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Data Science 4

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Master's Degree Programme in Cognitive Science

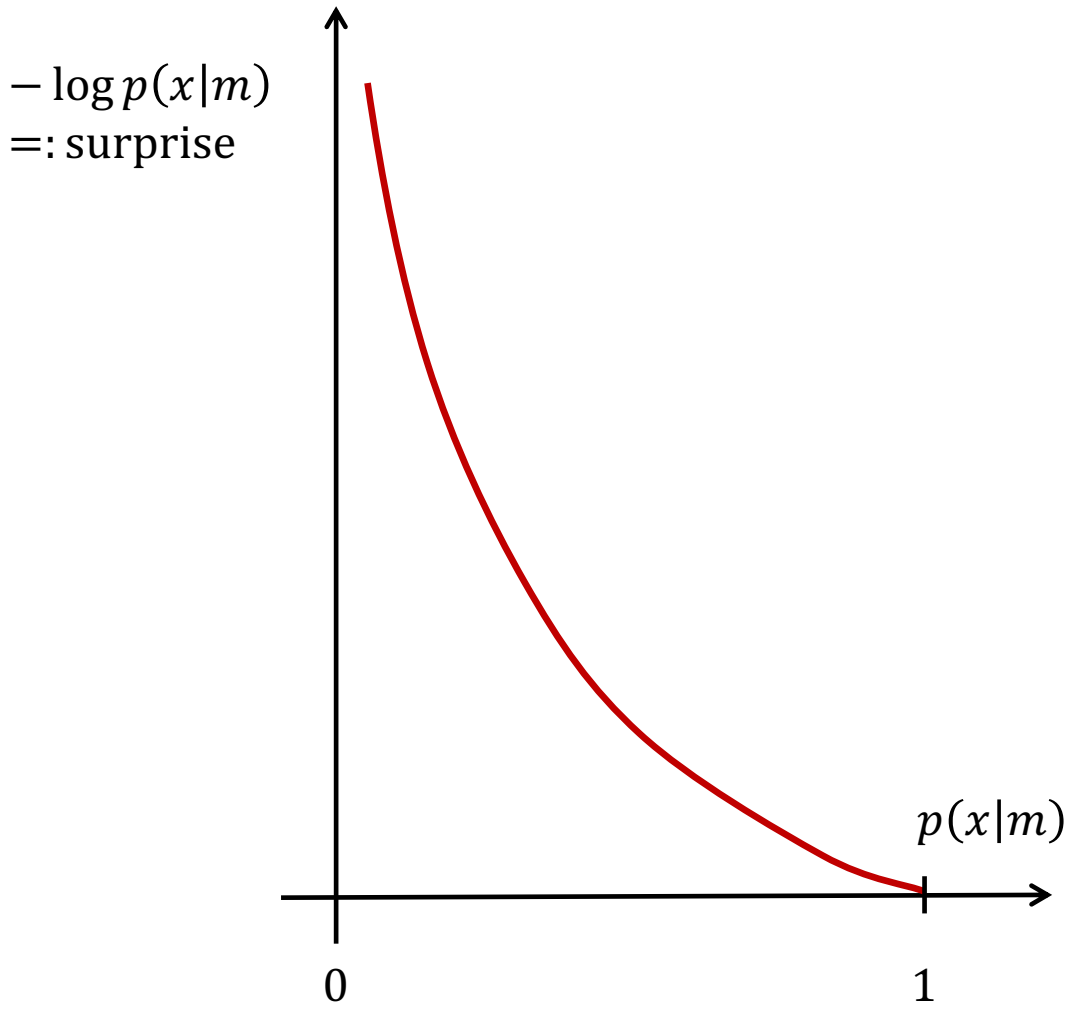
Spring 2022

General Principles of Model Fitting and Model Comparison

Optimizing (models, parameters,…) means *minimizing surprise*

- How surprising an event is felt to be depends on its probability.
- It makes intuitive sense to take the negative logarithm of $p(x|m)$ as a measure of surprise.
- If $p(x|m) = 1$, the outcome was certain and there is no surprise at all $(-\log\big(p(x|m)\big) = 0)$.
- If $p(x|m) = 0$, the outcome was impossible and surprise is infinite $(-\log\big(p(x|m)\big) = \infty)$.
- In between, surprise is greater than zero and increases for less probable observations.

