# Introduction to Bayesian Statistics - 8

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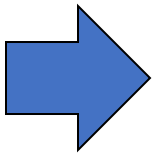
# Our next important topic: Bayesian estimates often require complex numerical integrals. How do we confront this problem?



enter the Monte Carlo methods!

1. acceptance-rejection sampling
2. importance sampling
3. statistical bootstrap
4. Bayesian methods in a sampling-resampling perspective
5. Introduction to Markov chains and to Random Walks (RW)
6. Detailed balance and Boltzmann's H-theorem
7. The Gibbs sampler
8. More on Gibbs sampling
9. Simulated annealing and the Traveling Salesman Problem (TSP)
10. The Metropolis algorithm
11. Image restoration and Markov Random Fields (MRF)
12. The Metropolis-Hastings algorithm and Markov Chain Monte Carlo (MCMC)
13. The efficiency of MCMC methods
14. Affine-invariant MCMC algorithms (emcee)

# A simple view of the convergence of Gibbs sampling in the bivariate case.

We consider the following case: two discrete random variables with marginally Bernoulli distributions and with a joint probability distribution described by the following matrix

| $Y$ \ $X$ | 0 | 1 |
|---|---|---|
| 0 | $p_1$ | $p_2$ |
| 1 | $p_3$ | $p_4$ |

$$p_i \geq 0, p_1 + p_2 + p_3 + p_4 = 1$$

$$\begin{bmatrix} f_{x,y}(0,0) & f_{x,y}(1,0) \\ f_{x,y}(0,1) & f_{x,y}(1,1) \end{bmatrix} = \begin{bmatrix} p_1 & p_2 \\ p_3 & p_4 \end{bmatrix}$$

$$\begin{bmatrix} f_{x,y}(0,0) & f_{x,y}(1,0) \\ f_{x,y}(0,1) & f_{x,y}(1,1) \end{bmatrix} = \begin{bmatrix} p_1 & p_2 \\ p_3 & p_4 \end{bmatrix}$$

$$f_x = [f_x(0) \quad f_x(1)] = [p_1 + p_3 \quad p_2 + p_4]$$

marginal distribution

from the usual formula for conditional probabilities

$$f_{y|x}(y|x) = \frac{f(x,y)}{f_x(x)}$$

$$A_{y|x} = \begin{bmatrix} \frac{p_1}{p_1 + p_3} & \frac{p_3}{p_1 + p_3} \\ \frac{p_2}{p_2 + p_4} & \frac{p_4}{p_2 + p_4} \end{bmatrix}$$

$$A_{x|y} = \begin{bmatrix} \frac{p_1}{p_1 + p_2} & \frac{p_2}{p_1 + p_2} \\ \frac{p_3}{p_3 + p_4} & \frac{p_4}{p_3 + p_4} \end{bmatrix}$$

transition probabilities

Since we are only interested in the X sequence

$$P(X_1' = x_1 \mid X_0' = x_0) = \sum_y P(X_1' = x_1 \mid Y_1' = y) \times P(Y_1' = y \mid X_0' = x_0).$$

the transition matrix for the X sequence is

$$A_{x|x} = A_{y|x} A_{x|y}$$

This defines the transition probabilities for a single Markov chain in X-space and from the theory of Markov chains we know that iterating this produces a fixed probability distribution, i.e., our marginal distribution for X.

## What about the continuous case? Consider the bivariate case

Suppose that, for two random variables $X$ and $Y$, we know the conditional densities $f_{X|Y}(x \mid y)$ and $f_{Y|X}(y \mid x)$. We can determine the marginal density of $X$, $f_X(x)$, and hence the joint density of $X$ and $Y$, through the following argument. By definition,

$$f_X(x) = \int f_{XY}(x, y)\, dy,$$

where $f_{XY}(x, y)$ is the (unknown) joint density. Now using the fact that $f_{XY}(x, y) = f_{X|Y}(x \mid y) f_Y(y)$, we have

