Introduction to Bayesian Methods - 4

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Edwin T. Jaynes (1922-1998), introduced the method of maximum entropy in statistical mechanics: when we start from the informational entropy (Shannon's entropy) and we use it to introduce Boltzmann's entropy we obtain again the whole of statistical mechanics by maximizing entropy.

In a sense, statistical mechanics also arises from a comprehensive "principle of maximum entropy".

http://bayes.wustl.edu/etj/etj.html

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Information Theory and Statistical Mechanics

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Information theory provides a constructive criterion for setting up probability distributions on the basis of partial knowledge, and leads to a type of statistical inference which is called the maximum-entropy estimate. It is the least biased estimate possible on the given information; i.e., it is maximally noncommittal with regard to missing information. If one considers statistical mechanics as a form of statistical inference rather than as a physical theory, it is found that the usual computational rules, starting with the determination of the partition function, are an immediate consequence of the maximum-entropy principle. In the resulting "subjective statistical mechanics," the usual rules are thus justified independently of any physical argument, and in particular independently of experimental verification; whether or not the results agree with experiment, they still represent the best estimates that could have been made on the basis of the information available.

It is concluded that statistical mechanics need not be regarded as a physical theory dependent for its validity on the truth of additional assumptions not contained in the laws of mechanics (such as ergodicity, metric transitivity, equal *a priori* probabilities, etc.). Furthermore, it is possible to maintain a sharp distinction between its physical and statistical aspects. The former consists only of the correct enumeration of the states of a system and their properties; the latter is a straightforward example of statistical inference.

Here we apply the maximum entropy principle (MaxEnt) to solve problems and find prior distributions ...

The kangaroo problem (Jaynes)

•*Basic information*: one third of all kangaroos has blue eyes, and one third is left-handed.

•Question: which fraction of kangaroos has both blue eyes and is left-handed?

	left	~left
blue	1/9	2/9
~blue	2/9	4/9

no correlation

	left	~left
blue	0	1/3
~blue	1/3	1/3

maximum negative correlation

	left	~left
blue	1/3	0
~blue	0	2/3

maximum positive correlation

probabilities p_{bl} $p_{\bar{b}l}$ $p_{b\bar{l}}$ $p_{\overline{bl}}$

entropy (proportional to Shannon's entropy)

$$S = p_{bl} \ln \frac{1}{p_{bl}} + p_{\bar{b}l} \ln \frac{1}{p_{\bar{b}l}} + p_{b\bar{l}} \ln \frac{1}{p_{b\bar{l}}} + p_{\overline{bl}} \ln \frac{1}{p_{\overline{bl}}}$$

constraints (3 constraints, 4 unknowns)

$$p_{bl} + p_{\bar{b}l} + p_{b\bar{l}} + p_{\overline{bl}} = 1$$

$$p_{bl} + p_{b\bar{l}} = 1/3$$

$$p_{bl} + p_{\bar{b}l} = 1/3$$

entropy maximization with constraints

$$S_V = \left(p_{bl} \ln \frac{1}{p_{bl}} + p_{\bar{b}l} \ln \frac{1}{p_{\bar{b}l}} + p_{b\bar{l}} \ln \frac{1}{p_{b\bar{l}}} + p_{\overline{bl}} \ln \frac{1}{p_{\overline{bl}}} \right)$$

$$+\lambda_1 \left(p_{bl} + p_{\bar{b}l} + p_{b\bar{l}} + p_{\overline{bl}} - 1 \right) + \lambda_2 \left(p_{bl} + p_{b\bar{l}} - 1/3 \right) + \lambda_3 \left(p_{bl} + p_{\bar{b}l} - 1/3 \right)$$

$$\frac{\partial S_V}{\partial p_{bl}} = -\ln p_{bl} - 1 + \lambda_1 + \lambda_2 + \lambda_3 = 0$$

$$\frac{\partial S_V}{\partial p_{\bar{b}l}} = -\ln p_{\bar{b}l} - 1 + \lambda_1 + \lambda_3 = 0$$

$$\frac{\partial S_V}{\partial p_{b\bar{l}}} = -\ln p_{b\bar{l}} - 1 + \lambda_1 + \lambda_2 = 0$$

$$\frac{\partial S_V}{\partial p_{\overline{bl}}} = -\ln p_{\overline{bl}} - 1 + \lambda_1 = 0$$

$$p_{bl} = \exp\left(-1 + \lambda_1 + \lambda_2 + \lambda_3\right)$$

$$p_{\bar{b}l} = \exp\left(-1 + \lambda_1 + \lambda_3\right)$$

$$p_{b\bar{l}} = \exp\left(-1 + \lambda_1 + \lambda_2\right)$$

$$p_{\overline{bl}} = \exp\left(-1 + \lambda_1\right)$$

$$
\begin{cases}
p_{\bar{b}l} = p_{\overline{bl}} \exp(\lambda_3) \\
p_{b\bar{l}} = p_{\overline{bl}} \exp(\lambda_2) \\
p_{bl} = p_{\overline{bl}} \exp(\lambda_2 + \lambda_3)
\end{cases}
\quad \Rightarrow \quad p_{\bar{b}l} p_{b\bar{l}} = p_{bl} p_{\overline{bl}}
$$

$$
\begin{cases}
p_{bl} + p_{\bar{b}l} + p_{b\bar{l}} + p_{\overline{bl}} = 1 \\
p_{bl} + p_{b\bar{l}} = 1/3 \\
p_{bl} + p_{\bar{b}l} = 1/3 \\
p_{\bar{b}l} p_{b\bar{l}} = p_{bl} p_{\overline{bl}}
\end{cases}
\quad \Rightarrow \quad
\begin{cases}
p_{b\bar{l}} = p_{\bar{b}l} = 1/3 - p_{bl} \\
p_{\overline{bl}} = 1/3 + p_{bl} \\
(1/3 - p_{bl})^2 = p_{bl}/3 + p_{bl}^2 \\
1/9 - 2p_{bl}/3 + p_{bl}^2 = p_{bl}/3 + p_{bl}^2
\end{cases}
$$

$$
\Rightarrow \quad p_{bl} = \frac{1}{9}; \quad p_{b\bar{l}} = p_{\bar{b}l} = \frac{2}{9}; \quad p_{\overline{bl}} = \frac{4}{9}
$$

this solution coincides with the least informative distribution (no correlation)

Solution of underdetermined systems of equations

In this problem there are fewer equations than unknowns; the system of equations is underdetermined, and in general there is no unique solution.

The maximum entropy method helps us find a reasonable solution, the least informative one (least correlations between variables)

Example:

$$
\begin{aligned}
3x + 5y + 1.1z &= 10 \\
-2.1x + 4.4y - 10z &= 1
\end{aligned}
\qquad (x, y, z > 0)
$$

$$3x + 5y + 1.1z = 10$$

$$-2.1x + 4.4y - 10z = 1$$

$$(x, y, z > 0)$$

this ratio can be taken to be a "probability"

$$S = -\left(\frac{x}{x+y+z} \ln \frac{x}{x+y+z} + \frac{y}{x+y+z} \ln \frac{y}{x+y+z} + \frac{z}{x+y+z} \ln \frac{z}{x+y+z} \right)$$

$$= -\frac{1}{x+y+z}\left[x \ln x + y \ln y + z \ln z - (x+y+z)\ln(x+y+z) \right]$$

$$Q = S + \lambda(3x + 5y + 1.1z - 10) + \mu(-2.1x + 4.4y - 10z - 1)$$

$$\frac{\partial Q}{\partial x} = -\frac{\ln x - \ln(x+y+z)}{x+y+z} + \frac{x \ln x + y \ln y + z \ln z - (x+y+z)\ln(x+y+z)}{(x+y+z)^2} + 3\lambda - 2.1\mu$$

$$= \frac{(y+z)\ln x + y \ln y + z \ln z}{(x+y+z)^2} + 3\lambda - 2.1\mu = 0$$

$$\frac{\partial Q}{\partial x} = \frac{(y+z)\ln x + y\ln y + z\ln z}{(x+y+z)^2} + 3\lambda - 2.1\mu = 0$$

$$\frac{\partial Q}{\partial y} = \frac{x\ln x + (x+z)\ln y + z\ln z}{(x+y+z)^2} + 5\lambda + 4.4\mu = 0$$

$$\frac{\partial Q}{\partial z} = \frac{x\ln x + y\ln y + (x+y)\ln z}{(x+y+z)^2} + 1.1\lambda - 10\mu = 0$$

$$10 = 3x + 5y + 1.1z$$

$$1 = -2.1x + 4.4y - 10z$$

$$x = 0.606275; \quad y = 1.53742; \quad z = 0.449148;$$

$$\lambda = 0.0218739; \quad \mu = -0.017793$$

this is an example of an “ill-posed” problem

the solution that we found is a kind of

regularization of the ill-posed problem

Finding priors with the maximum entropy method

$$S = \sum_k p_k \ln \frac{1}{p_k} = -\sum_k p_k \ln p_k$$

Shannon entropy

entropy maximization when all information is missing, and normalization is the only constraint:

$$\frac{\partial}{\partial p_k}\left[-\sum_k p_k \ln p_k + \lambda\left(\sum_k p_k - 1\right)\right] = -\left(\ln p_k + 1\right) + \lambda = 0$$

$$p_k = e^{\lambda-1}; \quad \sum_k p_k = \sum_k e^{\lambda-1} = N e^{\lambda-1} = 1 \quad \Rightarrow \quad p_k = 1/N$$

entropy maximization when the mean is known μ

$$\frac{\partial}{\partial p_k}\left[-\sum_k p_k \ln p_k + \lambda_0\left(\sum_k p_k - 1\right) + \lambda_1\left(\sum_k x_k p_k - \mu\right)\right]$$
$$= -\left(\ln p_k + 1\right) + \lambda_0 + \lambda_1 x_k = 0$$

incomplete solution...

