

Predictability, Complexity and Learning

Ilya Nemenman

Co-authored with: William Bialek, Naftali Tishby

August 26, 2003

<http://xxx.lanl.gov/abs/physics/0007070>

Outline

- A curious observation.
- Why a new learning and complexity theory is needed?
- Why and how to use information theory?
- Predictive information and its properties.
- Calculating predictive information for different processes.
- Unique complexity measure through predictive information.
- Possible applications.

Entropy of words in a spin chain

$$S(N) = - \sum_{k=0}^{2^N-1} P_N(W_k) \log_2 P_N(W_k)$$

For this chain, $P(W_0) = P(W_1) = P(W_3) = P(W_7) = P(W_{12}) = P(W_{14}) = 2$, $P(W_8) = P(W_9) = 1$, and all other frequencies (probabilities) are zero. Thus, $S(4) \approx 2.95$ bits.

Entropy of 3 generated chains

- $J_{ij} = \delta_{i,j+1}$
- $J_{ij} = J_0 \delta_{i,j+1}$, J_0 is taken
at random from $\mathcal{N}(0, 1)$
every 400000 spins
- J_{ij} is taken at random
from $\mathcal{N}(0, \frac{1}{i-j})$
every 400000 spins

$1 \cdot 10^9$ spins total.

Entropy is extensive! It shows no distinction between the cases.

Subextensive component of the entropy

This component is usually neglected in physics and information theory.

Subextensive entropy shows a qualitative distinction between the cases! What is the significance of this difference?

Problems in learning and complexity theories

- many frameworks to study learning
 - all very specialized
- many frameworks to study complexity
 - probabilistic or deterministic?
 - description length (Kolmogorov-style complexities) — but are all bits relevant?
- no clear connection between learning and complexity
- over-universal complexity definitions
- complexity must be zero for a completely random signal, and some measures get it wrong

There is very little known about connections between various views on learning and complexity.

We need a *universal* paradigm created, of which all studied problems are special cases.

We base this approach on the notion of predictability.

Why predictability?

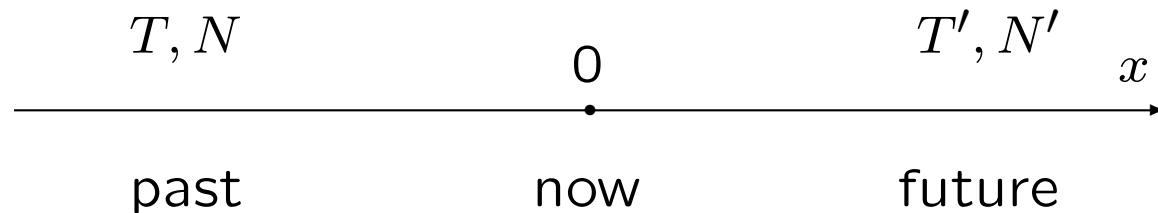
- we learn (estimate parameters, extrapolate, classify, ...) not for the sake of learning; the problem of learning is to *generalize* and *predict* from training examples, and estimation of parameters is only an intermediate step
- nonpredictive features in any signal are useless since we observe *now* and react in the *future*
- high predictability means more features to predict, not easier prediction — this is a problem of intuitively higher complexity
- it is impossible to predict a totally random string, so if complexity is based on predictability, for such a string it is zero

Quantifying predictability

- learning is accrual of *information*
- Shannon's information theory is *the only* nonmetric way to quantify information

Thus we will use information theory to study predictability and will define *predictive information* as *the information that the observed data provides about the data that is coming.*

Definitions



$$\begin{aligned}
 \mathcal{I}_{\text{pred}}(T, T') &= \left\langle \log_2 \left[\frac{P(x_{\text{future}} | x_{\text{past}})}{P(x_{\text{future}})} \right] \right\rangle \\
 &= S(T) + S(T') - S(T + T') \\
 S(T) &= \mathcal{S}_0 \cdot T + S_1(T)
 \end{aligned}$$

extensive component cancels in predictive information
 predictability is a deviation from extensivity!

