Predictive information: From definition to applications to biological systems

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Outline

- A curious observation.
- Quantifying predictability.
- Predictability and optimization in sensory information processing.
- Learning and predictive information.
- Testing models used by animals.
- Bonus material.
Entropy of words in a spin chain

\[ W_0 = 0 0 0 0 \]
\[ W_1 = 0 0 0 \]
\[ W_2 = 0 0 1 \]
\[ \ldots \]
\[ W_{15} = 1 1 1 \]
Entropy of words in a spin chain

\[ S(N) = - \sum_{k=0}^{2^N-1} P_N(W_k) \log_2 P_N(W_k) \]
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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.
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Entropy is extensive!
It shows no distinction between the cases.
Subextensive component of the entropy

... shows a qualitative distinction between the cases!
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Other examples:
- **const** periodic sequences, chaotic sequences (finite correlation length)
- **log** systems at phase transitions, or at the onset of chaos (divergent correlation length)
- **power** natural texts, DNA sequences, (possibly) some exotic transitions, (many divergent correlation lengths)
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- Entropy density or channel capacity do not distinguish these cases.
- Theory of phase transitions may not distinguish between the last two cases.
- Complexity of underlying dynamics intuitively increases from \textbf{const} to \textbf{power}. 

\[ S_1 = \text{const}_1 + \text{const}_2 N^{0.5} \]
\[ S_1 = \text{const}_1 + \frac{1}{2} \log N \]
\[ S_1 = \text{const} \]
Objectives

- unified description of complexity and learning
- make distinction between useful and unusable data
- do this using physical quantities
- understand models used by organisms to represent the world
- understand biological designs by means of optimization principles
Solution – predictability

- we learn (estimate parameters, extrapolate, classify, ...) to generalize and predict from training examples; estimation of parameters is only an intermediate step
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- high predictability sources (more details to predict, not easier predictions) are generated by more complex sources (in particular, regular and random sources have low complexity)
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- optimizing predictive information may be the design principle
Quantifying predictability

Information theory: non-metric, universal way to quantify learning

\[ T, N \quad \rightarrow \quad 0 \quad \rightarrow \quad T', N' \quad x \]

past \quad \rightarrow \quad now \quad \rightarrow \quad future
Quantifying predictability

Information theory: non-metric, universal way to quantify learning

\[ I_{\text{pred}}(T, T') = \left\langle \log_2 \left[ \frac{P(x_{\text{future}}|x_{\text{past}})}{P(x_{\text{future}})} \right] \right\rangle = S(T) + S(T') - S(T + T') \]
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Information theory: non-metric, universal way to quantify learning

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\mathcal{I}_{\text{pred}}(T, T') = \langle \log_2 \left[ \frac{P(x_{\text{future}} | x_{\text{past}})}{P(x_{\text{future}})} \right] \rangle \\
= S(T) + S(T') - S(T + T')
\]

\[
S(T) = S_0 \cdot T + S_1(T)
\]

Extensive component cancels in predictive information.

Predictability is a deviation from extensivity!
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\[
I_{\text{pred}}(T) \equiv I_{\text{pred}}(T, \infty) = S_1(T)
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Properties of $I_{\text{pred}}(T)$

- $I_{\text{pred}}(T)$ is information, so $I_{\text{pred}}(T) \geq 0$
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- it relates to and generalizes many relevant quantities
  - learning: universal learning curves
  - complexity: complexity measures
  - coding: model coding length
How can $I_{\text{pred}}$ behave?

$$\lim_{N \to \infty} I_{\text{pred}} = \text{const}$$

no long-range structure

- simply predictable (periodic, constant, etc.) processes
- fully stochastic (Markov) processes
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$$\lim_{N \to \infty} I_{\text{pred}} = \text{const} \times \log_2 N$$
precise learning of a fixed set of parameters
- learning finite-parameter densities
- well known as $I(N, \text{parameters}) = I_{\text{pred}}(N)$
- physical system at criticality
- (possibly) nonextensive statistics systems
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\[ \lim_{N \to \infty} I_{\text{pred}} = \text{const} \times N^\xi \]  
learning more features as $N$ grows
- learning continuous densities
- language
- some critical phenomena (wetting transitions)
- not well studied
$I_{\text{pred}}$ optimization in biology