$$p_k = e^{\lambda_0 + \lambda_1 x_k - 1};$$

We must satisfy two constraints now ...

$$p_k = e^{\lambda_0 + \lambda_1 x_k - 1}$$

$$\sum_k p_k = \sum_k e^{\lambda_0 + \lambda_1 x_k - 1} = e^{\lambda_0 - 1} \sum_k e^{\lambda_1 x_k} = 1$$

$$\sum_k x_k p_k = \sum_k x_k e^{\lambda_0 + \lambda_1 x_k - 1} = e^{\lambda_0 - 1} \sum_k x_k e^{\lambda_1 x_k} = \mu$$

$$e^{\lambda_0 - 1} = \frac{1}{\sum_k e^{\lambda_1 x_k}}; \qquad \frac{\sum_k x_k e^{\lambda_1 x_k}}{\sum_k e^{\lambda_1 x_k}} = \mu$$

no analytic solution, only numerical

Example : the biased die

(E. T. Jaynes: *Where do we stand on Maximum Entropy?* In *The Maximum Entropy Formalism*; Levine, R. D. and Tribus, M., Eds.; MIT Press, Cambridge, MA, 1978)

mean value of throws for an unbiased die

$$\frac{1}{6}(1+2+3+4+5+6)=\frac{21}{6}=3.5$$

mean value for a biased die

$$3.5(1+\varepsilon)$$

Problem: for a given mean value of the biased die, what is the probability distribution of each value?

The mean value is insufficient information, and we use the maximum entropy method to find the most likely distribution (the least informative one).

entropy maximization with the biased die:

$$\frac{\partial}{\partial p_k}\left[-\sum_{k=1}^{6} p_k \ln p_k + \lambda_0\left(\sum_{k=1}^{6} p_k - 1\right) + \lambda_1\left(\sum_{k=1}^{6} k p_k - \frac{7}{2}(1+\varepsilon)\right)\right]$$

$$= -\left(\ln p_k + 1\right) + \lambda_0 + k\lambda_1 = 0$$

$$p_k = e^{\lambda_0 + \lambda_1 k - 1}$$

$$\sum_{k=1,6} p_k = e^{\lambda_0 - 1} \sum_{k=1,6} e^{\lambda_1 k} = 1$$

$$\sum_{k=1,6} k p_k = e^{\lambda_0 - 1} \sum_{k=1,6} k e^{\lambda_1 k} = \frac{7}{2}(1+\varepsilon)$$

$$e^{\lambda_0 - 1} = \frac{1}{\sum_{k=1,6} e^{\lambda_1 k}}; \quad \frac{\sum_{k=1,6} k p_k}{\sum_{k=1,6} e^{\lambda_1 k}} = \frac{7}{2}(1+\varepsilon)$$

we still have to satisfy the constraints ...

$$e^{\lambda_0 - 1} \sum_{k=1,6} e^{\lambda_1 k} = e^{\lambda_0 - 1} \left(\sum_{k=0,6} e^{\lambda_1 k} - 1 \right) = e^{\lambda_0 - 1} \left(\frac{1 - e^{7\lambda_1}}{1 - e^{\lambda_1}} - 1 \right) = 1$$

$$\frac{\sum_{k=1,6} k e^{\lambda_1 k}}{\sum_{k=1,6} e^{\lambda_1 k}} = \frac{\partial}{\partial \lambda_1} \ln \sum_{k=1,6} e^{\lambda_1 k} = \frac{\partial}{\partial \lambda_1} \ln \left(e^{\lambda_1} \sum_{k=0,5} e^{\lambda_1 k} \right)$$

$$= \frac{\partial}{\partial \lambda_1} \left[\lambda_1 + \ln\left(1 - e^{6\lambda_1}\right) - \ln\left(1 - e^{\lambda_1}\right) \right]$$

$$= 1 - \frac{6 e^{6\lambda_1}}{1 - e^{6\lambda_1}} + \frac{e^{\lambda_1}}{1 - e^{\lambda_1}} = \frac{7}{2}(1 + \varepsilon)$$

The Lagrange multipliers are obtained from nonlinear equations, and we must use numerical methods

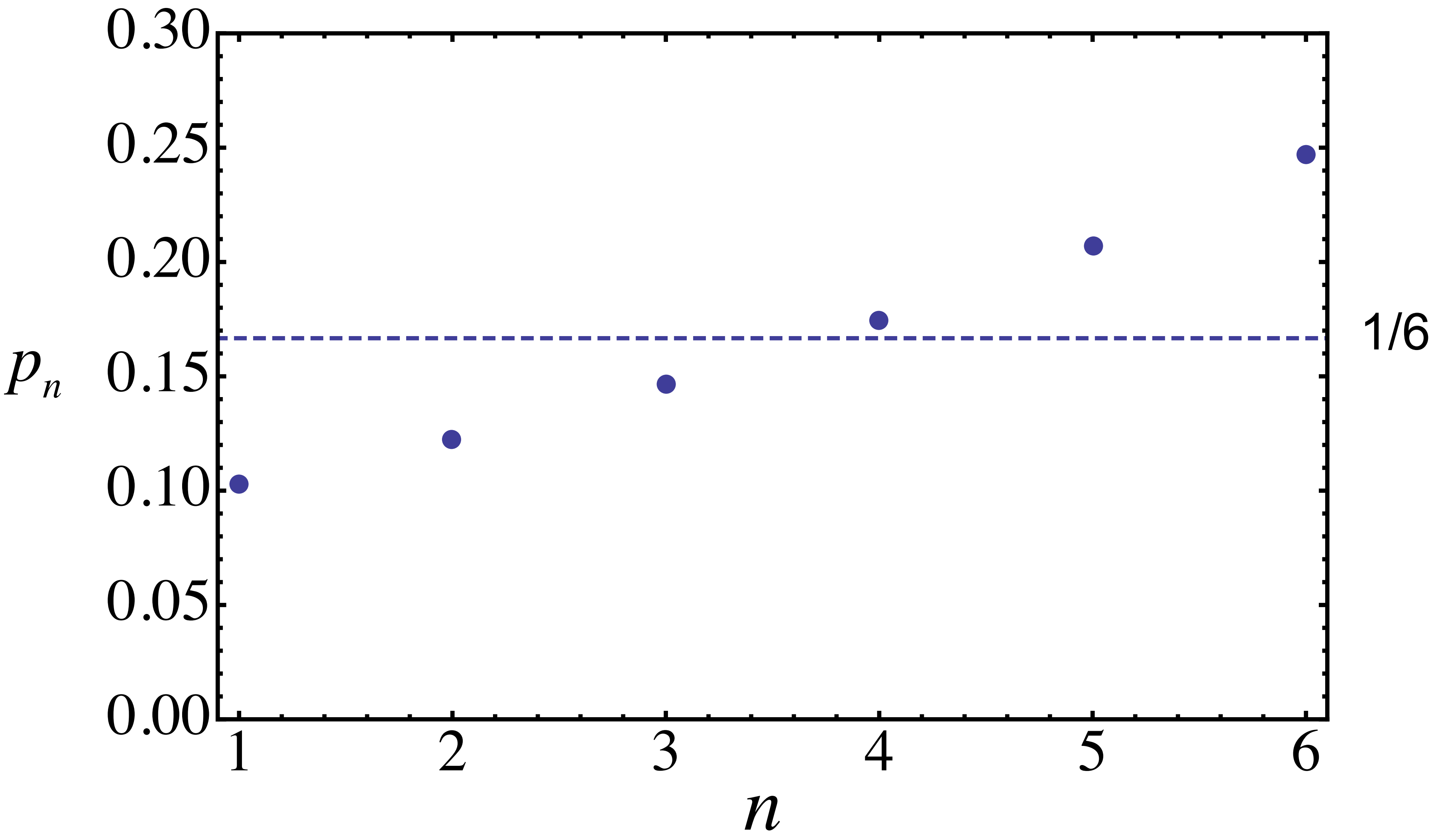
numerical solution

media	p_1	p_2	p_3	p_4	p_5	p_6
3.0	0.246782	0.20724	0.174034	0.146148	0.122731	0.103065
3.1	0.22929	0.199582	0.173723	0.151214	0.131622	0.114568
3.2	0.212566	0.191659	0.172808	0.155811	0.140487	0.126669
3.3	0.196574	0.183509	0.171313	0.159928	0.149299	0.139377
3.4	0.181282	0.175168	0.16926	0.163551	0.158035	0.152704
3.5	0.166667	0.166667	0.166667	0.166667	0.166666	0.166666
3.6	0.152704	0.158035	0.163551	0.16926	0.175168	0.181282
3.7	0.139377	0.149299	0.159928	0.171313	0.183509	0.196574
3.8	0.126669	0.140487	0.155811	0.172808	0.191659	0.212566
3.9	0.114568	0.131622	0.151214	0.173723	0.199582	0.22929
4.0	0.103065	0.122731	0.146148	0.174034	0.20724	0.246782

with a biased die we obtain skewed distributions.

These are examples of UNINFORMATIVE PRIORS

Example: mean = 4



Entropy with continuous probability distributions

(relative entropy, Kullback-Leibler divergence)

$$S \to -\int_a^b \left[p(x)dx\right]\ln\left[p(x)dx\right]$$

this diverges!

$$S_{p|m} = -\sum_k p_k \ln\frac{p_k}{m_k}$$

relative entropy

$$S_{p|m} = -\int_a^b p(x)\ln\frac{p(x)}{m(x)}dx$$

this does not diverge!

