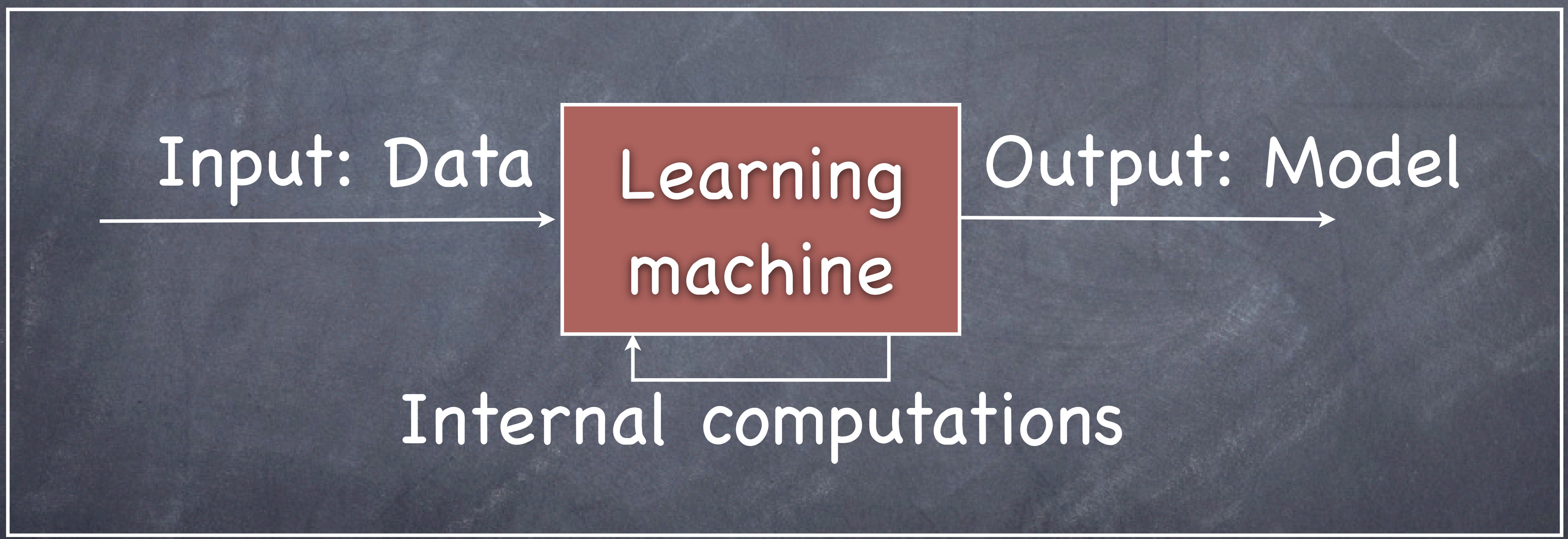
Optimal predictive inference

Susanne Still
University of Hawaii at Manoa
Information and Computer Sciences

S. Still, J. P. Crutchfield. Structure or Noise? http://lanl.arxiv.org/abs/0708.0654
S. Still, J. P. Crutchfield, C. J. Ellison. Optimal Causal Inference. http://lanl.arxiv.org/abs/0708.1580

The modeling (and machine learning) challenge:



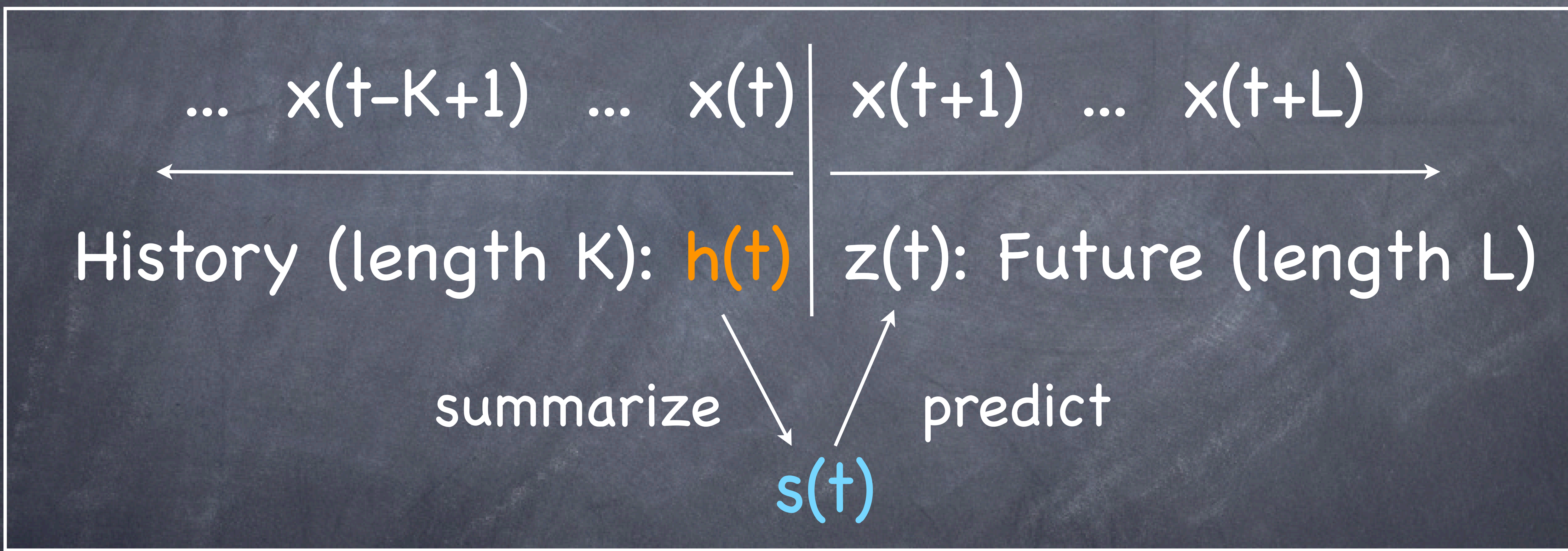
Fundamental question:
What is a good model?