$$f_X(x) = \int f_{X|Y}(x \mid y) f_Y(y)\, dy,$$

and if we similarly substitute for $f_Y(y)$, we have

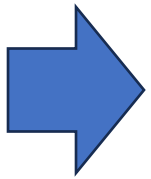
$$\begin{aligned} f_X(x) &= \int f_{X|Y}(x \mid y) \int f_{Y|X}(y \mid t) f_X(t)\, dt\, dy \\ &= \int \left[ \int f_{X|Y}(x \mid y) f_{Y|X}(y \mid t)\, dy \right] f_X(t)\, dt \\ &= \int h(x, t) f_X(t)\, dt, \end{aligned}$$

where $h(x, t) = [\int f_{X|Y}(x \mid y) f_{Y|X}(y \mid t)\, dy]$.

this is a continuous transition kernel

Let's consider the integral equation, how would it look like in a discrete setting? (in a computer, for instance)

$$
\begin{aligned}
f_X(x) &= \int f_{X|Y}(x \mid y) \int f_{Y|X}(y \mid t) f_X(t)\, dt\, dy \\
&= \int \left[ \int f_{X|Y}(x \mid y) f_{Y|X}(y \mid t)\, dy \right] f_X(t)\, dt \\
&= \int h(x, t) f_X(t)\, dt,
\end{aligned}
$$



$$[f_X]_i = \sum_j [h]_{ij} [f_X]_j = \sum_j [f_X]_j [h^T]_{ji}$$

or also in vector-matrix notation

$$\mathbf{f}_X = \mathbf{f}_X \mathbf{h}^T$$

**this corresponds to recasting the continuous problem to a discrete problem and we obtain again the eigenvalue problem that must be solved to find the asymptotic distribution in Markov processes.**

# Question: how do we determine the number of steps needed to reach the stationary state?

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Consider the diagonalized representation of the N-step transition kernel (eigenvalues on the diagonal), such that all N-step transition probabilities are positive in the non-diagonalized version of the kernel (all states can be reached)

$$P^N = \begin{pmatrix} 1 & 0 & 0 & \dots \\ 0 & \lambda_2 & 0 & \dots \\ 0 & 0 & \lambda_3 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \qquad (1 > \lambda_2 > \lambda_3 > \dots > 0)$$

and the corresponding representation of the initial state vector in terms of eigenvectors

$$\boldsymbol{\pi} = \alpha^* \boldsymbol{\pi}^* + \alpha_2 \boldsymbol{\pi}_2 + \alpha_3 \boldsymbol{\pi}_3 + \dots$$

Then, we see that the repeated action of the N-step transition kernel preserves the stationary state, while it gradually reduces the amplitude of the other states by a factor

$$\lambda_k^{nN}$$

after $nN$ steps.

# Question: how do we determine the number of steps needed to reach the stationary state?

In the case of the Land of Oz wheather model, we find the following diagonalized 2-step transition kernel

$$\mathbf{P}^2 = \begin{pmatrix} 0.25 & 0.375 & 0.375 \\ 0.25 & 0.5 & 0.5 \\ 0.125 & 0.3125 & 0.3125 \end{pmatrix} \Rightarrow \begin{pmatrix} 1. & 0. & 0. \\ 0. & 0.0625 & 0. \\ 0. & 0. & -4.44 \times 10^{-18} \end{pmatrix}$$

# The impact of sampling.

Consider the following expectation value

$$E_y[f(x|y)] = \int_Y f(x|y)f(y)dy = \int_Y f(x,y)dy = f(x)$$

we can estimate *f*(*x*) with the sum

$$\hat{f}(x) = \frac{1}{m}\sum_{i=1}^{m} f(x|y_i)$$

where the y's are generated according to their marginal distribution; we conclude that the Gibbs sampling provides representative samples that correspond to the marginal distribution of the x's. (for a mathematically accurate proof, check the paper by Casella&George)