Surprise in a graph



Entropy

- A concept closely related to surprise is entropy
- The more ignorant we are about a quantity, the greater is the surprise we may expect when observing it.
- Expected surprise is called the **entropy** S of a probability distribution p:

$$S[p] \coloneqq -\int p(x) \log p(x) \, \mathrm{d}x$$

- Entropy is a **measure of ignorance.**
- Its name is due to an analogous quantity in thermodynamics.

Entropy example

- As a simple example, let's look at a coin toss.
- There are two possible outcomes: $x \in \{\text{heads}, \text{tails}\}$
- Since outcomes are discrete and binary, we use a sum instead of an integral and the binary logarithm to define the entropy:

$$S[p] \coloneqq -\sum_{y} p(x) \log_2 p(x)$$

- For a fair coin (i.e., $p(\text{heads}) = p(\text{tails}) = \frac{1}{2}$), $S[p] = 1$
- However, for $p(\text{heads}) = \frac{9}{10}$, $p(\text{tails}) = \frac{1}{10}$, we get $S[p] \approx 0.47$ because expected surprise is much lower.

Varieties of free energy

In information theory, free energy A is the surprise of given model m at a particular (set of) observation(s) x:

$$A \coloneqq -\log p(x|m)$$

However, at least four kinds of free energy have to be kept apart:

- The free energy of thermodynamics
- The free energy of statistical physics
- Informational free energy (as above)
- Variational free energy

Free energy in thermodynamics and statistical mechanics

Two kinds: Gibbs and Helmholtz (him again!)

Helmholtz free energy:

$$A \coloneqq U - TS$$

U: internal energy; T: temperature; S: entropy

[Gibbs free energy: $G \coloneqq U + pV - TS$]

In **statistical mechanics**, the Boltzmann distribution describes the **relation between energy and probability**. If particles in a system can be in states $s_1, s_2, s_3, \ldots$ corresponding to energy levels $E_1, E_2, E_3, \ldots$, then the probability p_i of finding a particle in state s_i is

$$p_i = \frac{\exp(-E_i/kT)}{\sum_j \exp\left(-E_j/kT\right)} = \frac{\exp(-E_i/kT)}{Z},$$

where T is *temperature* and k is *Boltzmann's constant*, and $Z \coloneqq \sum_j \exp\left(-E_j/kT\right)$ is the *partition function*.

Free energy in thermodynamics and statistical mechanics

Taking the logarithm on both sides and rearranging gives us

$$-kT \log Z = E_i + kT \log p_i$$

Taking the expectation value on both sides, we get

$$\sum_i p_i \left(-kT \log Z\right) = \sum_i p_i E_i + \sum_i p_i kT \log p_i$$

$$-kT \log Z = \langle E \rangle - T\left(-k \sum_i p_i \log p_i\right) = \langle E \rangle - TS$$

with entropy $S \coloneqq -k \sum_i p_i \log p_i$.

In analogy to the definition $A \coloneqq U - TS$ of Helmholtz free energy from thermodynamics, this motivates the definition

$$A \coloneqq -kT \log Z$$

of free energy in statistical mechanics.

Informational free energy

Returning to information theory, we take the definition of informational free energy and perform a series of algebraic operations on it:

$$A \coloneqq -\log p(x|m) = -\int p(\vartheta|x,m)\log p(x|m)\,\mathrm{d}\vartheta$$

$$= -\int p(\vartheta|x,m)\log\frac{p(x,\vartheta|m)}{p(\vartheta|x,m)}\mathrm{d}\vartheta$$

$$= \underbrace{-\int p(\vartheta|x,m)\log p(x,\vartheta|m)\,\mathrm{d}\vartheta}_{=\langle E\rangle} \underbrace{-\left(-\int p(\vartheta|x,m)\log p(\vartheta|x,m)\,\mathrm{d}\vartheta\right)}_{=S}$$