$S_\phi(\omega) \propto \omega^{-\alpha}$

input, $\phi$ \hspace{1cm} “bug” \hspace{1cm} output, $\nu$
\( I_{\text{pred}} \) optimization in biology

\[ S_\phi(\omega) \propto \omega^{-\alpha} \]

\[ \tau \frac{dv}{dt} = -v + g\phi(t) + g\eta(t), \quad \langle \eta(t)\eta(0) \rangle = 1/I_0 \delta(t) \]
Ilya Nemenman, IBM – Functional Genomics and System Biology Seminar, March 4, 2004

$I_{\text{pred}}$ \textbf{optimization in biology}

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\[ \tau \frac{dv}{dt} = -v + g\phi(t) + g\eta(t), \quad \langle \eta(t)\eta(0) \rangle = 1/I_0 \delta(t) \]

\[ \mathcal{I}([\phi], [v]) = \lim_{T \to \infty} \frac{1}{2T} \int_{-T/2}^{T/2} \frac{d\omega}{2\pi} \log \left( 1 + \frac{S_\phi(\omega)}{1/I_0} \right) \]

Maximization w.r.t. $\tau$ is meaningless.
Predictive information maximization
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\[ I([v_{\text{past}}], [\phi_{\text{future}}]) \] – too difficult
Predictive information maximization

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\[ I(v_0, \phi_0) = \log \frac{\langle \phi^2 \rangle}{\langle \phi^2 \rangle - \frac{g^2 \langle \phi_f^2 \rangle^2}{\langle v^2 \rangle}} \]
Predictive information maximization

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Solution – matching filter: \( \tau = I_0^{-1/\alpha} \).
Specific examples: problem setup

\[ Q(\vec{x}|\alpha) \] 
p. d. f. for \( \vec{x} \) parameterized by unknown parameters \( \alpha \)
\[ \text{dim} \, \alpha = K \] 
dimensionality of \( \alpha \), may be infinite
\[ P(\alpha) \] 
prior distribution of parameters
\[ \vec{x}_1 \cdots \vec{x}_N \] 
random samples from the distribution
Specific examples: problem setup

\( Q(\vec{x}|\alpha) \) p. d. f. for \( \vec{x} \) parameterized by unknown parameters \( \alpha \)

\[ \text{dim } \alpha = K \] dimensionality of \( \alpha \), 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 terms

\[ S_0 = \int d^K \alpha \mathcal{P}(\alpha) \left[ -\int d\vec{x} \frac{Q(\vec{x}|\alpha)}{Q(\vec{x}|\alpha)} \log_2 Q(\vec{x}|\alpha) \right] \]

\[ S_1(N) = -\int d^K \bar{\alpha} d^N \vec{x}_i \mathcal{P}(\bar{\alpha}) \prod Q(\vec{x}_i|\bar{\alpha}) \log_2 \int d^K \alpha \mathcal{P}(\alpha) e^{-N \mathcal{E}_N} \]
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\[ \mathcal{E}_N \equiv \frac{1}{N} \sum_i \log \left[ \frac{Q(\vec{x}_i | \bar{\alpha})}{Q(\vec{x}_i | \alpha)} \right] \longrightarrow \int d\vec{x} Q(\vec{x} | \bar{\alpha}) \log \frac{Q(\vec{x} | \bar{\alpha})}{Q(\vec{x} | \alpha)} \]

Annealed approximation (almost) always works.
Density of states

\[ Z(\bar{\alpha}; N) = \int d\epsilon \rho(\epsilon; \bar{\alpha}) \exp[-N\epsilon] \]

\[ \rho(\epsilon; \bar{\alpha}) = \int d^K \alpha \mathcal{P}(\alpha) \delta[\epsilon - D_{KL}(\bar{\alpha} \parallel \alpha)] \]
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The density \(\rho\) could be very different for different targets.

Learning is annealing at decreasing temperature.

Nonzero \(\rho \implies\) consistency in learning.
Density at $\epsilon \to 0$, $I_{\text{pred}}$, and learning