## *8. Another view of Gibbs sampling*

Consider again the sequence that generates a "Gibbs sequence" of random variables

$$Y'_0, X'_0, Y'_1, X'_1, Y'_2, X'_2, \ldots, Y'_k, X'_k$$

where one initial value is specified and the others are computed with the rule

$$X'_j \sim f(x|Y'_j = y'_j)$$
$$Y'_{j+1} \sim f(y|X'_j = x'_j)$$

# Example: bivariate Gaussian distribution

- Bivariate Gaussian likelihood

$$p(y_1, y_2|\theta_1, \theta_2) = \frac{1}{2\pi\sqrt{|\det V|}} \exp\left[-\frac{1}{2}(\mathbf{y}-\boldsymbol{\theta})^T V^{-1}(\mathbf{y}-\boldsymbol{\theta})\right]$$

where the known covariance matrix is

$$V = \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}$$

- Posterior pdf from Bayes theorem with improper priors, with a single datapoint ($y_1$,$y_2$)

$$p(\theta_1, \theta_2|y_1, y_2) \propto p(y_1, y_2|\theta_1, \theta_2)$$

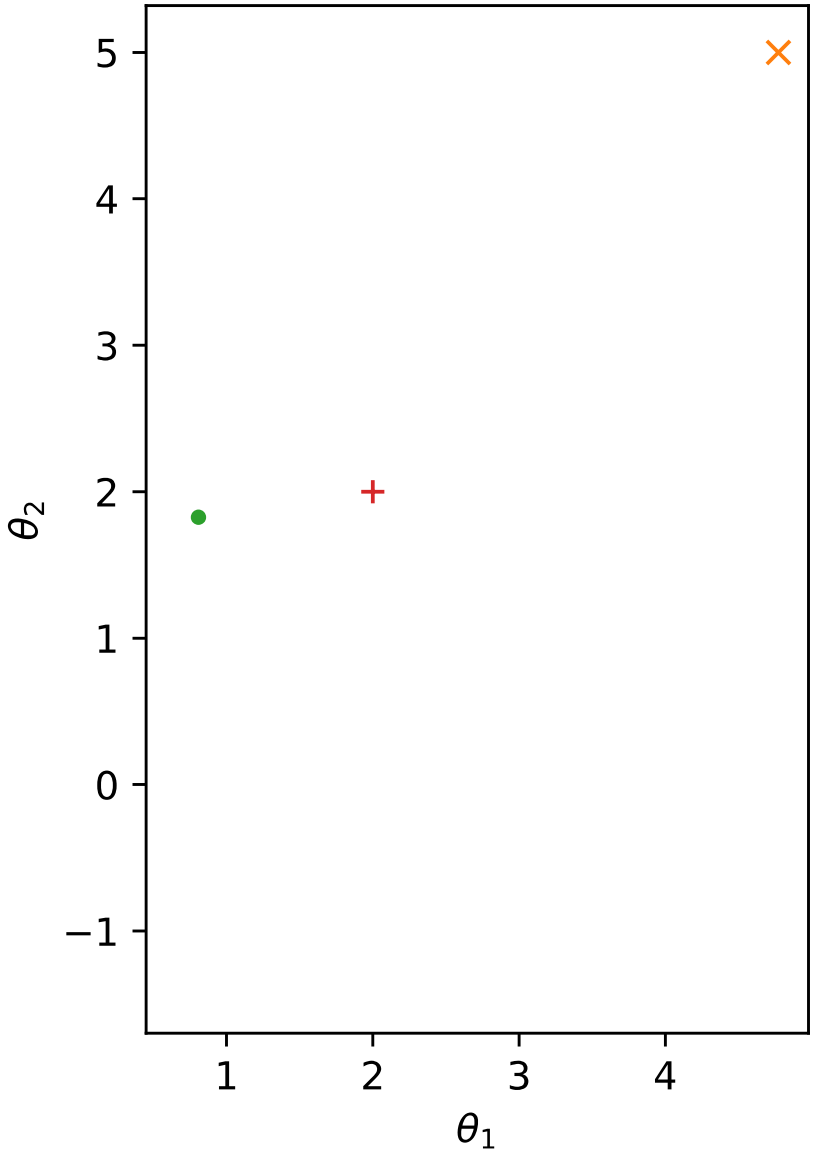
- Expanding, we find

$$p(\theta_1, \theta_2 | y_1, y_2) \sim \exp\left\{ -\frac{1}{2(1-\rho^2)} \left[ (\theta_1 - y_1)^2 - 2\rho(\theta_1 - y_1)(\theta_2 - y_2) + (\theta_2 - y_2)^2 \right] \right\}$$

- Then, from the Gaussian structure of the posterior, we find the marginals

$$p(\theta_1 | \theta_2, y_1, y_2) \sim \exp\left[ -\frac{1}{2(1-\rho^2)} \left( \theta_1 - (y_1 + \rho(\theta_2 - y_2)) \right)^2 \right]$$

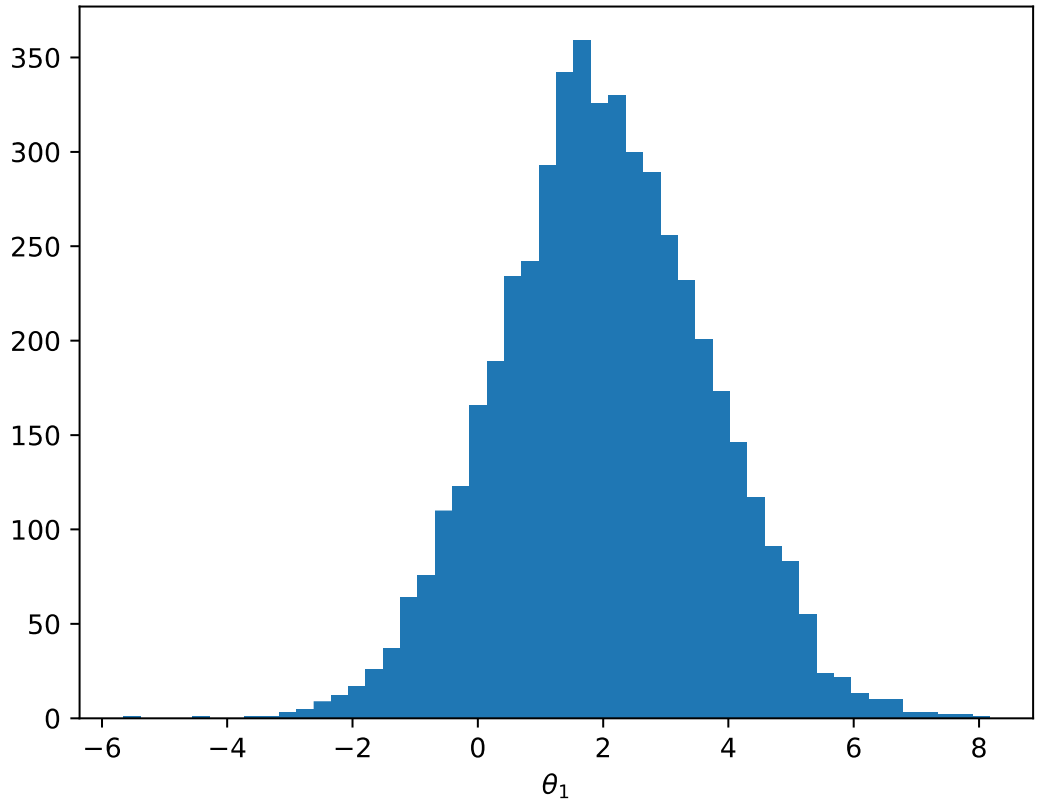
$$p(\theta_2 | \theta_1, y_1, y_2) \sim \exp\left[ -\frac{1}{2(1-\rho^2)} \left( \theta_2 - (y_2 + \rho(\theta_1 - y_1)) \right)^2 \right]$$