Entropy maximization with additional conditions (partial knowledge of moments of the prior distribution)

$$\langle x^k \rangle = \int_a^b x^k p(x) dx$$

function (functional) that must be maximized

$$Q[p] = -\int_a^b p(x) \ln \frac{p(x)}{m(x)} dx + \sum_k \lambda_k \left\{ \int_a^b x^k p(x) dx - M_k \right\}$$

variation

$$\delta Q = -\int_a^b \delta p \left\{ \ln \frac{p(x)}{m(x)} + 1 - \sum_k \lambda_k x^k \right\} dx = 0$$

$$\Rightarrow \quad \ln \frac{p(x)}{m(x)} + 1 - \sum_k \lambda_k x^k = 0$$

$$\Rightarrow \quad p(x) = m(x) \exp\left(\sum_k \lambda_k x^k - 1 \right)$$

$$p(x) = m(x)\exp\left(\sum_n \lambda_n x^n - 1\right)$$

p(x) is determined by the choice of *m(x)* and by the constraints

The constraints can be the moments themselves:

$$M_k = \int_a^b x^k m(x)\exp\left(\sum_n \lambda_n x^n - 1\right) dx$$

1. no moment is known, normalization is the only constraint, and *p(x)* is defined in the interval (*a*,*b*)

$$M_0 = \int_a^b m(x)\exp(\lambda_0 - 1)dx = 1$$

we take a reference distribution which is uniform on (*a*,*b*), i.e.,

$$m(x) = \frac{1}{b-a}$$

$$M_0 = \frac{1}{b-a}\int_a^b \exp(\lambda_0 - 1)dx = \exp(\lambda_0 - 1) = 1$$

$$\Rightarrow \qquad \lambda_0 = 1; \quad p(x) = m(x)\exp\left(\sum_{n=0}^{0}\lambda_n x^n - 1\right) = \frac{1}{b-a}$$

2. only the first moment – the mean – is known, and *p(x)* is defined on (*a*,*b*)

$$M_0 = \frac{1}{b-a}\int_a^b \exp\left(\lambda_0 + \lambda_1 x - 1\right)dx = 1$$

$$M_1 = \frac{1}{b-a}\int_a^b x\exp\left(\lambda_0 + \lambda_1 x - 1\right)dx$$

$$M_0 = 1 = \frac{\exp\left(\lambda_0 - 1\right)}{b-a}\int_a^b \exp\left(\lambda_1 x\right)dx = \frac{\exp\left(\lambda_0 - 1\right)}{b-a}\cdot\frac{\exp\left(\lambda_1 b\right) - \exp\left(\lambda_1 a\right)}{\lambda_1}$$

$$M_1 = \frac{\exp\left(\lambda_0 - 1\right)}{b-a}\int_a^b x\exp\left(\lambda_1 x\right)dx = \frac{\exp\left(\lambda_0 - 1\right)}{b-a}\left[\frac{1}{\lambda_1}\left(b\exp\left(\lambda_1 b\right) - a\exp\left(\lambda_1 a\right)\right) - \frac{1}{\lambda_1^2}\left(\exp\left(\lambda_1 b\right) - \exp\left(\lambda_1 a\right)\right)\right]$$

in general, these equations can only be solved numerically...

special case:

$$a \to -\frac{L}{2}; \quad b \to \frac{L}{2}; \quad M_1 = 0$$

$$\frac{\exp(\lambda_0 - 1)}{L} \cdot \frac{\exp(\lambda_1 L/2) - \exp(-\lambda_1 L/2)}{\lambda_1} = 1$$

$$\Rightarrow \frac{\exp(\lambda_0 - 1)}{L}\left[\frac{1}{\lambda_1}\left(\frac{L}{2}\exp(\lambda_1 L/2) + \frac{L}{2}\exp(-\lambda_1 L/2)\right) - \frac{1}{\lambda_1^2}\left(\exp(\lambda_1 L/2) - \exp(-\lambda_1 L/2)\right)\right] = 0$$

$$\frac{\exp(\lambda_0 - 1)}{L} \cdot \frac{\exp(\lambda_1 L/2) - \exp(-\lambda_1 L/2)}{\lambda_1} = 1$$

$$\Rightarrow \frac{L}{2}\left(\exp(\lambda_1 L/2) + \exp(-\lambda_1 L/2)\right) - \frac{1}{\lambda_1}\left(\exp(\lambda_1 L/2) - \exp(-\lambda_1 L/2)\right) = 0$$

$$\exp(\lambda_0 - 1)\frac{\sinh(\lambda_1 L/2)}{\lambda_1 L/2} = 1$$

$$L\cosh(\lambda_1 L/2) - \frac{2}{\lambda_1}\sinh(\lambda_1 L/2) = 0$$

$$\Rightarrow \quad (\lambda_1 L/2) = \tanh(\lambda_1 L/2) \quad \Rightarrow \quad \lambda_1 = 0; \quad \lambda_0 = 1$$

$$p(x) = m(x)\exp\left(\sum_{k=0}^{1}\lambda_k x^k - 1\right) = \frac{1}{L}$$

nonzero mean

$$a \to -\frac{L}{2}; \quad b \to \frac{L}{2}; \quad M_1 = \varepsilon$$

$$\frac{\exp(\lambda_0 - 1)}{L} \cdot \frac{\exp(\lambda_1 L/2) - \exp(-\lambda_1 L/2)}{\lambda_1} = 1$$

$$\frac{\exp(\lambda_0 - 1)}{\lambda_1 L}\left[\frac{L}{2}\left(\exp(\lambda_1 L/2) + \exp(-\lambda_1 L/2)\right) - \frac{1}{\lambda_1}\left(\exp(\lambda_1 L/2) - \exp(-\lambda_1 L/2)\right)\right] = \varepsilon$$

$$\frac{\exp(\lambda_0 - 1)}{(\lambda_1 L/2)} \cdot \sinh(\lambda_1 L/2) = 1$$

$$\frac{L}{2}\frac{1}{\tanh(\lambda_1 L/2)} - \frac{1}{\lambda_1} = \varepsilon$$

$$\tanh\left(\lambda_1 L/2\right) = \left(\frac{1}{\lambda_1 L/2} + \frac{2\varepsilon}{L}\right)^{-1} \qquad \tanh(z) = \left(\frac{1}{z} + \frac{2\varepsilon}{L}\right)^{-1}$$

we find an approximate solution

$$z - \frac{z^3}{3} \approx \left(\frac{1}{z} + \frac{2\varepsilon}{L}\right)^{-1} \quad \Rightarrow \quad \left(z - \frac{z^3}{3}\right)\left(\frac{1}{z} + \frac{2\varepsilon}{L}\right) \approx 1 + \frac{2\varepsilon}{L} z - \frac{z^2}{3} = 1$$

$$\Rightarrow \quad \frac{2\varepsilon}{L} - \frac{z}{3} \approx 0 \quad \Rightarrow \quad z \approx \frac{6\varepsilon}{L}$$

$$\frac{\lambda_1 L}{2} \approx \frac{6\varepsilon}{L} \quad \Rightarrow \quad p(x) \approx \frac{1}{L}\exp\left(\lambda_1 x\right) \approx \frac{1}{L}\left(1 - \frac{12\varepsilon}{L} x\right)$$

another special case $a = 0; \quad b \to \infty$

$$M_0 = \frac{1}{b-a}\int_a^b \exp\left(\lambda_0 + \lambda_1 x - 1\right)dx = 1$$

$$M_1 = \frac{1}{b-a}\int_a^b x\exp\left(\lambda_0 + \lambda_1 x - 1\right)dx$$

$$M_0 = 1 = m_0 \exp\left(\lambda_0 - 1\right)\cdot\frac{1}{\left(-\lambda_1\right)}$$

$$M_1 = m_0 \exp\left(\lambda_0 - 1\right)\left[\frac{1}{\lambda_1^2}\right] = \left(-\lambda_1\right)\left[\frac{1}{\lambda_1^2}\right] = -\frac{1}{\lambda_1} = \langle x \rangle$$

then

$$m_0 \exp(\lambda_0 - 1) = -\lambda_1 = \frac{1}{\langle x \rangle}$$

and we obtain the exponential distribution

$$p(x) = m(x) \exp\left(\sum_n \lambda_n x^n - 1 \right)$$

$$= m_0 \exp(\lambda_0 - 1) \exp(\lambda_1 x) = \frac{1}{\langle x \rangle} \exp\left(-\frac{x}{\langle x \rangle} \right)$$