Occam factor, generalization error, prediction error, fluctuation determinant:

$$\mathcal{D}(\bar{\alpha}; N) \approx -\log \int d\epsilon \rho(\epsilon; \bar{\alpha})e^{-N\epsilon}$$
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Predictive information:

$$I_{\text{pred}}(N) \approx \int d^K \bar{\alpha} \mathcal{P}(\bar{\alpha}) D(\bar{\alpha}, N)$$
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Universal learning curves:

$$\Lambda(\bar{\alpha}; N) \equiv D_{\text{KL}}(\bar{\alpha}||\alpha_{\text{est}}) \approx \frac{dD(\bar{\alpha}; N)}{dN}$$

$$\Lambda(N) \equiv \int d\bar{\alpha} \mathcal{P}(\bar{\alpha}) \Lambda(\bar{\alpha}; N) \approx \frac{dI_{\text{pred}}}{dN}$$
Finite number of states and finite $I_{\text{pred}}$

$$\rho(\epsilon; a_1) = \sum_{i=1}^{M} P_i \delta(d_i - \epsilon)$$
Finite number of states and finite $I_{\text{pred}}$ 

$$\rho(\epsilon; a_1) = \sum_{i=1}^{M} P_i \delta(d_i - \epsilon)$$

$$\mathcal{D}(a_1; N) = C_1 - C_2 \exp[-NC_3]$$

$$\Lambda(a_1; N) \approx C_2 C_3 \exp[-NC_3]$$

$I_{\text{pred}}$ saturates as $N \to \infty$
Power–law density function

$$\rho(\epsilon \to 0; \bar{\alpha}) \approx A(\bar{\alpha})\epsilon^{(d-2)/2}$$
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Example: *sound* finite parameter models, \(\dim \alpha = d\).

\[ D_{\text{KL}}(\bar{\alpha}||\alpha) \xrightarrow{\alpha \to \bar{\alpha}} \frac{1}{2} \sum_{\mu\nu} (\bar{\alpha}_\mu - \alpha_\mu)F_{\mu\nu}(\bar{\alpha}_\nu - \alpha_\nu) + \cdots \]

\[ \rho(\epsilon; \bar{\alpha}) \xrightarrow{\epsilon \to 0} \mathcal{P}(\bar{\alpha}) \frac{2\pi^{d/2}}{\Gamma(d/2)} (\det F)^{-1/2} \epsilon^{(d-2)/2} \]

\[ I_{\text{pred}} \approx S_1^{(a)} \approx \frac{d}{2} \log_2 N \]
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Speed of approach to this asymptotics is rarely investigated.
Another example

Learning $Q(\vec{x}_1 \cdots \vec{x}_N|\alpha)$, a finite parameter Markov process with long range intrinsic correlations such that

$$S[\{\vec{x}_i}\mid\alpha] \equiv -\int d^N \vec{x} Q(\{\vec{x}_i\}\mid\alpha) \log_2 Q(\{\vec{x}_i\}\mid\alpha)$$

$$\rightarrow NS_0 + S^*_0; \quad S^*_0 = \frac{K'}{2} \log_2 N$$
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$$S^{(\text{a})}_1(N) \approx \frac{K + K'}{2} \log_2 N$$
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$$S^{(a)}_1(N) \approx \frac{K + K'}{2} \log_2 N$$

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

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

\[ S_1^{(a)}(N) \propto N^{\mu/(\mu+1)} \]
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- 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 \( \mu \to \infty \) complexity grows and then vanishes to the leading order when \( S_1^{(a)} \) becomes extensive
Example of the power–law $I_{\text{pred}}$

Learning a smooth nonparameteric density $Q(x) = 1/l_0e^{-\phi(x)}$, $x \in [0, L]$ (Bialek, Callan, and Strong 1996), Complete model.

$$P[\phi(x)] = \frac{1}{Z} \exp \left[ -\frac{l}{2} \int dx \left( \frac{\partial \phi}{\partial x} \right)^2 \right] \delta \left[ \frac{1}{l_0} \int dx \ e^{-\phi(x)} - 1 \right]$$
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$$\rho(D \to 0; \bar{\phi}) = A[\bar{\phi}(x)]\epsilon^{-3/2} \exp \left( -\frac{B[\bar{\phi}(x)]}{\epsilon} \right)$$

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- increasing number of “effective parameters” (bins) of adaptive size $\sim \sqrt{l/N} Q(x)$
- heuristic arguments for the dimensionality $\zeta$ and the smoothness exponent $\eta$ give $S_1(N) \sim N^{\zeta/2\eta}$ — demonstrates a crossover from complexity to randomness
Nonuniform $\mathcal{D}$

Nested finite parameter models, $r = 1 \ldots \infty$, $K = K(r)$, $\mathcal{P}(r)$:

\[
\mathcal{P}(\alpha_\mu | r) = \begin{cases} 
p(\alpha_\mu), & \mu \leq K(r) \\
\delta(\alpha_\mu), & \mu > K(r) \end{cases}
\]