Intuition behind the approach we take

1. A good model predicts well
   -> find maximally predictive model.
   Keep predictive information!

2. A good model is compact
   -> do not keep irrelevant information.

- System -> Produces observable x(t)
- Observer: Has access to a history h(t) of length K.
  Makes a representation of the system
  by creating internal states s(t).



- What information do we need to keep for prediction?
- Simplifying assumptions: discrete time; finite states.

Making a model

- Natural processes execute computations and produce information.
- The "predictive information", or "excess entropy" measures the information that the past carries about the future.

$$I_{\text{pred}} = \langle \log \frac{p(\text{future};\text{past})}{p(\text{future})p(\text{past})} \rangle$$

Quantifying the intuition

Objectives	Quantified by
Good generalization <=> Good prediction	Predicted Information I[s;z] s: internal state at time t z: future starting at t
Minimal coding cost (complexity)	Coding Rate I[s;h] h: history up to time t

Information about future, predicted by model:

$$I[s;z] = H[z] - H[z|s]$$

- Measures the reduction in uncertainty about the future, when the model state is known.
- If the state tells us nothing about future, then $H[z|s] = H[z]$ and $I[s;z] = 0$
- If knowing the state reduces the uncertainty about the future to $H[z|s] = 0$, then I is maximal: $I[s;z] = H[z]$.

Coding rate = historical information that is retained by the model:

$$I[s;h] = H[s] - H[s|h]$$

- $H[s]$: measures the "statistical complexity" of the model (Crutchfield and Young, '89). Computational mechanics.
- $H[s|h]$: measures how uncertain we are about whether the history h should be represented by the state s.
- Maximum entropy solution (Rose, 1990): max $H[s|h]$
- min $I[s;h]$ -> prefers model with minimal statistical complexity and maximal entropy.
- ($H[s|h] = 0$ for deterministic maps - the case in computational mechanics. Then $I[s;h] = H[s]$)

Making a model

- Finite state machine with internal states s
- Probabilistic map from input space to internal states: $p(s|h)$
- Together with prediction from model state s $p(z|s) = \langle p(z|h)p(h|s) \rangle$
- Objective: Construct s such that it is a maximally predictive and efficient summary of historical information.
- Find the optimal probabilistic map $p(s|h)$.

Optimization principle:

$$\max_{p(s|h)} \left(I[s;z] - \lambda I[s;h] \right)$$

This is rate-distortion theory!!!

- Maps directly onto the "Information Bottleneck Method" (*N. Tishby, F. Pereira and W. Bialek (1999) http://lanl.arxiv.org/abs/physics/0004057*)
- past = data to compress
- future = relevant quantity

- Note: Objective function is equivalent to constructing the states such that they implement "causal shielding", a property of the causal states in computational mechanics.

$$\min_{p(s|h)} \left(I[s;h] + \beta I[z;h|s] \right)$$

- Rate distortion theory with the distortion function

$$d(h,s) = D_{\mathrm{KL}}[p(z|h) \| p(z|s)]$$

- because of the Markov condition, p(z|h;s) = p(z|h):

$$\begin{aligned} I[z;h|s] &= \langle\langle \log \left[\frac{p(z;h|s)}{p(z|s)p(h|s)} \right] \rangle_{p(z|h,s)} \rangle_{p(h,s)} \\ &= \langle\langle \log \left[\frac{p(z|h)p(h|s)}{p(z|s)p(h|s)} \right] \rangle_{p(z|h)} \rangle_{p(h,s)} \\ &= \langle D_{\mathrm{KL}}[p(z|h) \| p(z|s)] \rangle_{p(h,s)} \end{aligned}$$

Optimization principle:

$$\max_{p(s|h)} \left(I[s;z] - \lambda I[s;h] \right)$$

Family of solutions:

$$p(s|h) = \frac{p(s)}{Z(h,\lambda)} \exp\left(-\frac{1}{\lambda} D_{KL}[p(z|h)||p(z|s)] \right)$$

Iterative Algorithm

$$
\begin{aligned}
p^{(j)}(s|h) &= \frac{p^{(j)}(s)}{Z(h,\lambda)} \exp\left(-\frac{1}{\lambda} D_{KL}[p(z|h)||p^{(j)}(z|s)]\right) \\
p^{(j+1)}(s) &= \sum_h p^{(j+1)}(s|h)p(h) \\
p^{(j+1)}(z|s) &= \frac{1}{p^{(j+1)}(s)} \sum_h p(z|h)p^{(j)}(s|h)p(h)
\end{aligned}
$$

Blahut-Arimoto type algorithm (same as "Information Bottleneck" algorithm). Converges to local optimum.

Theorem: In the low temperature regime ($\lambda \to 0$) the causal state partition is found.