3. both mean and variance are known, and the interval is the whole real axis

$$M_0 = m_0 \int_a^b \exp\left(\lambda_0 + \lambda_1 x + \lambda_2 x^2 - 1\right) dx = 1$$

$$M_1 = m_0 \int_a^b x \exp\left(\lambda_0 + \lambda_1 x + \lambda_2 x^2 - 1\right) dx$$

$$M_2 = m_0 \int_a^b x^2 \exp\left(\lambda_0 + \lambda_1 x + \lambda_2 x^2 - 1\right) dx$$

$$\begin{aligned} \exp\left(\lambda_0 + \lambda_1 x + \lambda_2 x^2 - 1\right) &= \exp\left[\lambda_2\left(x^2 + 2\frac{\lambda_1}{\lambda_2}x + \frac{\lambda_1^2}{\lambda_2^2}\right) + \left(\lambda_0 - 1 - \frac{\lambda_1^2}{\lambda_2}\right)\right] \\ &= \exp\left(\lambda_0 - 1 - \frac{\lambda_1^2}{\lambda_2}\right) \exp\left[\lambda_2\left(x + \frac{\lambda_1}{\lambda_2}\right)^2\right] \end{aligned}$$

$$M_0 = m_0 \exp\left(\lambda_0 - 1 - \frac{\lambda_1^2}{\lambda_2}\right)\int_{-\infty}^{+\infty} \exp\left[-\frac{1}{2(-1/2\lambda_2)}\left(x + \frac{\lambda_1}{\lambda_2}\right)^2\right]dx = m_0 \exp\left(\lambda_0 - 1 - \frac{\lambda_1^2}{\lambda_2}\right)\sqrt{-\frac{\pi}{\lambda_2}} = 1$$

$$M_1 = m_0 \exp\left(\lambda_0 - 1 - \frac{\lambda_1^2}{\lambda_2}\right)\int_{-\infty}^{+\infty} x \exp\left[-\frac{1}{2(-1/2\lambda_2)}\left(x + \frac{\lambda_1}{\lambda_2}\right)^2\right]dx = m_0 \exp\left(\lambda_0 - 1 - \frac{\lambda_1^2}{\lambda_2}\right)\sqrt{-\frac{\pi}{\lambda_2}}\left(-\frac{\lambda_1}{\lambda_2}\right) = -\mu$$

$$M_2 = m_0 \exp\left(\lambda_0 - 1 - \frac{\lambda_1^2}{\lambda_2}\right)\int_{-\infty}^{+\infty} x^2 \exp\left[-\frac{1}{2(-1/2\lambda_2)}\left(x + \frac{\lambda_1}{\lambda_2}\right)^2\right]dx = m_0 \exp\left(\lambda_0 - 1 - \frac{\lambda_1^2}{\lambda_2}\right)\sqrt{-\frac{\pi}{\lambda_2}}\left(-\frac{1}{2\lambda_2} + \frac{\lambda_1^2}{\lambda_2^2}\right) = \sigma^2 + \mu^2$$

$$M_0 = m_0 \exp\left(\lambda_0 - 1 - \frac{\lambda_1^2}{\lambda_2}\right)\sqrt{-\frac{\pi}{\lambda_2}} = 1$$

$$M_1 = \frac{\lambda_1}{\lambda_2} = \mu$$

$$M_2 = \left(-\frac{1}{2\lambda_2} + \frac{\lambda_1^2}{\lambda_2^2}\right) = \sigma^2 + \mu^2$$

$$\Rightarrow \quad \lambda_1 = -\frac{\mu}{2\sigma^2}; \quad \lambda_2 = -\frac{1}{2\sigma^2}; \quad m_0 \exp\left(\lambda_0 - 1 - \frac{\lambda_1^2}{\lambda_2}\right) = \frac{1}{\sqrt{2\pi\sigma^2}}$$

$$
\begin{aligned}
p(x) &= m_0 \exp\left(\lambda_0 + \lambda_1 x + \lambda_2 x^2 - 1\right) \\
&= m_0 \exp\left(\lambda_0 - 1 - \frac{\lambda_1^2}{\lambda_2}\right) \exp\left[-\frac{1}{2\left(-1/2\lambda_2\right)}\left(x + \frac{\lambda_1}{\lambda_2}\right)^2\right] \\
&= \frac{1}{\sqrt{2\sigma^2\pi}} \exp\left[\frac{1}{2\sigma^2}\left(x - \mu\right)^2\right]
\end{aligned}
$$

... in this case where mean and variance are known, the entropic prior is Gaussian

An alternative form of entropy that incorporates the normalization constraint from the start

$$Q[p;m] = -\int_X dx\ p(x)\ln\frac{p(x)}{m(x)} + \lambda\left(\int_X dx p(x) - \int_X dx m(x)\right)$$

$$= \int_X dx\left(-p(x)\ln\frac{p(x)}{m(x)} + \lambda p(x) - \lambda m(x)\right)$$

$$\delta Q = \int_X \delta p\, dx\left(-\ln\frac{p(x)}{m(x)} - 1 + \lambda\right) = 0$$

$$p(x) = m(x)\exp(\lambda - 1)$$

$$\int_X dx\ p(x) = \int_X dx\ m(x)\exp(\lambda-1) = \exp(\lambda-1)\int_X dx\ m(x) = \exp(\lambda-1) = 1$$

$$\Rightarrow \quad \lambda = 1$$

$$Q[p;m] = \int_X dx\left(-p(x)\ln\frac{p(x)}{m(x)} + p(x) - m(x)\right)$$

Until now we have emphasized the role of the momenta of the distribution, however other information can be incorporated in the same way in the entropic prior.

A "crystallographic" example (Jaynes, 1968)

Consider a simple version of a crystallographic problem, where a 1-D crystal has atoms at the positions

$$x_j = jL \quad (L = 1, \ldots, n)$$

and such that these positions may be occupied by impurities.

From X-ray experiments it has been determined that impurity atoms prefer sites where

$$\cos\left(kx_j\right) > 0$$

furthermore we take, as an example,

$$\left\langle \cos\left(kx_j\right) \right\rangle = 0.3$$

which means that we have the constraint

$$\left\langle \cos\left(kx_j\right) \right\rangle = \sum_{j=1}^{n} p_j \cos\left(kx_j\right) = 0.3$$

where p_j is the probability that an impurity atom is at site j.

Then the constrained entropy that must be maximized is

$$Q = -\sum_{j=1}^{n} p_j \ln p_j + \lambda_0 \left(\sum_{j=1}^{n} p_j - 1 \right) + \lambda_1 \left(\sum_{j=1}^{n} p_j \cos\left(kx_j\right) - 0.3 \right)$$

from which we find the maximization condition

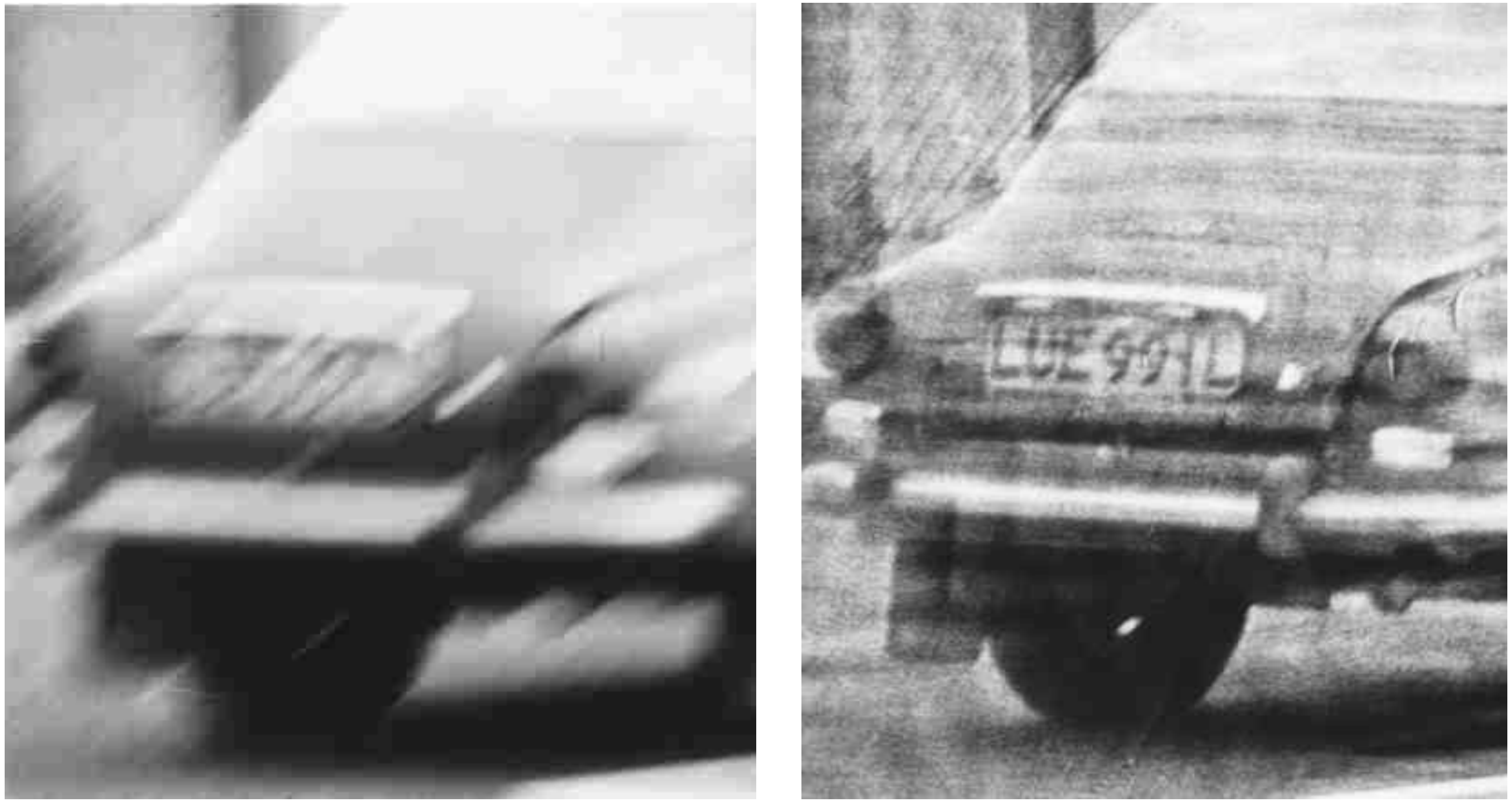
$$\frac{\partial Q}{\partial p_j} = -\left(\ln p_j + 1\right) + \lambda_0 + \lambda_1 \cos\left(kx_j\right) = 0$$