This gives us an **information theoretic analogon** to the definition of Helmholtz free energy in statistical mechanics. Compare:

$$A \coloneqq -kT\log Z = -kT\log\left(\sum_j \exp\left(-E_j/kT\right)\right)$$

$$A \coloneqq -\log p(x|m) = -\log\int p(x,\vartheta|m)\mathrm{d}\vartheta$$

This is the same if we set $kT = 1$ and **interpret the negative logarithm of the joint probability distribution as an energy**:

$$E_\vartheta \equiv -\log p(x,\vartheta|m)$$

Variational free energy

The problem with informational free energy is that we cannot calculate it except in trivial cases. Whenever models are complicated enough to be interesting, the integrals involved are intractable.

$$A \coloneqq \underbrace{-\int p(\vartheta|x,m)\log p(x,\vartheta|m)\,\mathrm{d}\vartheta}_{=\langle E\rangle} \underbrace{-\left(-\int p(\vartheta|x,m)\log p(\vartheta|x,m)\,\mathrm{d}\vartheta\right)}_{=S}$$

The solution to this is variational free energy, where we replace the true posterior $p(\vartheta|x,m)$ by an approximation $q(\vartheta)$:

$$A_v \coloneqq \underbrace{-\int q(\vartheta)\log p(x,\vartheta|m)\,\mathrm{d}\vartheta}_{\coloneqq E_v} \underbrace{-\left(-\int q(\vartheta)\log q(\vartheta)\,\mathrm{d}\vartheta\right)}_{\coloneqq S_v}$$

Variational free energy

What makes variational free energy A_v such an extremely useful concept is the following theorem:

$$A_v \geq A \text{ for all } q(\vartheta)$$

This means that **whatever $q(\vartheta)$ we plug into A_v, we get an A_v that is greater than A**. So without having to know anything about A, we can vary $q(\vartheta)$ such that it minimizes A_v.

$$A_v := -\int q(\vartheta) \log p(x, \vartheta|m) \, \mathrm{d}\vartheta + \int q(\vartheta) \log q(\vartheta) \, \mathrm{d}\vartheta$$

The branch of mathematics that describes how to carry out the minimization of A_v with respect to $q(\vartheta)$ is called **variational calculus**, hence "variational" free energy.

Minimizing A_v with respect to $q(\vartheta)$ leads to an approximation of $p(\vartheta|x, m)$ by $q(\vartheta)$ because of the theorem above and because $A_v = A$ for $q(\vartheta) = p(\vartheta|x, m)$.

The remarkable thing here is that we can use variational calculus to find a $q(\vartheta)$ that approximates $p(\vartheta|x, m)$ **without ever having to know $p(\vartheta|x, m)$ itself**.

This is how the brain can build, update, and compare models of the world without ever "seeing behind the scenes" of its sensory input.

Variational free energy

Proof that $A_v \geq A$ for all $q(\vartheta)$:

$$
\begin{aligned}
A &:= -\log p(x|m) \\
&= -\log \int p(x,\vartheta|m)\mathrm{d}\vartheta \\
&= -\log \int q(\vartheta)\frac{p(x,\vartheta|m)}{q(\vartheta)}\mathrm{d}\vartheta \\
&\leq -\int q(\vartheta)\log\frac{p(x,\vartheta|m)}{q(\vartheta)}\mathrm{d}\vartheta \\
&= -\int q(\vartheta)\log p(x,\vartheta|m)\,\mathrm{d}\vartheta + \int q(\vartheta)\log q(\vartheta)\,\mathrm{d}\vartheta \\
&=: A_v
\end{aligned}
$$