$$I_{\text{pred}}(T) \equiv \mathcal{I}_{\text{pred}}(T, \infty) = S_1(T)$$

Properties of $I_{\text{pred}}(T)$

- $I_{\text{pred}}(T)$ is information, so $I_{\text{pred}}(T) \geq 0$
- $I_{\text{pred}}(T)$ is subextensive, $\lim_{T \rightarrow \infty} \frac{I_{\text{pred}}(T)}{T} = 0$
- diminishing returns, $\lim_{T \rightarrow \infty} \frac{I_{\text{pred}}(T)}{S(T)} = 0$
- prediction and postdiction are symmetric
- it relates to and generalizes many relevant quantities
 - learning: universal learning curves
 - complexity: complexity measures
 - coding: coding length

How can I_{pred} behave?

$\lim_{N \rightarrow \infty} I_{\text{pred}} = \text{const}$ no long-range structure

- simply predictable (periodic, constant, etc.) processes
- fully stochastic (Markov) processes

$\lim_{N \rightarrow \infty} I_{\text{pred}} = \text{const} \times \log_2 N$ precise learning of a fixed set of parameters

- learning finite-parameter densities
- analyzed as $I(N, \text{parameters}) = I_{\text{pred}}(N)$

$\lim_{N \rightarrow \infty} I_{\text{pred}} = \text{const} \times N^\xi$ learning more features as N grows

- learning continuous densities
- not well studied

Problem setup

$Q(x|\alpha)$ probability density function for \vec{x} parameterized by unknown parameters α

$\dim \alpha = K$ dimensionality of α , may be infinite

$\mathcal{P}(\alpha)$ prior distribution of parameters

$\vec{x}_1 \cdots \vec{x}_N$ random samples from the distribution

$$P(\vec{x}_1, \vec{x}_2, \cdots, \vec{x}_N | \alpha) = \prod_{i=1}^N Q(\vec{x}_i | \alpha)$$

$$P(\vec{x}_1, \vec{x}_2, \cdots, \vec{x}_N) = \int d^K \alpha \mathcal{P}(\alpha) \prod_{i=1}^N Q(\vec{x}_i | \alpha)$$

$$S(\vec{x}_1, \vec{x}_2, \cdots, \vec{x}_N) \equiv S(N) = - \int d\vec{x}_1 \cdots d\vec{x}_N P(\{\vec{x}_i\}) \log_2 P(\{\vec{x}_i\})$$

Separating the extensive term

$$\begin{aligned}
 S(N) &= - \int d^K \bar{\alpha} \mathcal{P}(\bar{\alpha}) \left\{ d^N \vec{x} \prod_{j=1}^N Q(\vec{x}_j | \bar{\alpha}) \log_2 \int d^K \alpha \mathcal{P}(\alpha) \prod_{i=1}^N Q(\vec{x}_i | \alpha) \right\} \\
 &= - \int d^K \bar{\alpha} \mathcal{P}(\bar{\alpha}) \left\{ d^N \vec{x} \prod_{j=1}^N Q(\vec{x}_j | \bar{\alpha}) \right. \\
 &\quad \times \log_2 \prod_{j=1}^N Q(\vec{x}_j | \bar{\alpha}) \int d^K \alpha \mathcal{P}(\alpha) \left. \overbrace{\prod_{i=1}^N \left[\frac{Q(\vec{x}_i | \alpha)}{Q(\vec{x}_i | \bar{\alpha})} \right]}^{\exp[-N\mathcal{E}_N(\alpha; \{\vec{x}_i\})]} \right\}
 \end{aligned}$$

This separates $S(N)$ into the extensive and the subextensive terms

$$\begin{aligned}
 \mathcal{S}_0 &= \int d^K \alpha \mathcal{P}(\alpha) \left[- \int d^D x Q(\vec{x} | \alpha) \log_2 Q(\vec{x} | \alpha) \right], \\
 S_1(N) &= - \int d^K \bar{\alpha} d^N \vec{x}_i \mathcal{P}(\bar{\alpha}) \log_2 \left[\int d^K \alpha \mathcal{P}(\alpha) e^{-N\mathcal{E}_N} \right]
 \end{aligned}$$

