{T_1} = 1 - \frac{T_2}{T_1}$$

# Heat to Work I, Sensor with Back Action (Ideal Actuator)

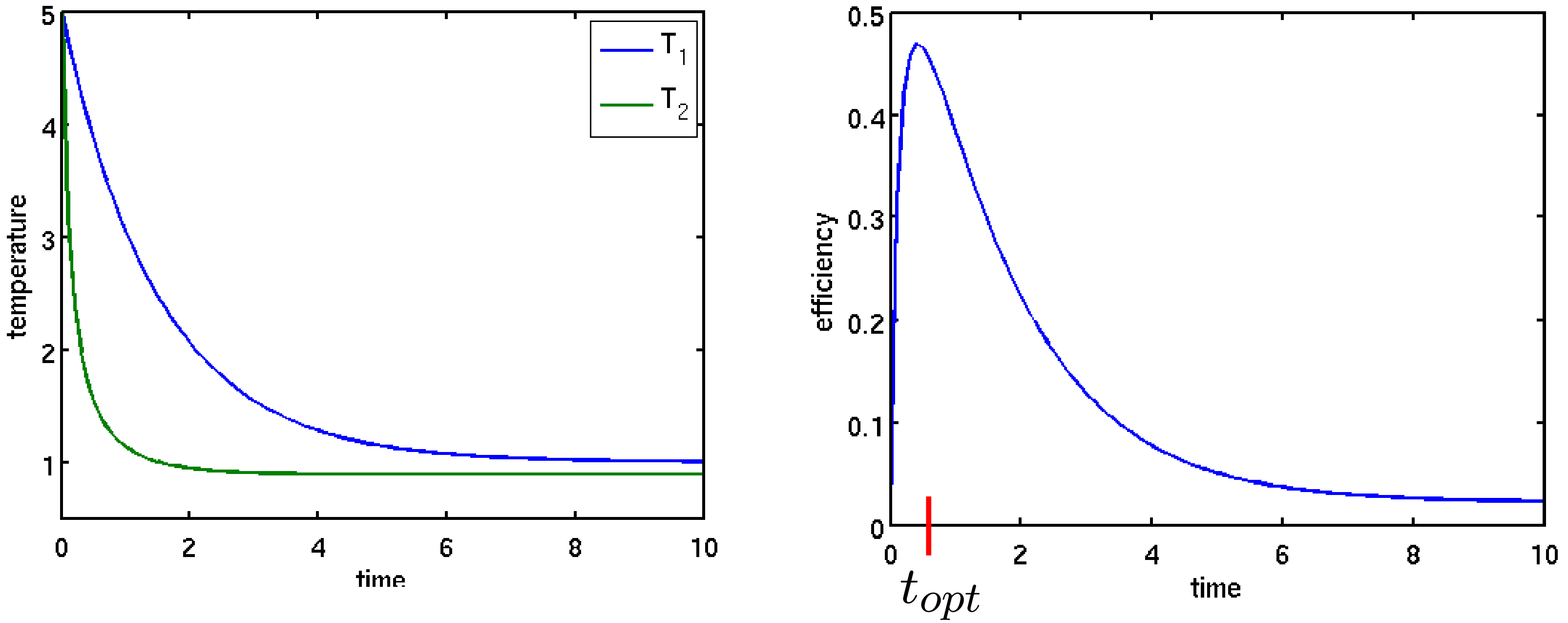
- **More realism**: Use a linear measurement device of temperature $T_m$ *and* a Kalman filter to obtain $\bar{x}_1(0)$




Tradeoffs:

- **Measure long time**: Dissipation in measurement device
- **Measure short time**: Bad estimate

# Example: Expected Work from Heated Capacitor Using Kalman Filter ($T_m$=1, $T_1(0)$=5, R=3, C=1)




- $T_1(t)$ – Temperature of capacitor
- $T_2(t)$ – Uncertainty (or temperature) of estimate
- "Efficiency" – $\frac{\text{expected work}}{\text{initial heat}} = \frac{T_1(t) - T_2(t)}{T_1(0)}$
- There is an optimal amount of time to measure before pulling out work ($t_{opt} \approx 0.4$)!