Jensen's inequality

□

Three ways to decompose A_v

$$A_v := -\int q(\vartheta)\log\frac{p(x,\vartheta|m)}{q(\vartheta)}\,\mathrm{d}\vartheta$$

$$= \underbrace{-\int q(\vartheta)\log p(x,\vartheta|m)\,\mathrm{d}\vartheta}_{\text{Expected energy } E_v} \underbrace{-\left(-\int q(\vartheta)\log q(\vartheta)\,\mathrm{d}\vartheta\right)}_{\text{Entropy } S_v}$$

$$= -\int q(\vartheta)\log\frac{p(\vartheta|x,m)p(x|m)}{q(\vartheta)}\,\mathrm{d}\vartheta = KL[q(\vartheta),p(\vartheta|x,m)]\underbrace{-\log p(x|m)}_{=A}$$

$$= -\int q(\vartheta)\log\frac{p(x|\vartheta,m)p(\vartheta|m)}{q(\vartheta)}\,\mathrm{d}\vartheta = \underbrace{KL[q(\vartheta),p(\vartheta|m)]}_{\text{Complexity}} \underbrace{-\int q(\vartheta)\log p(x|\vartheta,m)\,\mathrm{d}\vartheta}_{\text{Accuracy}}$$

The first decomposition of A_v

$$A_v = -\int q(\vartheta) \log p(x, \vartheta|m) \, \mathrm{d}\vartheta - \left(-\int q(\vartheta) \log q(\vartheta) \, \mathrm{d}\vartheta \right)$$

$$= E_v - S_v$$

$$= \text{Expected energy} - \text{Entropy}$$

This first decomposition illustrates the mathematical analogy to statistical mechanics.

More importantly, it only contains quantities known to the model-builder: the joint density $p(x, \vartheta|m)$, consisting of likelihood and prior, and the arbitrary density $q(\vartheta)$.

Because it only contains known quantities, this decomposition shows that A_v is, in principle, computable up to an arbitrarily small error.

The second decomposition of A_v

$$A_v = KL[q(\vartheta), p(\vartheta|x,m)] \underbrace{- \log p(x|m)}_{=A}$$

$$= \text{Divergence between approximate and true posterior} + \text{log–model evidence}$$

The **Kullback-Leibler divergence** between two distributions is defined as

$$KL[p_1, p_2] := \int p_1(\vartheta) \log \frac{p_1(\vartheta)}{p_2(\vartheta)} \mathrm{d}\vartheta$$

It is zero if and only if $p_1 = p_2$, otherwise positive. It is not symmetric (i.e., $KL[p_1, p_2] \neq KL[p_2, p_1]$ in general).

This second decomposition again shows that $A_v \geq A$ for all $q(\vartheta)$ (because the divergence is non-negative).

Crucially, it again shows that **minimizing A_v with respect to $q(\vartheta)$ leads to an approximation of $p(\vartheta|x,m)$ by $q(\vartheta)$**.

The third decomposition of A_v

$$A_v = KL[q(\vartheta), p(\vartheta|m)] - \int q(\vartheta) \log p(x|\vartheta, m) \, \mathrm{d}\vartheta$$

$$= \text{Complexity} - \text{Accuracy}$$

The expected log-likelihood $\log p(x|\vartheta, m)$ under the approximate posterior $q(\vartheta)$ is a measure of the accuracy we may expect under the current model.

The divergence between the approximate posterior $q(\vartheta)$ and the prior $p(\vartheta|m)$ is a measure for how much the data x have forced the model to adapt. As such, it is a measure of **model complexity.**

It is important to note that complexity cannot be assessed in the absence of data. Different data will lead to different complexity. One way to remind oneself of this is to think of model complexity as the **complexity of the data under the current model.**

The third decomposition of A_v

$$A_v = KL[q(\vartheta), p(\vartheta|m)] - \int q(\vartheta) \log p(x|\vartheta, m) \, \mathrm{d}\vartheta$$

$$= \text{Complexity} - \text{Accuracy}$$

This decomposition illustrates why A_v is a good measure of model quality: a good model is one that makes good predictions.

This means that inferences based on currently available data have to generalize to new data.

There are two dangers to this: seeing patterns where there are none (i.e., too much complexity) and missing patterns (i.e., too little accuracy).