Annealed approximation

Under some conditions we may have

$$\begin{aligned}
 \psi(\alpha, \bar{\alpha}; \{x_i\}) &\equiv \underbrace{\mathcal{E}_N(\alpha; \{\vec{x}_i\})}_{\text{quenched energy}} - \underbrace{D_{\text{KL}}(\bar{\alpha}||\alpha)}_{\text{annealed energy}} \\
 &\equiv -\frac{1}{N} \sum_{i=1}^N \ln \left[\frac{Q(\vec{x}_i|\alpha)}{Q(\vec{x}_i|\bar{\alpha})} \right] + \int d\vec{x} Q(\vec{x}|\bar{\alpha}) \ln \left[\frac{Q(\vec{x}|\alpha)}{Q(\vec{x}|\bar{\alpha})} \right] \\
 &\leadsto 0
 \end{aligned}$$

$$S_1(N) \leadsto S_1^{(\text{a})}(N) \equiv - \int d^K \bar{\alpha} \mathcal{P}(\bar{\alpha}) \underbrace{\log_2 \frac{\overbrace{\int d^K \alpha P(\alpha) e^{-N D_{\text{KL}}}}^{\text{annealed partition function, } Z(\bar{\alpha}; N)}}{\text{annealed free energy, } F(\bar{\alpha}; N)}}_{\text{annealed free energy, } F(\bar{\alpha}; N)}$$

Density of states

We can rewrite the partition function

$$\begin{aligned} Z(\bar{\alpha}; N) &= \int dD \rho(D; \bar{\alpha}) \exp[-ND] \\ \rho(D; \bar{\alpha}) &= \int d^K \alpha \mathcal{P}(\alpha) \delta[D - D_{\text{KL}}(\bar{\alpha} || \alpha)] \\ \int dD \rho(D; \bar{\alpha}) &= \int d^K \alpha \mathcal{P}(\alpha) = 1 \end{aligned}$$

The density ρ could be very different for different targets.

Thus learning is annealing at decreasing temperature; properties of predictive information (and learning) almost always depend on $D = 0$ behavior of the density.

Power-law density function

For this case:

$$\begin{aligned}\rho(D \rightarrow 0; \bar{\alpha}) &\approx A(\bar{\alpha}) D^{(d-2)/2} \\ S_1^{(a)} &\approx \frac{d}{2} \log_2 N\end{aligned}$$

If $d = d(\bar{\alpha})$, then we can get non half-integer coefficients in front of the logarithm term.

- this behavior is known in MDL and other literature
- speed of approach to this asymptotics is rarely investigated

Examples of the logarithmic predictive information

- Finite parameter models, $\dim \alpha = K$. Then for $\alpha \approx \bar{\alpha}$ and for *sound* parameterization

$$D_{\text{KL}}(\bar{\alpha}||\alpha) \approx \frac{1}{2} \sum_{\mu\nu} (\bar{\alpha}_\mu - \alpha_\mu) \mathcal{F}_{\mu\nu} (\bar{\alpha}_\nu - \alpha_\nu) + \dots$$

$$\rho(D \rightarrow 0; \bar{\alpha}) \approx \mathcal{P}(\bar{\alpha}) \frac{2\pi^{K/2}}{\Gamma(K/2)} (\det \mathcal{F})^{-1/2} D^{(K-2)/2}$$

\mathcal{F} — Fisher information matrix

To avoid complications with *soundness*, we can *define* the phase space dimensionality of the model family through the exponent of the density function.

- Finite parameter Markov process, learn $Q(\vec{x}_1 \cdots \vec{x}_N | \alpha)$. If energy is extensive,

$$D_{\text{KL}} [Q(\{\vec{x}_i\} | \bar{\alpha}) || Q(\{\vec{x}_i\} | \alpha)] \rightarrow N D_{\text{KL}} (\bar{\alpha} || \alpha) + o(N) .$$

and extensive term is replaced by

$$\begin{aligned} S[\{\vec{x}_i\} | \alpha] &\equiv - \int d^N \vec{x} Q(\{\vec{x}_i\} | \alpha) \log_2 Q(\{\vec{x}_i\} | \alpha) \\ &\rightarrow N S_0 + S_0^*; \quad S_0^* = \frac{K'}{2} \log_2 N \end{aligned}$$

then

$$S_1^{(a)}(N) = \frac{K + K'}{2} \log_2 N$$

Predictive information does not distinguish predictability coming from unknown parameters and from intrinsic long-range correlations. This is similar to describing physical systems with correlations using order parameters.