(S. Still, J. P. Crutchfield, C. Ellison. Optimal Causal Inference. arXiv:0708.1580)

- The causal states reflect the underlying states of the system -> physically meaningful solution.

  (J. P. Crutchfield and K. Young (1989) PRL 63:105–108)

- Causal states are unique and minimal sufficient statistics.

  (J. P. Crutchfield and C. R. Shalizi (1999) Phys.Rev.E 59(1): 275–283)

Proof Sketch:

Recall: $$p(s|h) = \frac{p(s)}{Z(h,\lambda)} \exp\left(-\frac{1}{\lambda} D_{KL}[p(z|h)||p(z|s)]\right)$$

1. In low temp. regime -> deterministic partition:

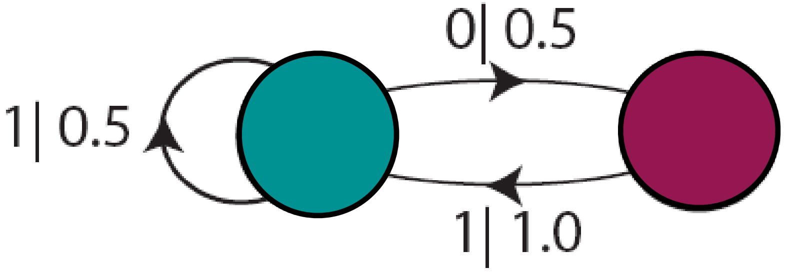
$$p(s|h) = \delta_{ss^*}$$

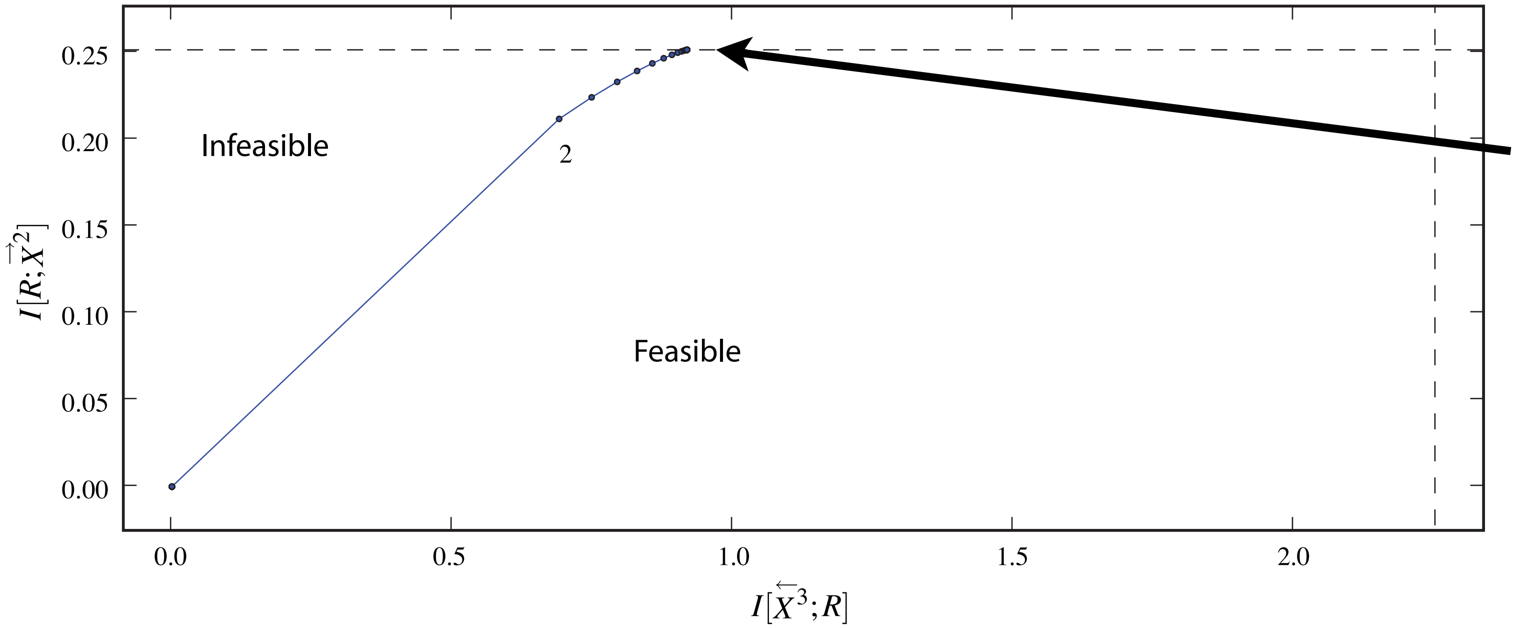
with: $$s^* = \arg\min_s D_{KL}[p(z|h)||p(z|s)]$$

2. Histories h with same conditional future distributions, p(z|h) = p(z|s), are assigned to the same category s. This defines an equivalence relation, or probabilistic "bisimulation" (Milner, '84), which is precisely the causal state partition of computational mechanics.