A_v is a measure that balances these two opposing demands because it rewards accuracy while penalizing complexity.

The third decomposition of A_v

$$A_v = KL[q(\vartheta), p(\vartheta|m)] - \int q(\vartheta) \log p(x|\vartheta, m) \, \mathrm{d}\vartheta$$

$$= \text{Complexity} - \text{Accuracy}$$

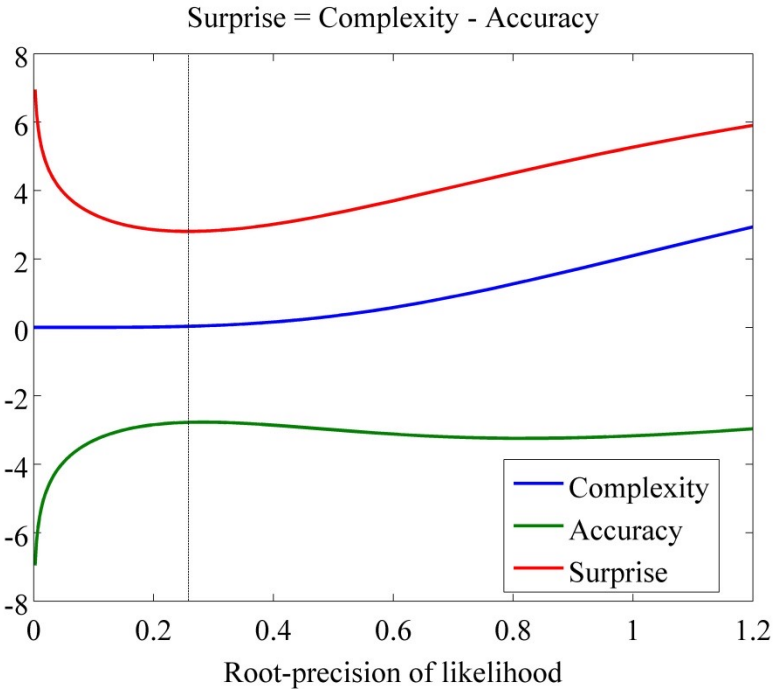
The principled reason why A_v is a good measure of model quality is that the difference in A_v is an approximation to the log-Bayes factor.

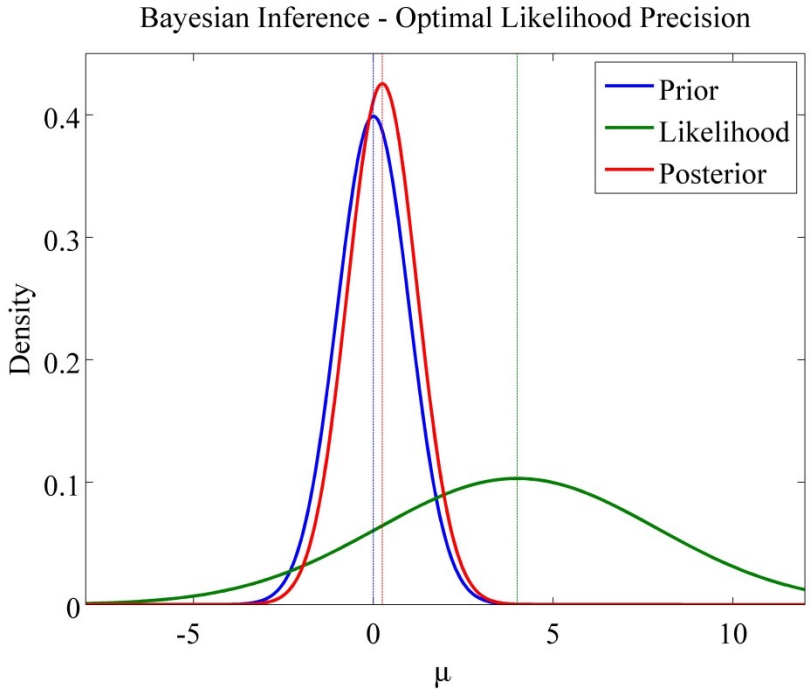
AIC (the Akaike Information Criterion) and BIC (the Bayesian Information Criterion) are approximations to A_v where the complexity term is replaced by a function of the number of parameters.