i.e.,

$$p_j = \exp\left[1 - \lambda_0 - \lambda_1 \cos\left(kx_j\right)\right]$$

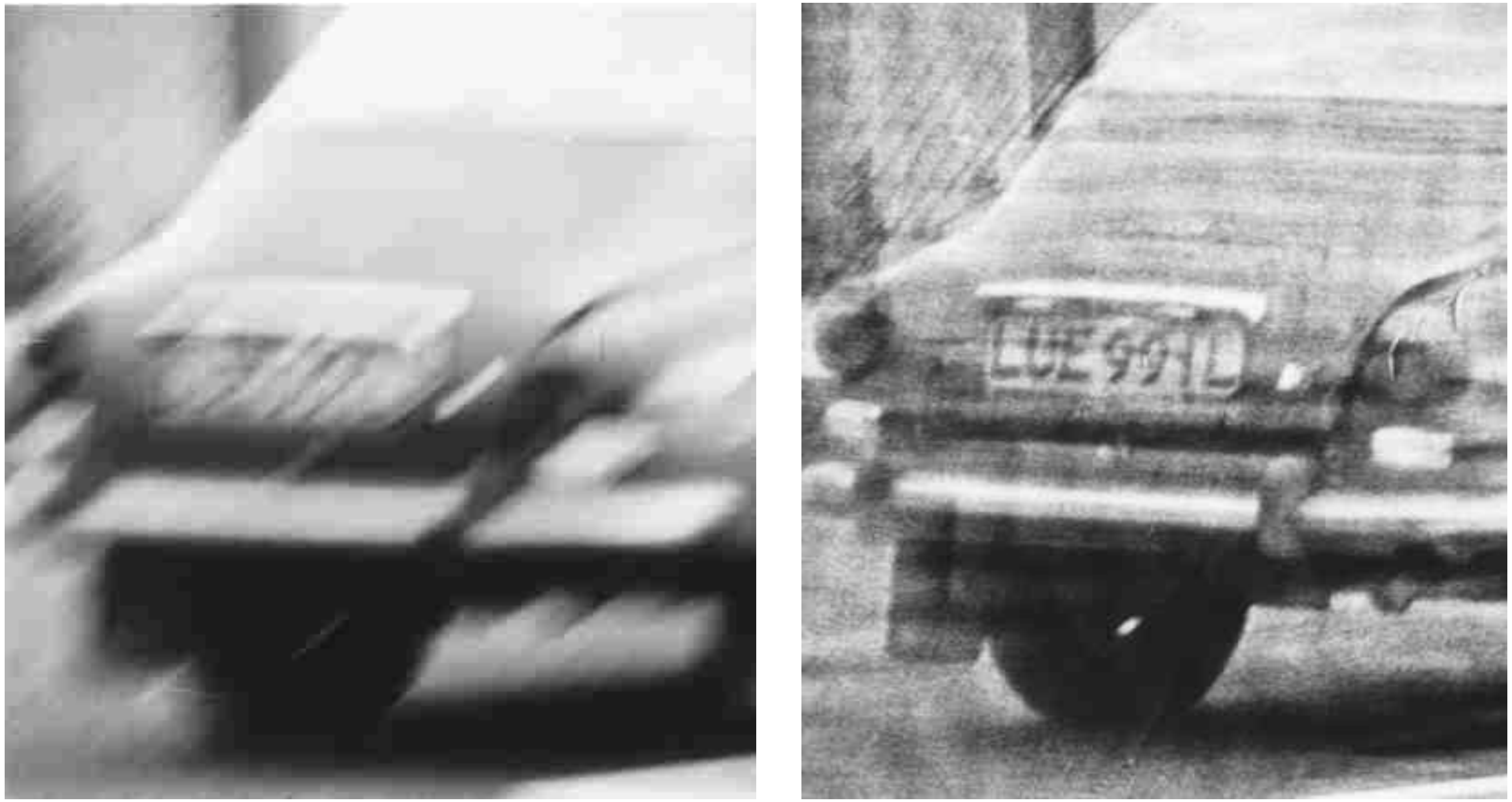
The rest of the solution proceeds either by approximation or by numerical calculation.

Example of MaxEnt in action:
unconstrained problem in image restoration



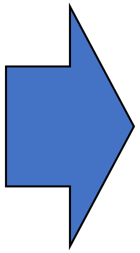
J. Skilling, Nature 309 (1984) 748

Car movement introduces linear correlations among pixels. The model of linear corrections does not allow direct inversion to find the corrected image because the number of variables is larger than the number of equations. The MaxEnt methods regularizes the problem and finds a reasonable solution.



J. Skilling, Nature 309 (1984) 748

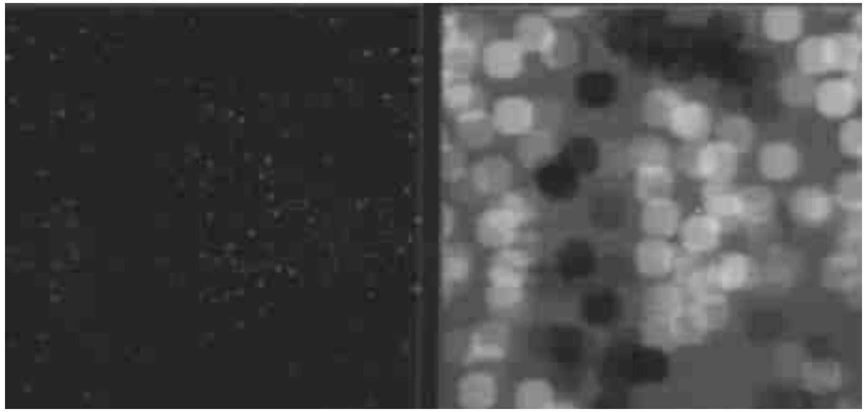
Reconstruction of missing data
(from http://www.maxent.co.uk)