Example: Golden Mean

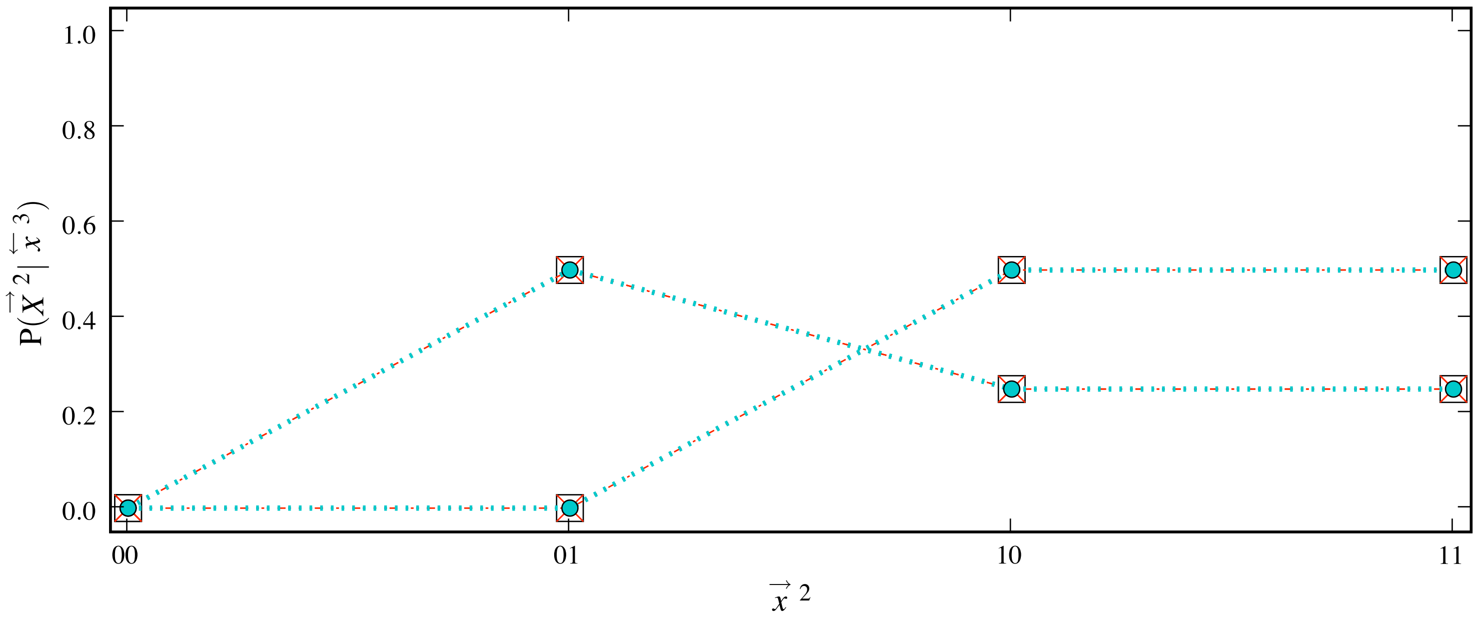
Produces all binary sequences except those with 00





Algorithm finds the 2 states that describe the process fully.

Conditional future distributions associated with 2 state model



Hierarchy of optimal models

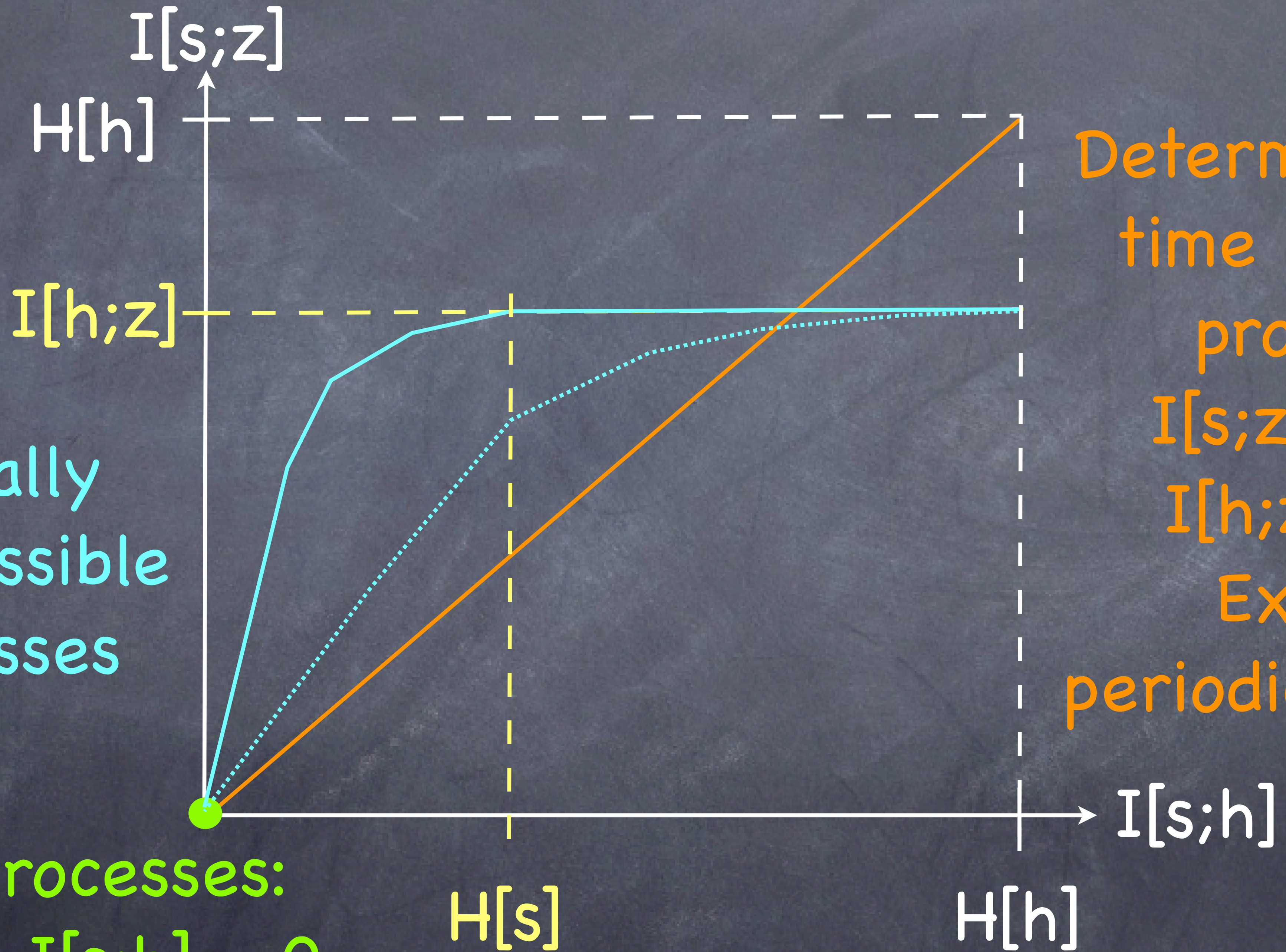
- As temperature -> 0, we find causal states. Those capture the full predictive information!
- But, in general we may not want to keep all detail!
- We can find more compact models. Those have larger prediction error.
- Compared to computational mechanics, here we have an extension to non-deterministic models.