The third decomposition of A_v

$$A_v = KL[q(\vartheta), p(\vartheta|m)] - \int q(\vartheta) \log p(x|\vartheta, m)\, \mathrm{d}\vartheta$$

$$= \text{Complexity} - \text{Accuracy}$$





How do you compare models?

Related questions:

- How do you quantify the goodness of a model?
- What are the trade-offs involved in improving model fit?
- Do models have an inherent degree of complexity?
- Is complexity good or bad?

Model comparison: A_v in relation to Bayes factors, AIC, BIC

$$\textbf{Bayes factor} := \frac{p(x|m_1)}{p(x|m_0)} = \exp\left(\log\frac{p(x|m_1)}{p(x|m_0)}\right) = \exp(\log p(x|m_1) - \log p(x|m_0))$$

$$\approx \exp\left(A_{v_0} - A_{v_1}\right)$$

Bayes factor

Posterior odds

Prior odds

[Meaning of the Bayes factor: $\frac{p(m_1|x)}{p(m_0|x)} = \frac{p(x|m_1)}{p(x|m_0)}\frac{p(m_1)}{p(m_0)}$]

$$\boldsymbol{A_v} = KL[q(\vartheta), p(\vartheta|m)] - \int q(\vartheta)\log p(x|\vartheta, m)\,\mathrm{d}\vartheta$$

$$= \text{Complexity} - \text{Accuracy}$$

Number of parameters

$$\textbf{AIC} := 2(\mathrm{p} - \text{Accuracy})$$

Number of data points

$$\textbf{BIC} := 2\left(\frac{p}{2}\log N - \text{Accuracy}\right)$$

What to do in practice

- When available: use **log-model evidence** (or an approximation like variational free energy)
- **Nested cross-validation** (https://scikit-learn.org/stable/auto_examples/model_selection/plot_nested_cross_validation_iris.html#)
- R package 'loo': expected log-predictive density (**elpd** – an approximation to log-model evidence using sampling and cross-validation)

R package 'loo'

Stat Comput (2017) 27:1413–1432
DOI 10.1007/s11222-016-9696-4

Practical Bayesian model evaluation using leave-one-out cross-validation and WAIC

Aki Vehtari[1] · Andrew Gelman[2] · Jonah Gabry[2]

R package 'loo'

$$\text{lpd} = \text{log pointwise predictive density}$$
$$= \sum_{i=1}^{n} \log p(y_i|y) = \sum_{i=1}^{n} \log \int p(y_i|\theta)\, p(\theta|y) d\theta. \quad (2)$$

The lpd of observed data y is an overestimate of the elpd for future data (1). To compute the lpd in practice, we can evaluate the expectation using draws from $p_{\text{post}}(\theta)$, the usual posterior simulations, which we label θ^s, $s = 1, \ldots, S$:

$$\widehat{\text{lpd}} = \text{computed log pointwise predictive density}$$
$$= \sum_{i=1}^{n} \log \left(\frac{1}{S} \sum_{s=1}^{S} p(y_i|\theta^s) \right). \quad (3)$$

R package 'loo'

The Bayesian LOO estimate of out-of-sample predictive fit is

$$\text{elpd}_{\text{loo}} = \sum_{i=1}^{n} \log p(y_i|y_{-i}), \tag{4}$$

where

$$p(y_i|y_{-i}) = \int p(y_i|\theta)p(\theta|y_{-i})d\theta \tag{5}$$

is the leave-one-out predictive density given the data without the ith data point.

Comparison of neural networks

- Cross-entropy loss function leads to minimizing surprise
- Regularization techniques (all of them) are equivalent to placing priors on parameters
- Hyperparameters determine model structure (e.g., number of layers and nodes, correspond to priors (e.g., regularization parameter), or affect optimization algorithm (e.g., learning rate)
- **Out-of-sample predictive performance approximates model evidence**