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\mathcal{P}(\alpha | r) = \prod_{\mu=1}^{R} \mathcal{P}(\alpha_\mu | r)
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\[
\rho(\epsilon; \bar{\alpha}) = \sum_{r: D_r(\bar{\alpha}) \leq \epsilon} \mathcal{P}(r) \mathcal{P}(\hat{\alpha}_r | r)
\]

\[
= \frac{2\pi^{K(r)/2}}{\Gamma[K(r)/2]} \frac{[\epsilon^2 - D_r^2(\bar{\alpha})][K(r)-2]/4}{\sqrt{\det \mathcal{F}_{K(r)}}}
\]
Nonuniform $\mathcal{D}$

Nested finite parameter models, $r = 1 \ldots \infty$, $K = K(r)$, $\mathcal{P}(r)$:

\[
\begin{align*}
\mathcal{P}(\alpha_\mu | r) &= \begin{cases} 
    p(\alpha_\mu), & \mu \leq K(r) \\
    \delta(\alpha_\mu), & \mu > K(r)
\end{cases} \\
\mathcal{P}(\alpha | r) &= \prod_{\mu=1}^{R} \mathcal{P}(\alpha_\mu | r) \\
\rho(\epsilon; \bar{\alpha}) &= \sum_{r: D_r(\bar{\alpha}) \leq \epsilon} \mathcal{P}(r) \mathcal{P}(\hat{\alpha}_r | r)
\end{align*}
\]

Another complete model!
Density near atypical solutions

\[
\rho(\epsilon; \bar{\alpha}) \sim \epsilon^{\frac{-1}{(2\eta - 1)}} \ell^{-1}
\]

\[
\mathcal{D} \propto N^{1/2\eta} \left( \frac{\log N}{\ell} \right)^{1-1/2\eta}
\]
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- nested model is at most log worse than the QFT
- QFT may be a power law worse
Density near atypical solutions

\[ \rho(\epsilon; \bar{\alpha}) \sim \epsilon^{-(1/(2\eta-1))\ell-1} \]

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- nested model is at most log worse than the QFT
- QFT may be a power law worse
- for natural (structured) data nested case is better
- alignment may be imperfect for finite precision \( \epsilon \)
Which model is being used?

- for QFT or nested asymptotics kicks in fast
- asymptotic decay rate should signify the model
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(Gallistel et al., 2001)
Which model is being used?

- for QFT or nested asymptotics kicks in fast
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- noisy learning
- maybe FDT? \( \frac{\partial A}{\partial N} = -\zeta_N \Lambda^\nu \)

(Gallistel et al., 2001)
Fluctuations (drifting target) and dissipation (learning curve)
Fluctuations (drifting target) and dissipation (learning curve)

$$\Delta_{\text{rms}} = \left\{ \nu^{1/\nu} \frac{\Gamma\left(\frac{3}{2\nu}\right)}{\Gamma\left(\frac{1}{2\nu}\right)} \right\}^{1/2} \left(\frac{\Omega}{\zeta}\right)^{1/(2\nu)}$$
The hidden extras...
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
Complexity measure

- some kind of entropy (we proclaim Shannon’s postulates: monotonicity, continuity, additivity)
Complexity measure

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• invariant under invertible temporally local transformations ($x_k \rightarrow x_k + \xi x_{k-1}$: measuring device with inertia, article with misprints, same book in different languages – same universality class)

$$\log P_1(x) = \log P_2(x) + \text{loc. oper.} \Rightarrow C[P_1(x)] = C[P_2(x)]$$

This may present a problem in higher dimensions.
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The divergent subextensive term measures complexity uniquely!
Relations to other definitions . . .

. . . are mostly straightforward.
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- equivalence $=$ indistinguishable conditional distributions of futures

If sufficient statistics exist, then $C_K \approx I_{\text{pred}}$. Otherwise $C_K > I_{\text{pred}}$. $C_K$ is unique up to a constant.
Not finite size scaling!
What’s next?

**extraction** separating predictive information from non–predictive using the ‘relevant information’ technique

**physics** of phase transitions, connection to subextensive statistical mechanics

**statistics** extensions of MDL (predictive information *is* a property of the data, not of the model)

**learning** unification of approaches: Bayesian, SRM, MDL, Cucker-Smale. . .

**bioinformatics** what is predictive information of natural symbolic sequences? (DNA, languages, spike trains) can we use changes in predictability for data partitioning? for model building?

**dynamical systems theory** what is predictive information and complexity of various systems?