Causal compressibility

- Study the full range of optimal models to lear about the “causal compressibility” of a stochastic process at hand.
- Encoded in the rate-distortion curve.

- Not causally compressible:
  - Deterministic and time reversible processes (RD curve on the diagonal)
  - i.i.d. processes (RD curve degenerated to a point at the origin)
- Weakly causally compressible: RD curve is close to a straight line (small curvature).
- Strongly causally compressible: large curvature.
- Fully causally compressible: full predictive information can be kept with a model that has a complexity smaller than H[h].

Causal compressibility



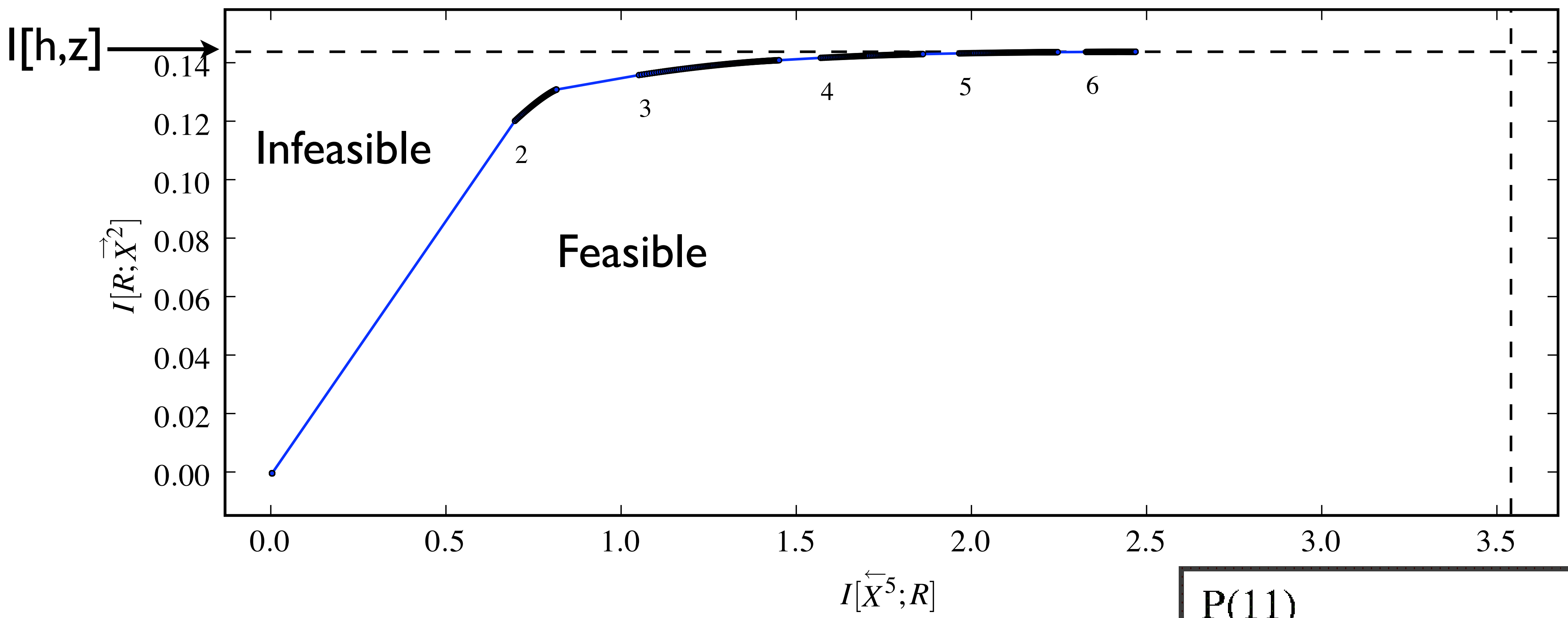
Causally compressible processes

Deterministic and time reversible processes:
I[s;z] = I[s;h]
I[h;z] = H[h]
Example: periodic processes