# Heat to Work I: Summary

- How to extract work from heat?
- First idea:
  - Linear time-invariant system;
  - Apply input in open loop;
  - Work extracted is $-\int u(t)^T y(t) dt$
- But: cannot convert heat into work
- Because: equation of mean and equation of variance are decoupled

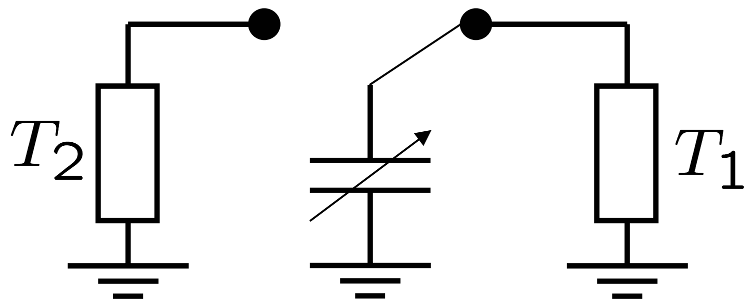
# Heat to Work I: Summary

- Second idea
  - Linear time-invariant system
  - Observe the output
  - Estimate the state
  - Apply an input

- Apparently: all heat into work
- Maxwell's demon
- But: Observation, estimation, actuation must be realized by (linear) physical systems
- Must be dissipative

- Kalman filter: linear time-varying

# Heat to Work II: Time-Varying Capacitor




- Brockett-Willems 1978
- How to modify capacity and connection to maximize work?
- Solution:
  - Capacitor connected to $T_1$ (high), capacitance increased slowly, energy $\frac{1}{2}T_1$
  - Capacitor disconnected, capacitance increased until energy $\frac{1}{2}T_2$
  - Capacitor connected to $T_2$ (low), capacitance decreased slowly, energy $\frac{1}{2}T_2$
  - Capacitor disconnected, capacitance decreased until energy $\frac{1}{2}T_1$
- Carnot cycle, efficiency $1 - \frac{T_2}{T_1}$

# General Formalism: Linear Time-Varying Systems

- Dissipative linear time-varying system:

$$\dot{x} = (A(t) - \sum_i M_i(t))x + \sum_i \sqrt{2T_i} F_i(t) v_i(t)$$

- Energy $U = \frac{1}{2} x^T K(t) x$
- We can choose $A(t),\ F_i(t),\ K(t)$
- Without loss of generality, $A^T K + KA = 0$
- How to extract work in an optimal way? (to be defined)
- Generalizes time-varying capacitor
- Generalizes Plant + Time-varying controller
- Nonlinear open-loop control in disguise

# Work and Heat

- Variance: $X = \mathbb{E}xx^T$
- Average energy: $U = \mathbb{E}\frac{1}{2}x^T Kx = \frac{1}{2}\text{Tr}KX$
- Energy equation:

$$\dot{U} = \frac{1}{2}\text{Tr}\dot{K}X + \frac{1}{2}\text{Tr}K\dot{X}$$

- Work extracted is $-\frac{1}{2}\text{Tr}\dot{K}X$

- Heat flow =

$$\frac{1}{2}\text{Tr}\dot{X}K = -\frac{1}{2}\sum_i \text{Tr}K(M_i X + XM_i) + \sum_i T_i \text{Tr}F_i F_i^T K$$

- Heat in-flow = fluctuation term = $\sum_i T_i \text{Tr}F_i F_i^T K$

# Efficiency

- During a cycle:

$$\text{Efficiency} = \frac{\text{Work}}{\text{Heat received}} = \frac{-\frac{1}{2}\int \text{Tr}\dot{K}X}{\sum_i T_i \int \text{Tr} F_i F_i^T K}$$

- If one temperature, efficiency $= 0$

- If two temperatures, efficiency $\leq 1 - \frac{T_{low}}{T_{high}}$

- Design the optimal cycle? In finite time?

- Given an open system, design the optimal controller?

# Entropy

- To prove efficiency bounds: entropy
- Entropy is

$$S = \frac{1}{2} \log \det X(t)$$

- Second Law

$$\dot{S} \geq \sum_i \frac{\dot{Q}_i}{T_i} = -\sum_i \frac{1}{T_i} (\frac{1}{2} \mathrm{Tr} K(M_i X + X M_i) + T_i \mathrm{Tr} F_i F_i^T K)$$

- In control and in physics,
  - entropy not interesting for itself
  - gives bound on work and heat

# Related Work

- *Willems and Brockett* (1978): Carnot cycles
- *Brockett* (1999): Control of stochastic ensembles
- *Newton and Mitter*: Kalman filter, information theory, and thermodynamics.
- *Lloyd and Touchette*: Control and information theory
- *Haddad, Chellaboina, and Nersesov*: Thermodynamics using storage function concepts.
- *Willems* (2006): Connections to behaviors
- "Finite-time thermodynamics"

# Summary

- **Limitation I**: Dissipative devices give noise when realized physically (from uncertainty in initial state). Example: measurement devices

- **Limitation II**: Measurements disturb the measured system (*back action*) through conservation of energy

- **Limitation III**: Work can be partly extracted from heated system using (noisy) measurements and models. (Compare with Carnot)

- **Limitation IV**: Work can be partly extracted from heated system by allowing time-varying systems (compare with Carnot)

- Possible connections to Bode-Shannon?