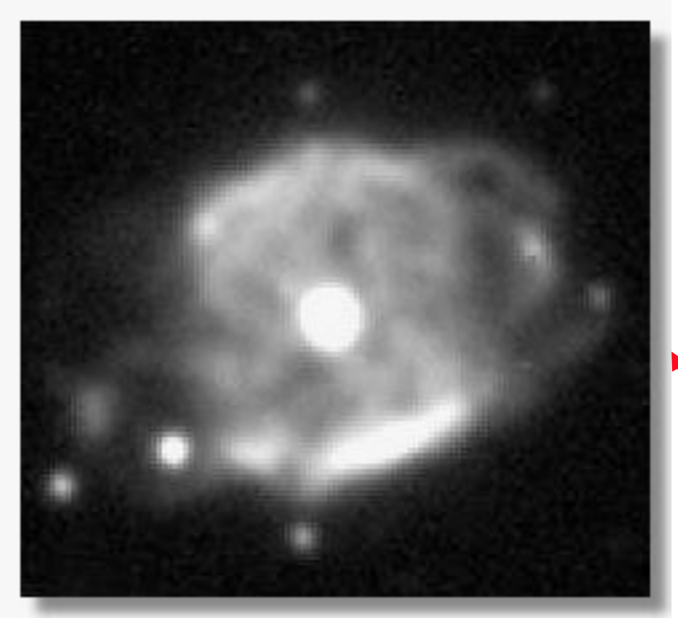


50%

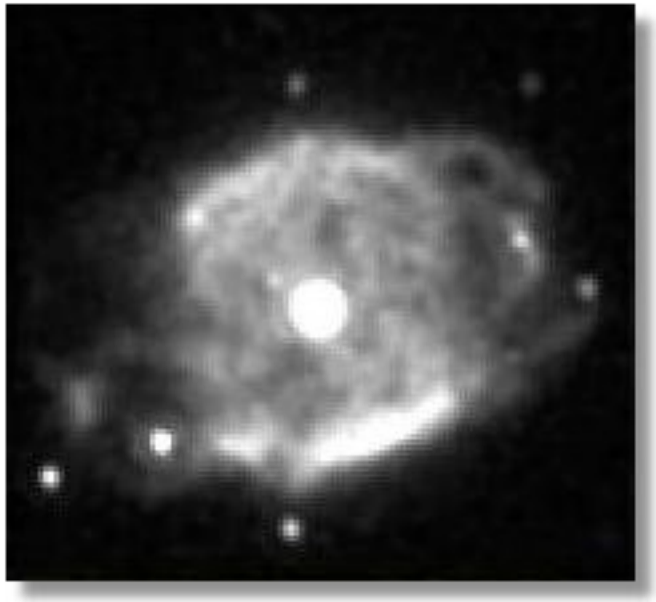
95%

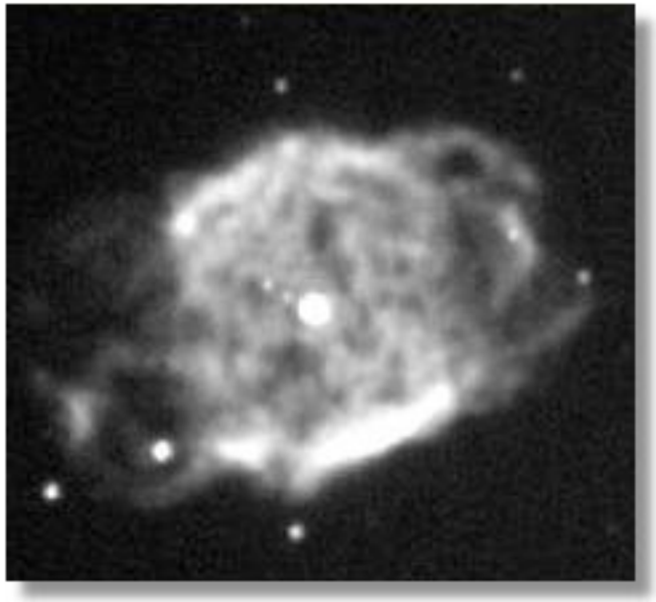
99%





NGC 40



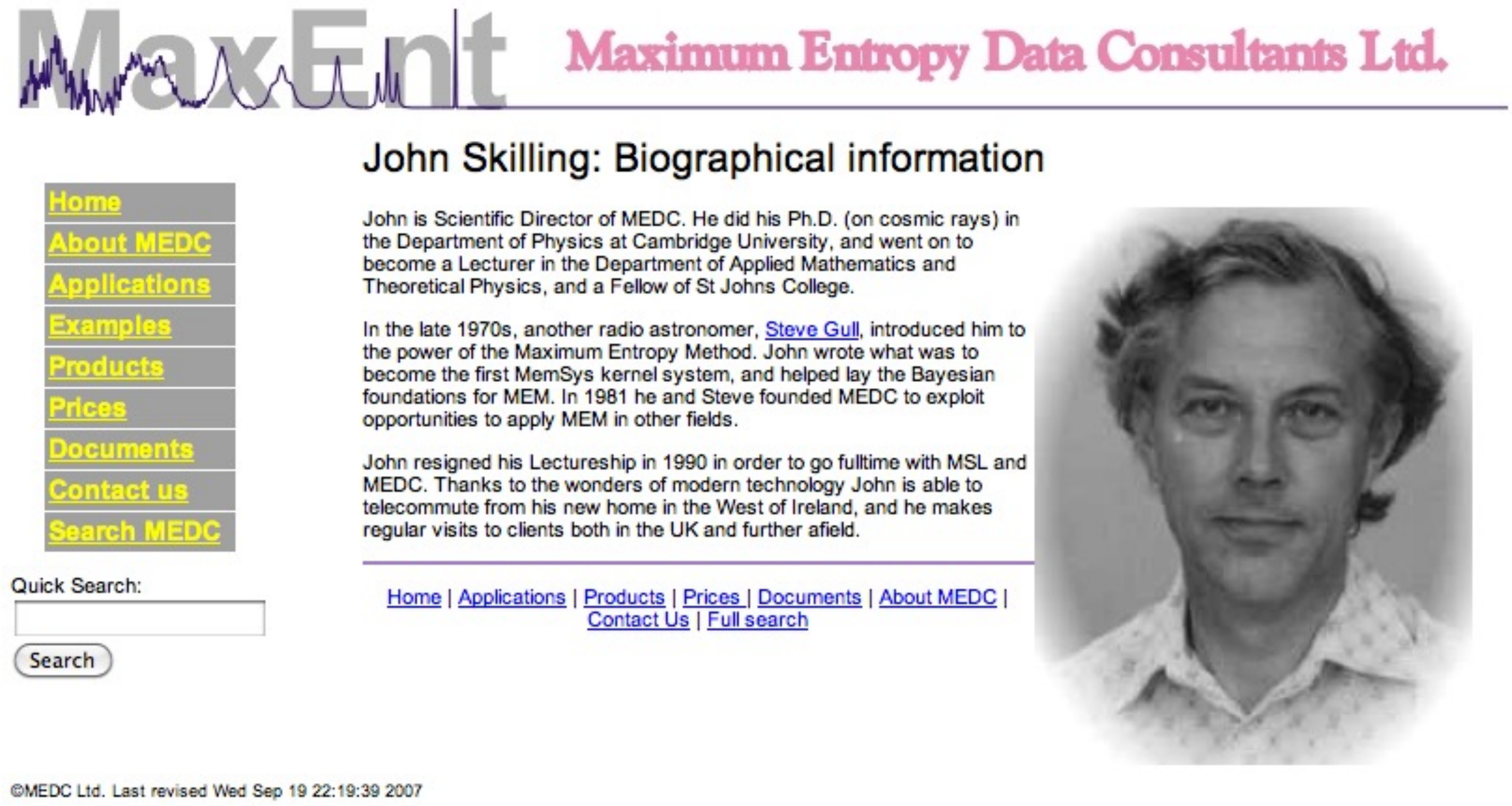


low resolution (MEM enhanced)

low resolution

high resolution

(from http://www.mirametrics.com)


MaxEnt Maximum Entropy Data Consultants Ltd.

John Skilling: Biographical information

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John is Scientific Director of MEDC. He did his Ph.D. (on cosmic rays) in the Department of Physics at Cambridge University, and went on to become a Lecturer in the Department of Applied Mathematics and Theoretical Physics, and a Fellow of St Johns College.

In the late 1970s, another radio astronomer, Steve Gull, introduced him to the power of the Maximum Entropy Method. John wrote what was to become the first MemSys kernel system, and helped lay the Bayesian foundations for MEM. In 1981 he and Steve founded MEDC to exploit opportunities to apply MEM in other fields.

John resigned his Lectureship in 1990 in order to go fulltime with MSL and MEDC. Thanks to the wonders of modern technology John is able to telecommute from his new home in the West of Ireland, and he makes regular visits to clients both in the UK and further afield.

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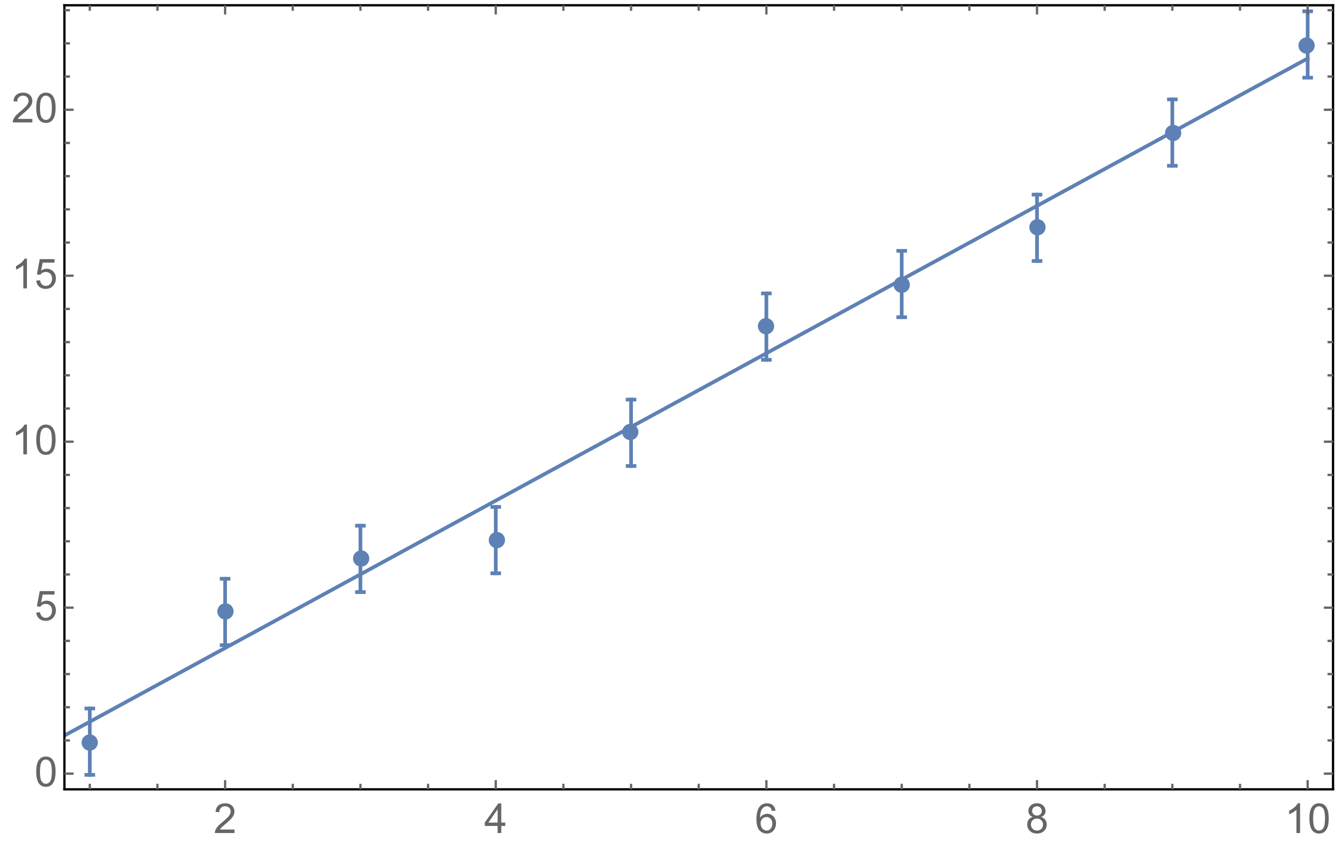
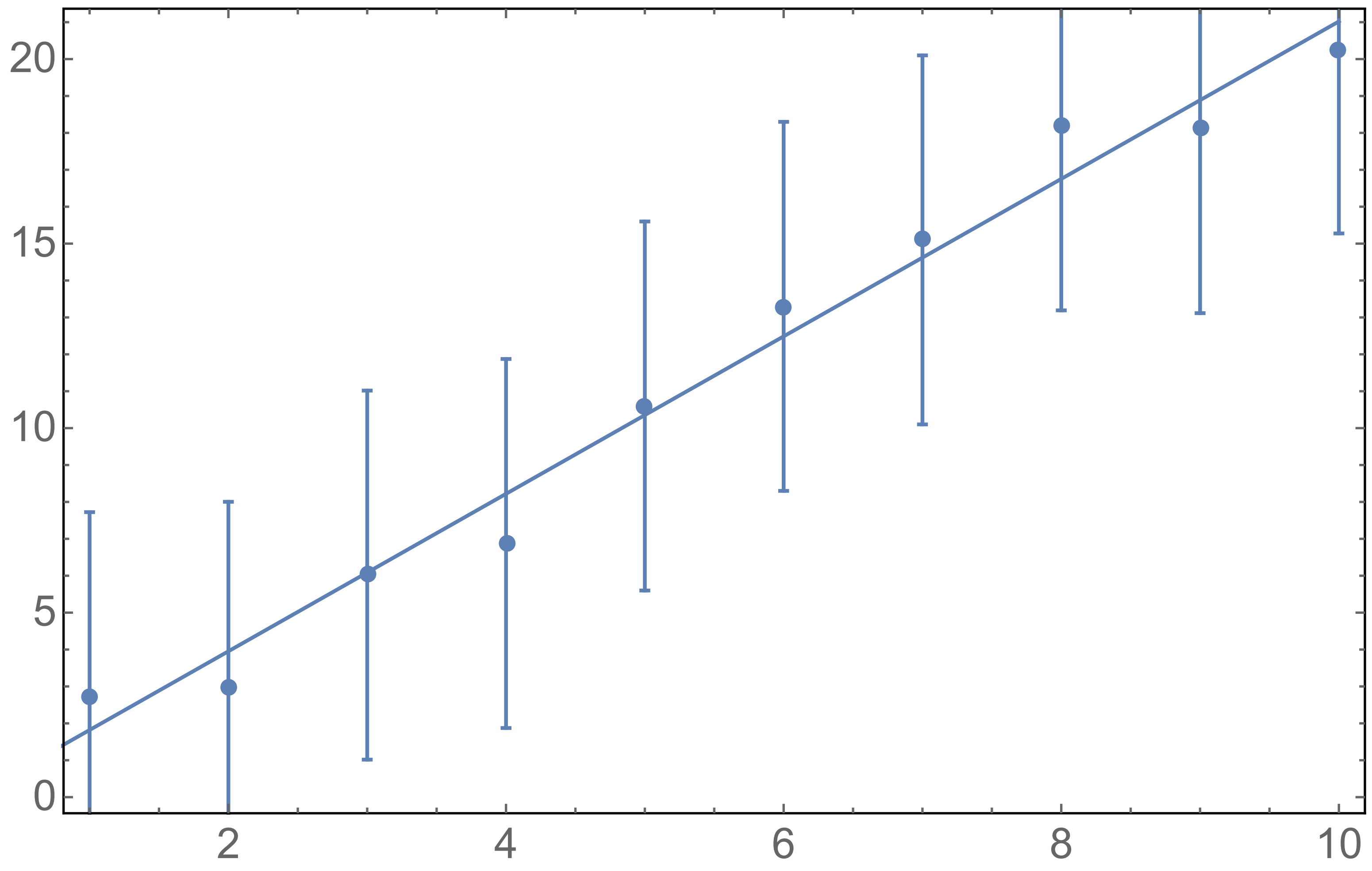
http://www.maxent.co.uk/
(the company no longer exists and the website has disappeared from the web)