i.i.d. processes:
I[s;z] = I[s;h] = 0

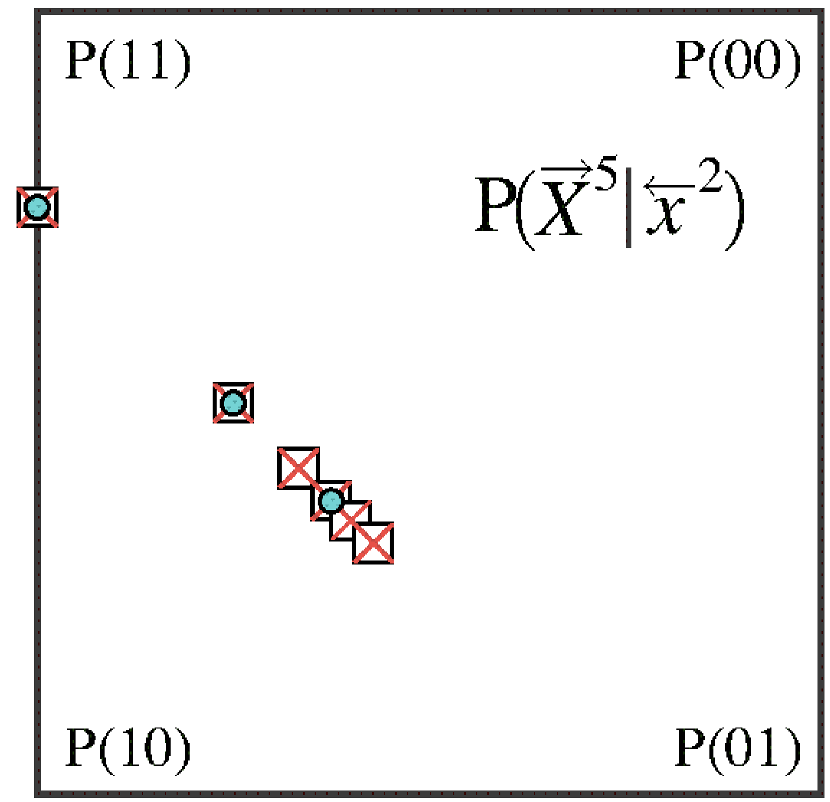
S. Still, J. P. Crutchfield. Structure or Noise? *http://lanl.arxiv.org/abs/0708.0654*

Example (SNS)



Future distributions:

- ✗ full historical information
- □ best 6-state model
- ● best 3-state model



Learning from finite data

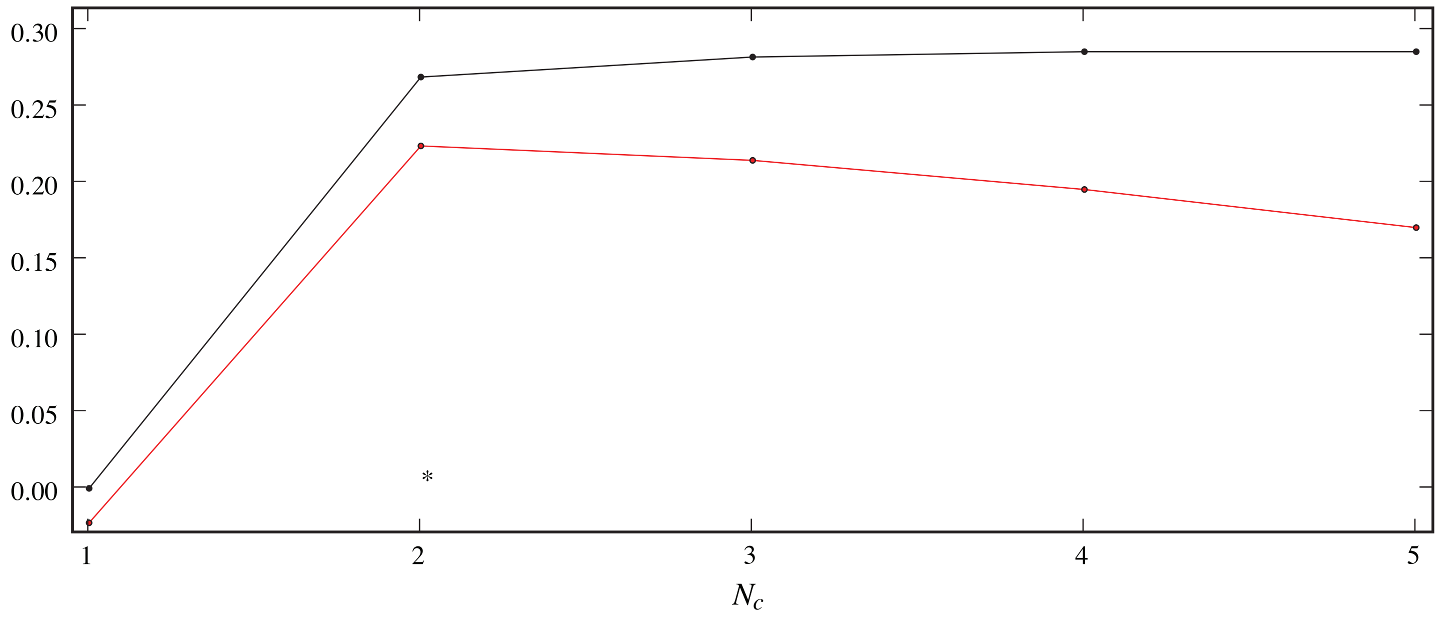
- So far, we assumed knowledge of $P(z|h)$
- In practice we have to estimate this distribution from finite data.
- Sampling errors result in overestimate of predictive information => could result in overfitting!
- It looks as if there are more causal states than there really are.