Essential singularity in the density function

As $d \rightarrow \infty$ we may imagine the following behavior

$$\rho(D \rightarrow 0; \bar{\alpha}) \approx A(\bar{\alpha}) \exp \left[-\frac{B(\bar{\alpha})}{D^\mu} \right], \quad \mu > 0$$

$$C(\bar{\alpha}) = [B(\bar{\alpha})]^{1/(\mu+1)} \left(\frac{1}{\mu^{\mu/(\mu+1)}} + \mu^{1/(\mu+1)} \right)$$

$$S_1^{(a)}(N) \approx \frac{1}{\ln 2} \langle C(\bar{\alpha}) \rangle_{\bar{\alpha}} N^{\mu/(\mu+1)}$$

- finite parameter model with increasing number of parameters $K \sim N^{\mu/(\mu+1)}$; $S_1(N) \sim N^{\mu/(\mu+1)}$, not $S_1(N) \sim \frac{N^{\mu/(\mu+1)}}{2} \log N$
- as $\mu \rightarrow \infty$ complexity grows and then vanishes to the leading order when $S_1^{(a)}$ becomes extensive

Example of the power-law I_{pred}

Learning a nonparametric (infinite parameter) density $Q(x) = 1/l_0 e^{-\phi(x)}$, $x \in [0, L]$, with some smoothness constraints (Bialek, Callan, and Strong 1996).

$$\mathcal{P}[\phi(x)] = \frac{1}{\mathcal{Z}} \exp \left[-\frac{l}{2} \int dx \left(\frac{\partial \phi}{\partial x} \right)^2 \right] \delta \left[\frac{1}{l_0} \int dx e^{-\phi(x)} - 1 \right]$$

$$\rho(D \rightarrow 0; \bar{\phi}) = A[\bar{\phi}(x)] D^{-3/2} \exp \left(-\frac{B[\bar{\phi}(x)]}{D} \right)$$

$$S_1^{(a)}(N) \approx \frac{1}{2 \ln 2} \sqrt{N} \left(\frac{L}{l} \right)^{1/2}$$

- increasing number of ‘effective parameters’ (bins) of adaptive size $\sim \sqrt{l/NQ(x)}$
- heuristic arguments for the dimensionality ζ and the smoothness exponent η give $S_1(N) \sim N^{\zeta/2\eta}$ — demonstrates a crossover from complexity to randomness

Which complexity do we want to define?

- complexity of dynamics that generates a time series (not computational or descriptive complexity); thus it must be zero for totally random and for easily predictable processes
- usable for Occam–style punishment in statistical inference
- expressible in conventional physical terms
- must be attached to an ensemble, not a single realization

Ensemble property?

All pictures could be just random, but we do not perceive them this way. Ensemble is implicit!

Unique measure of complexity!

Complexity measure must be:

- some kind of entropy (we proclaim Shannon's postulates)
 - monotonic in N for N equally likely signals
 - additive for statistically independent signals
 - a weighted sum of measure at branching points if measuring a leaf on a tree
- reparameterization, quantization invariant, thus subextensive
- invertible temporally local transformations (e. g., $x_k \rightarrow x_k + \xi x_{k-1}$ —measuring device with inertia) and prior insensitive

The divergent subextensive term measures complexity uniquely!

What's next?

- separating predictive information from non-predictive using the 'relevant information' technique
- reflection to physics — finding order parameters for phase transitions using behavior of the predictive information
- reflection to biology — large expansion from receptors to primary sensory cortices may be due to efficient representation of predictive information, not current state of the world
- reflection to psychology — experiments on learning distributions and language (power law complexity class) by humans; what expectations of the world do we have?
- reflection to statistics
 - nonparametric models may be simpler than finite parameter ones (relevant to biology)
 - predictive information is the property of the data (nonparametric extension of the MDL principle)

Summary

We have built a generalizing and unique theory of learning and complexity.