Example: miscalibrated Gaussian measurement errors, a Bayesian estimate using objective priors

Here, we consider the case where we must find the mean value with given measurement uncertainties that are systematically multiplied by an unknown scale factor, under the assumption of Gaussianity.





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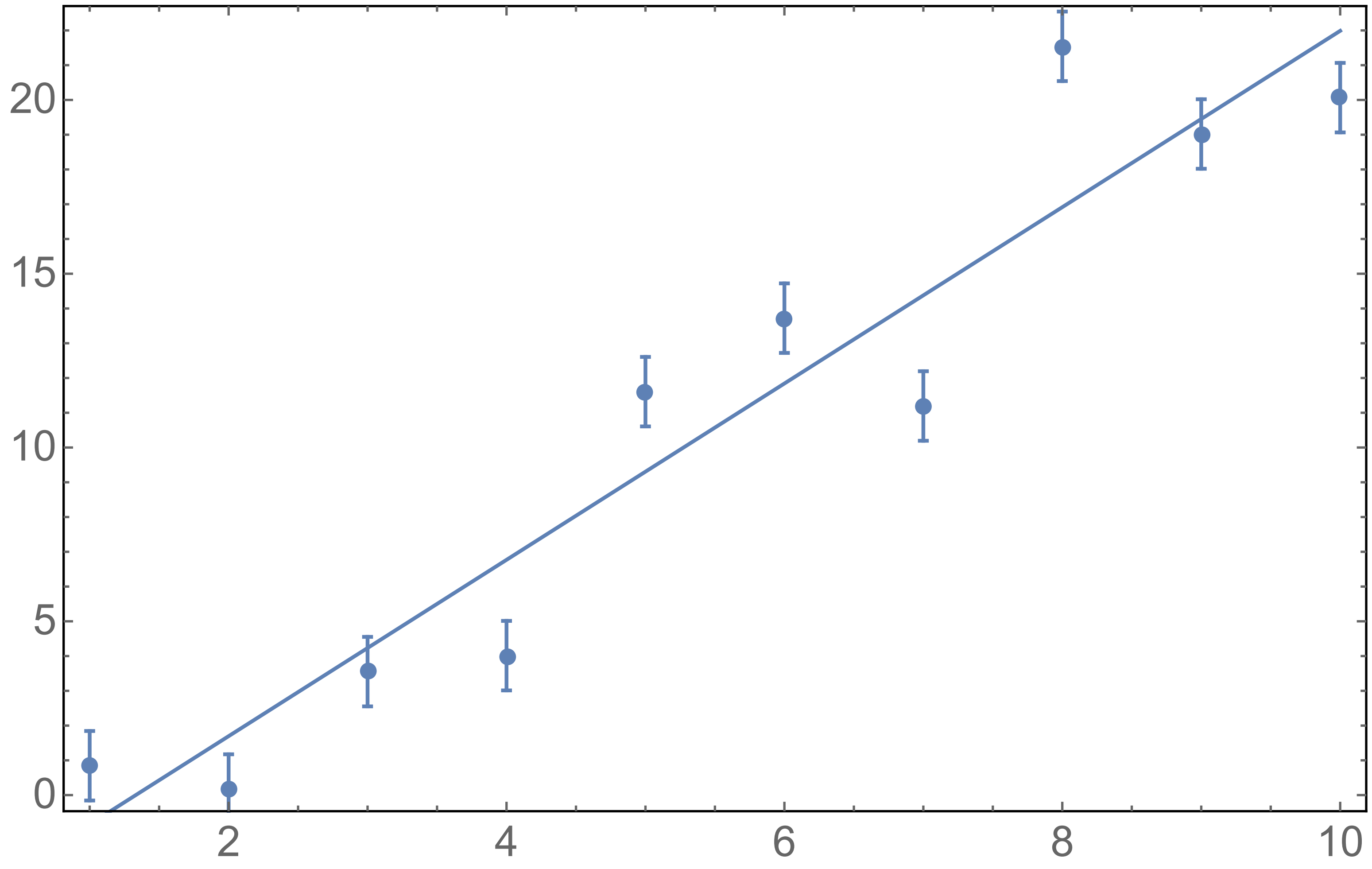

20
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The likelihood has a Gaussian structure

$$P\left(\mathbf{d} \mid \mu, \boldsymbol{\sigma}, \alpha\right) = \prod_{k=1}^{N} \frac{1}{\sqrt{2\pi\alpha^2\sigma_k^2}} \exp\left[-\frac{\left(d_k - \mu\right)^2}{2\alpha^2\sigma_k^2}\right]$$

$$= \frac{1}{\left(2\pi\right)^{N/2}\alpha^N} \left(\prod_{k=1}^{N} \frac{1}{\sigma_k}\right) \exp\left[-\frac{1}{2\alpha^2}\sum_{k=1}^{N} \frac{\left(d_k - \mu\right)^2}{\sigma_k^2}\right]$$

we must rearrange the exponent as usual ...

$$\sum_{k=1}^{N} \frac{(d_k - \mu)^2}{\sigma_k^2} = \sum_{k=1}^{N} \frac{d_k^2}{\sigma_k^2} - 2\mu \sum_{k=1}^{N} \frac{d_k}{\sigma_k^2} + \mu^2 \sum_{k=1}^{N} \frac{1}{\sigma_k^2} = \frac{ND}{\sigma_M^2} - 2\mu \frac{NM}{\sigma_M^2} + \mu^2 \frac{N}{\sigma_M^2}$$

$$= \frac{N}{\sigma_M^2}\left(D - 2\mu M + \mu^2\right)$$

dove $\displaystyle \frac{1}{\sigma_M^2} = \frac{1}{N}\sum_{k=1}^{N}\frac{1}{\sigma_k^2}; \quad M = \sum_{k=1}^{N}\frac{d_k}{\sigma_k^2} \Big/ \sum_{k=1}^{N}\frac{1}{\sigma_k^2}; \quad D = \sum_{k=1}^{N}\frac{d_k^2}{\sigma_k^2} \Big/ \sum_{k=1}^{N}\frac{1}{\sigma_k^2}$

therefore the likelihood is

$$P(\mathbf{d} \mid \mu, \boldsymbol{\sigma}, \alpha) = \frac{1}{(2\pi)^{N/2}\alpha^N}\left(\prod_{k=1}^{N}\frac{1}{\sigma_k}\right)\exp\left[-\frac{N}{2\alpha^2\sigma_M^2}\left(D - 2\mu M + \mu^2\right)\right]$$