Finite Data

- Find the maximum number of states we can use safely without overfitting.
- Idea: compensate for sampling error in the objective function! Taylor expansion gives estimate of error.
- Result: Corrected curve has a maximum => easy to detect optimal number of states.

S. Still and W. Bialek (2004) Neural Comp. 16(12):2483–2506

Golden Mean Process



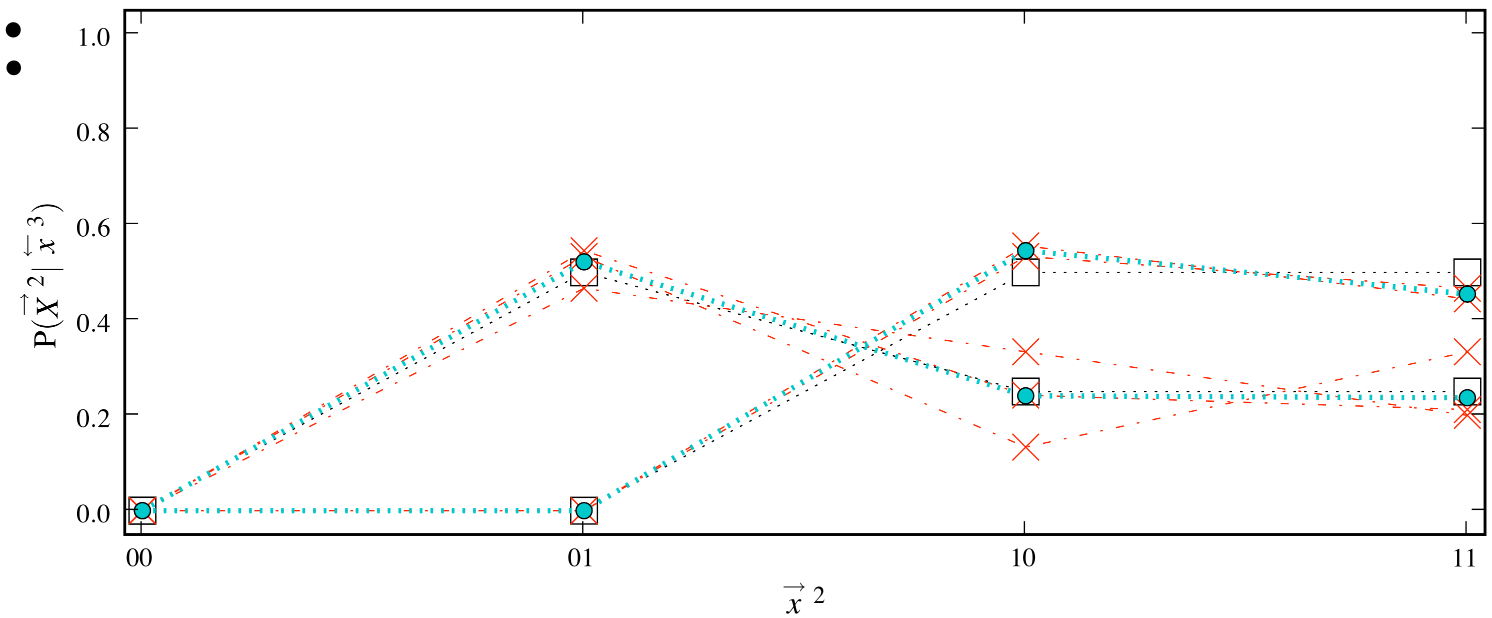
Correction finds optimal number of states (2)

Future distributions:

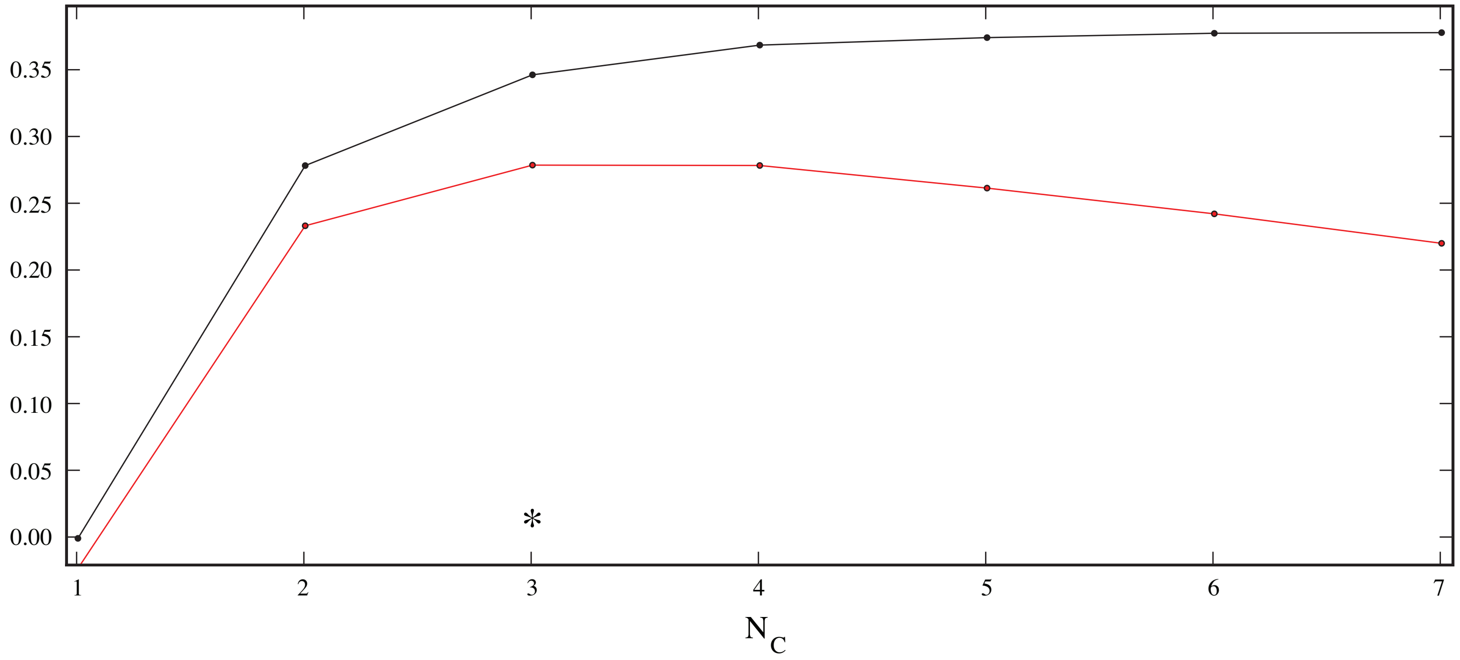
Finite Data

ideal (truth)

result (algorithm)

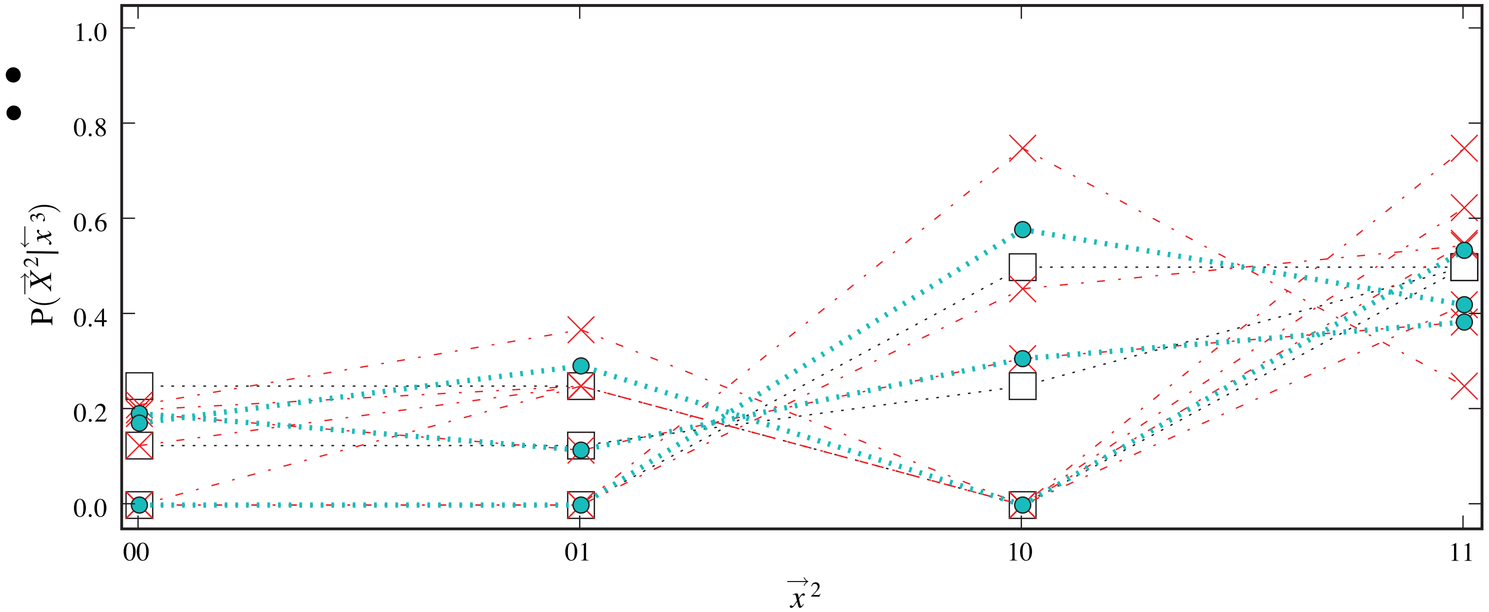


Even Process



Correction finds optimal number of states (3)

Future distributions:



Finite Data

ideal (truth)

result (algorithm)

Conclusion

Simple and intuitive principles allow us to:

1. Find optimal abstractions.

- construct maximally predictive models at fixed model complexity
- in the limit of full prediction we find the causal states (which constitute unique minimal sufficient statistics).
- correct for sampling errors due to finite data set size.

2. characterize a process in terms of its causal compressibility by studying the full range of optimal models.

Extensions

- Online learning: Reconstructing the "epsilon machine", including transition probabilities. (unpublished results)
- Active learning. (tomorrow's lecture)