Maximum entropy

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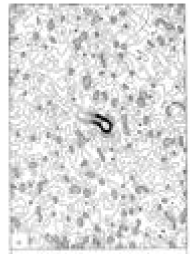


Radio map of a region of sky. Phases have been measured but, because of receiver noise, regions of negative intensity appear.

Maximum entropy reconstruction of the above map in which amplitudes have been adjusted to fit the expected distribution of errors.

Entropy

Thermodynamics
- measures the state of order of a system

Information theory
- measures the amount of information in a message

Probability theory
- measures the change in probability upon altering the conditions under which the probability is estimated

Image processing
- measures the amount of information in an image

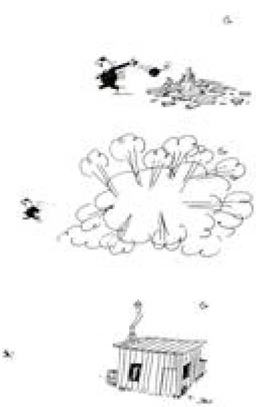
An increase in entropy means going from a less likely to a more likely state.

Thermodynamics
- temperature equalisation upon thermal contact

Information
- message contains errors after transmission

Probability
- probabilities move towards the mean as information becomes outdated

Images
- loss of resolution, contrast and increase in noise as image is transmitted



Maximum entropy in image processing

- Applied when data are inaccurate (experimental error) and / or incomplete (low resolution, missing phases, overlapped reflections
- Entropy is maximised within the constraints imposed by the data
- The image contains no information other than that given directly by the data
- Makes no assumptions about missing information
- Produces an unbiased estimate of the true image

Example of incomplete data

1. One third of all scientists are crystallographers.
2. One quarter of all scientists are left-handed.

Question: What proportion of all scientists are left-handed crystallographers?

$$a + b + c + d = 1$$
$$a + b = \tfrac{1}{3}$$
$$a + c = \tfrac{1}{4}$$

	lh	rh
cryst	a	b
non-cryst	c	d

eliminate b, c, d to give:

	lh	rh
cryst	a	$\frac{1}{3}-a$
non-cryst	$\frac{1}{4}-a$	$\frac{5}{12}+a$

Two extreme solutions

a = 0

no left-handed crystallographers

(smallest maximum)

	lh	rh
cryst	0	$\frac{4}{12}$
non-cryst	$\frac{3}{12}$	$\frac{5}{12}$

a = ¼

no left-handed non-crystallographers

(largest maximum)

	lh	rh
cryst	$\frac{3}{12}$	$\frac{1}{12}$
non-cryst	0	$\frac{8}{12}$

Additional criterion

Minimum variance - gives probabilities as close together as possible

$$V = a^2 + \left(\frac{1}{3}-a\right)^2 + \left(\frac{1}{4}-a\right)^2 + \left(\frac{5}{12}+a\right)^2$$

$$\frac{dV}{da} = 0 \text{ for a minimum}$$

solution gives $a = \frac{1}{24}$

	lh	rh
cryst	$\frac{1}{24}$	$\frac{7}{24}$
non-cryst	$\frac{5}{24}$	$\frac{11}{24}$

The result is biased:

$\frac{1}{8}$ of crystallographers are left-handed

$\frac{5}{16}$ of non-crystallographers are left-handed

The biased result occurs because of the inappropriate criterion

- a minimum variance has nothing at all to do with being a crystallographer or being left-handed.

A sensible result would be that ¼ of crystallographers are left-handed like the rest of scientists.

Maximum entropy solution

- should give an unbiased estimate of the proportion of left-handed crystallographers.

entropy:

$$S = -\sum_{i=1}^{m} p_i \log(p_i)$$

$$S = -a\log(a) - \left(\frac{1}{3}-a\right)\log\left(\frac{1}{3}-a\right) - \left(\frac{1}{4}-a\right)\log\left(\frac{1}{4}-a\right) - \left(\frac{5}{12}+a\right)\log\left(\frac{5}{12}+a\right)$$

$$\frac{dS}{da} = 0 \text{ for a maximum}$$

solution gives $a = \frac{1}{12}$

	lh	rh
cryst	$\frac{1}{12}$	$\frac{3}{12}$
non-cryst	$\frac{2}{12}$	$\frac{6}{12}$

Entropy and probability

The state of a system which is measured by entropy has a certain probability of occurring.

This may be written as $S = f(P)$

where the function f has to be determined

entropy of a complicated system = sum of entropies of the separate parts

In search of a function:

A system consists of 2 parts entropies S_1 S_2

probabilities P_1 P_2

entropy of combined system $= S = S_1 + S_2$

probability of combined system $= P = P_1 \times P_2$

since $S = f(P)$ $\qquad S_1 + S_2 = f(P_1 \times P_2)$

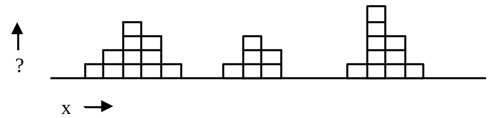
but, by definition $\qquad S_1 + S_2 = f(P_1) + f(P_2)$

so we have $\qquad f(P_1) + f(P_2) = f(P_1 \times P_2)$

compare with $\qquad \log(a) + \log(b) = \log(ab)$

so that $\qquad S = \log(P)$

Electron density maps



To apply maximum entropy to an electron density map, assume the density is made of discrete lumps.

A one-dimensional map may then look like the one above.

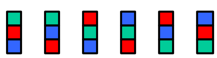
What is the probability of this map occurring?

The number of ways of arranging N lumps of density is:

$$N \times (N\text{-}1) \times (N\text{-}2) \times \ldots \times 3 \times 2 \times 1 = N!$$

Within each pile, the lumps can be rearranged to give an identical pile of the same height.

For a pile of n lumps, the number of rearrangements is $n!$

e.g.  $3! = 3 \times 2 \times 1 = 6$

The total number of rearrangements needs to be reduced by this factor.

The number of ways of producing the map is therefore:

$$\frac{N!}{n_1!\, n_2! \cdots n_m!}$$

This number is proportional to the probability of producing the map.

Ignoring constant terms, the entropy of the map is therefore:

$$S = \log\left(\frac{N!}{n_1!\, n_2! \cdots n_m!}\right)$$

Now use $\quad \log(N!) \approx N \log(N) - N \quad$ and $\quad \sum_{i=1}^{m} n_i = N$

So, again ignoring constant terms: $\quad S = -\sum_{i=1}^{m} n_i \log(n_i)$

For the electron density: $\quad S = -\sum_{i=1}^{m} r_i \log\left(\frac{r_i}{q_i}\right)$

where $q_i =$ expected value of r_i