Now we estimate the scale factor from Bayes' theorem

$$p(\alpha|\mathbf{d},\boldsymbol{\sigma}) = \frac{p(\mathbf{d}|\alpha,\boldsymbol{\sigma})}{\int_\alpha p(\mathbf{d}|\alpha',\boldsymbol{\sigma})p(\alpha')d\alpha'}p(\alpha)$$

however, we need first to marginalize the likelihood with respect to the mean, which in this case is a ***nuisance parameter***

we take a uniform prior for the mean

$$P(\mathbf{d}\,|\,\boldsymbol{\sigma},\alpha) = \int_\mu P(\mathbf{d}\,|\,\mu,\boldsymbol{\sigma},\alpha)P(\mu|\boldsymbol{\sigma},\alpha)\,d\mu$$

$$= \frac{1}{W}\int_{\mu_{\min}}^{\mu_{\max}} P(\mathbf{d}\,|\,\mu,\boldsymbol{\sigma},\alpha)\,d\mu$$

$$\approx \frac{1}{W}\frac{1}{(2\pi)^{N/2}\alpha^N}\left(\prod_{k=1}^{N}\frac{1}{\sigma_k}\right)\int_{-\infty}^{+\infty}\exp\left[-\frac{N}{2\alpha^2\sigma_M^2}\left(D-2\mu M+\mu^2\right)\right]d\mu$$

$$\left(W = \mu_{\max} - \mu_{\min}\right)$$

as usual ...

$$D - 2\mu M + \mu^2 = \mu^2 - 2\mu M + M^2 + D - M^2$$
$$= (\mu - M)^2 + D - M^2$$

... therefore the marginalized likelihood is:

$$P(\mathbf{d} \mid \boldsymbol{\sigma}, \alpha) \approx \frac{1}{W} \frac{1}{(2\pi)^{N/2} \alpha^N} \left(\prod_{k=1}^{N} \frac{1}{\sigma_k} \right) \int_{-\infty}^{+\infty} \exp\left\{ -\frac{N}{2\alpha^2 \sigma_M^2} \left[(\mu - M)^2 + D - M^2 \right] \right\} d\mu$$
$$= \frac{1}{W} \frac{1}{(2\pi)^{N/2} \alpha^N} \left(\prod_{k=1}^{N} \frac{1}{\sigma_k} \right) \exp\left(-\frac{N(D - M^2)}{2\alpha^2 \sigma_M^2} \right) \sqrt{\frac{2\pi\alpha^2\sigma_M^2}{N}}$$

$$p(\alpha|\mathbf{d},\boldsymbol{\sigma}) = \frac{p(\mathbf{d}|\alpha,\boldsymbol{\sigma})}{\int_\alpha p(\mathbf{d}|\alpha',\boldsymbol{\sigma})p(\alpha')d\alpha'}p(\alpha)$$

$$= \frac{\frac{1}{\alpha^{N-1}}\exp\left(-\frac{N(D-M^2)}{2\alpha^2\sigma_M^2}\right)}{\int_\alpha \frac{1}{\alpha'^{N-1}}\exp\left(-\frac{N(D-M^2)}{2\alpha'^2\sigma_M^2}\right)p(\alpha')d\alpha'}p(\alpha)$$

$$P(\alpha) \propto \frac{1}{\alpha}$$

for the standard deviation we take again a Jeffreys prior

$$p(\alpha|\mathbf{d},\boldsymbol{\sigma}) = \frac{\frac{1}{\alpha^{N-1}} \exp\left(-\frac{N(D-M^2)}{2\alpha^2\sigma_M^2}\right)\frac{1}{\alpha}}{\int_\alpha \frac{1}{\alpha'^{N-1}} \exp\left(-\frac{N(D-M^2)}{2\alpha'^2\sigma_M^2}\right)\frac{1}{\alpha'}d\alpha'}; \quad A^2 = \frac{N(D-M^2)}{2\sigma_M^2}$$

$$\Rightarrow \quad p(\alpha|\mathbf{d},\boldsymbol{\sigma}) \to \frac{\frac{1}{\alpha^N}\exp\left(-\frac{A^2}{\alpha^2}\right)}{\int_0^\infty \frac{1}{\alpha'^N}\exp\left(-\frac{A^2}{\alpha'^2}\right)d\alpha'}$$

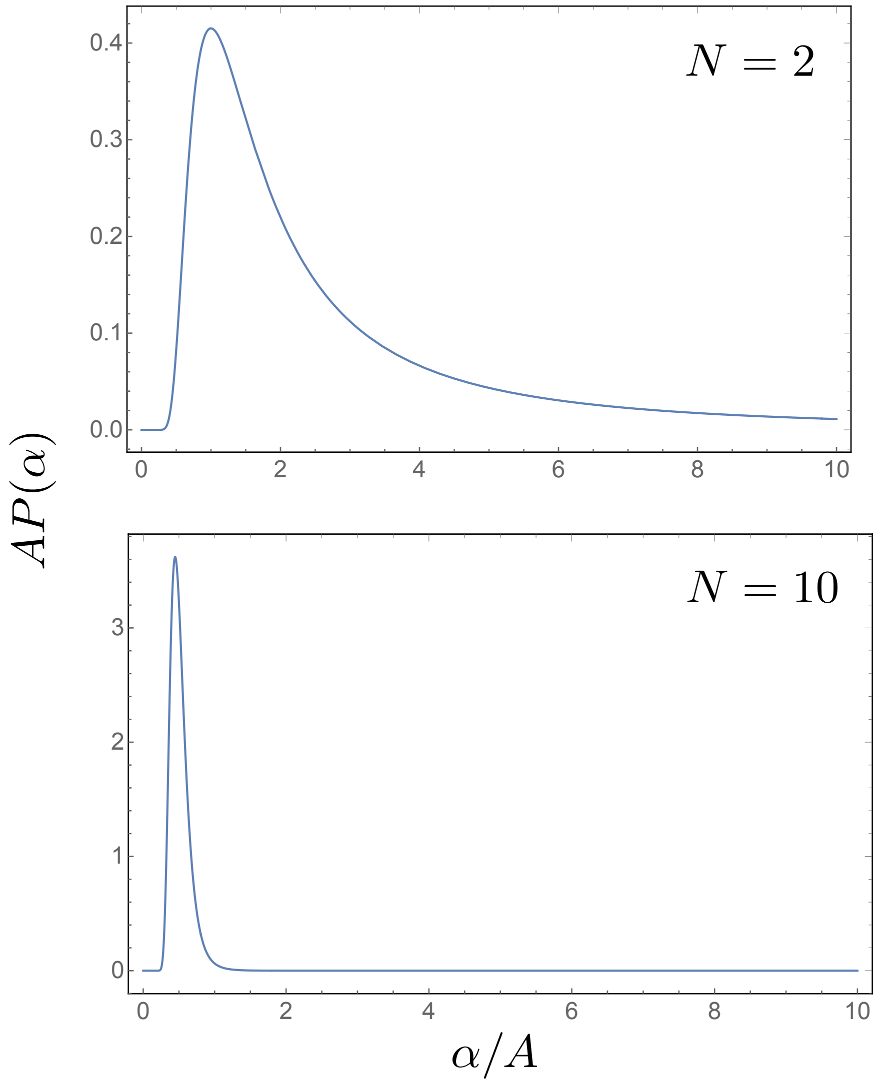
evaluation of $\int_0^\infty \frac{1}{\alpha'^N} \exp\left(-\frac{A^2}{\alpha'^2}\right) d\alpha'$

$$\frac{A^2}{\alpha^2} = x; \quad \alpha = \frac{A}{\sqrt{x}}; \quad d\alpha = -\frac{A}{2x^{3/2}} dx$$

$$\int_0^\infty \frac{x^{N/2}}{A^N} \exp(-x) \frac{A}{2x^{3/2}} dx = \frac{1}{2A^{N-1}} \int_0^\infty x^{\frac{N-1}{2}-1} \exp(-x) dx = \frac{1}{2A^{N-1}} \cdot \Gamma\left(\frac{N-1}{2}\right)$$

$$p(\alpha|\mathbf{d}, \boldsymbol{\sigma}) \to \frac{\frac{2A^{N-1}}{\alpha^N} \exp\left(-\frac{A^2}{\alpha^2}\right)}{\Gamma\left(\frac{N-1}{2}\right)}$$

$$P(\alpha|\mathbf{d},\boldsymbol{\sigma}) = \frac{(2A^{N-1}/\alpha^N)\exp(-A^2/\alpha^2)}{\Gamma\left[(N-1)/2\right]}$$



we take the MAP estimate of the scale parameter from the pdf

$$p(\alpha|\mathbf{d},\boldsymbol{\sigma}) = \frac{\dfrac{2A^{N-1}}{\alpha^N}\exp\left(-\dfrac{A^2}{\alpha^2}\right)}{\Gamma\left(\dfrac{N-1}{2}\right)}$$

$$\frac{d}{d\alpha}P(\alpha\,|\,\mathbf{d},\boldsymbol{\sigma}) \propto -\frac{N}{\alpha^{N+1}}\exp\left(-\frac{A^2}{\alpha^2}\right) + \frac{2A^2}{\alpha^{N+3}}\exp\left(-\frac{A^2}{\alpha^2}\right) = 0$$

$\Rightarrow$ $N\alpha^2 = 2A^2$ $\Rightarrow$ $\alpha_{MAP} = \sqrt{\frac{2}{N}}A = \sqrt{\frac{\left(D - M^2\right)}{\sigma_M^2}}$