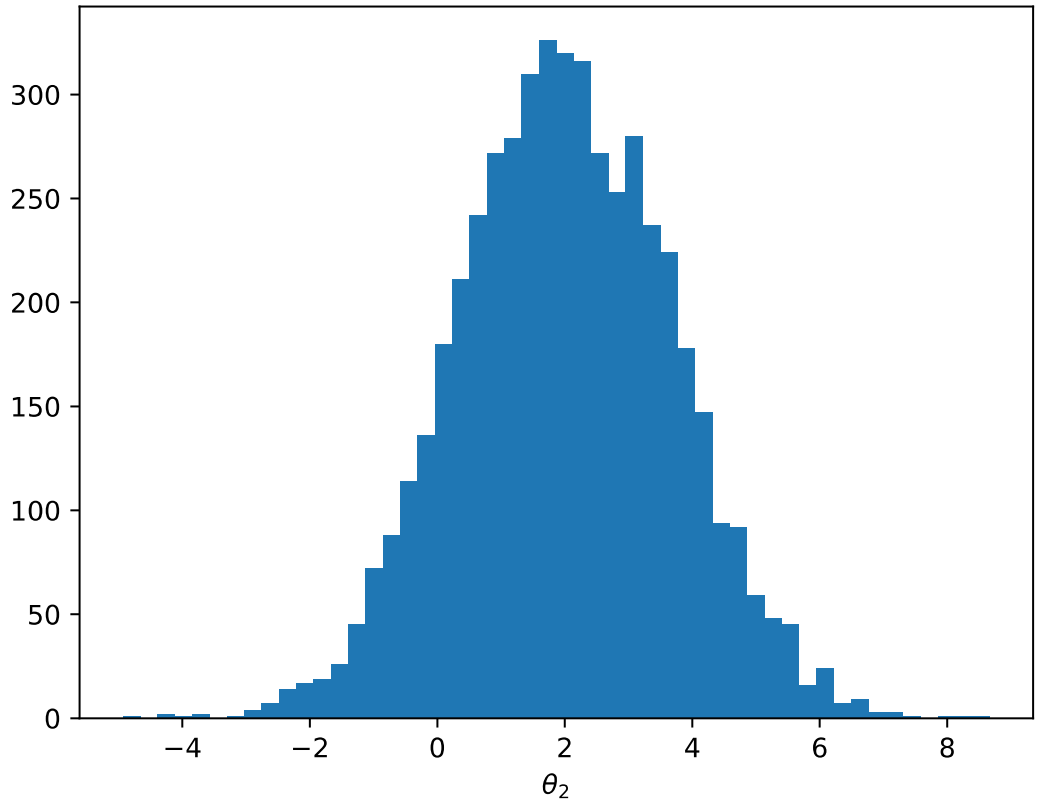



20 initial steps in a Gibbs sampler run:

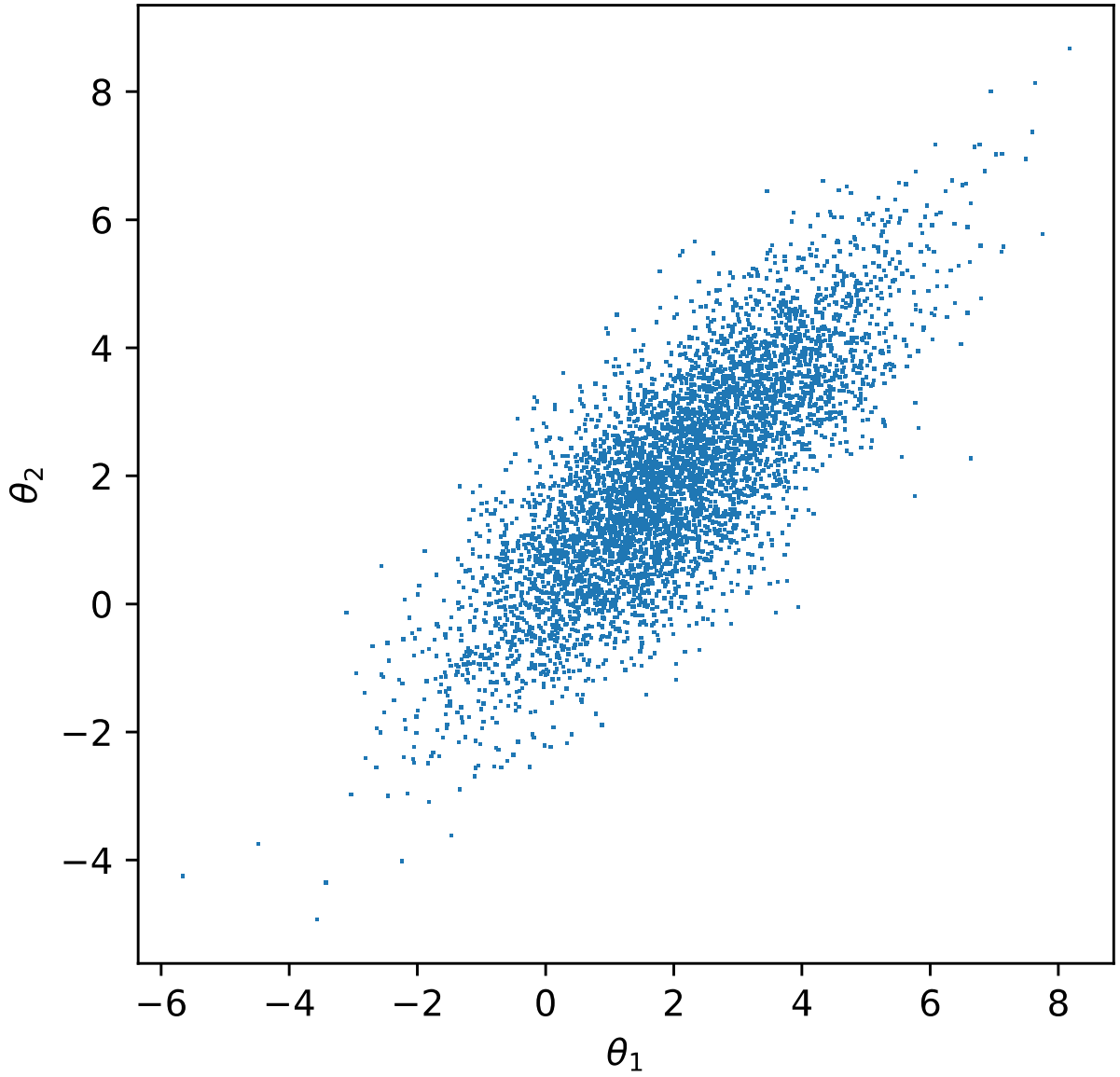
- orange cross: starting pair
- green dot: position after 20 steps
- red cross: bivariate mean

marginal distributions (second half of the simulation values in a run with 10000 generated pairs)



posterior distribution (second half of the simulation values in a run with 10000 generated pairs)




**Exercise**:

extend this treatment to more than one pair of measured $y$ values and write a computer program to implement it

# So, what's the use of all this?

Consider the case where we want to compute the marginal pdf

$$f(x) = \int \dots \int f(x, y_1, \dots, y_p)\, dy_1 \dots dy_p$$

in a situation where the multidimensional integral can be hard to compute.

**The Gibbs sampler completely bypasses the calculation of the multidimensional integral and affords an easy path to marginalization.**

Indeed, the procedure can be easily extended to multidimensional distributions, for example with two nuisance variables we produce the sequence

$$Y'_0, Z'_0, X'_0, Y'_1, Z'_1, X'_1, Y'_2, Z'_2, X'_2, \dots$$

by means of the conditional PDFs

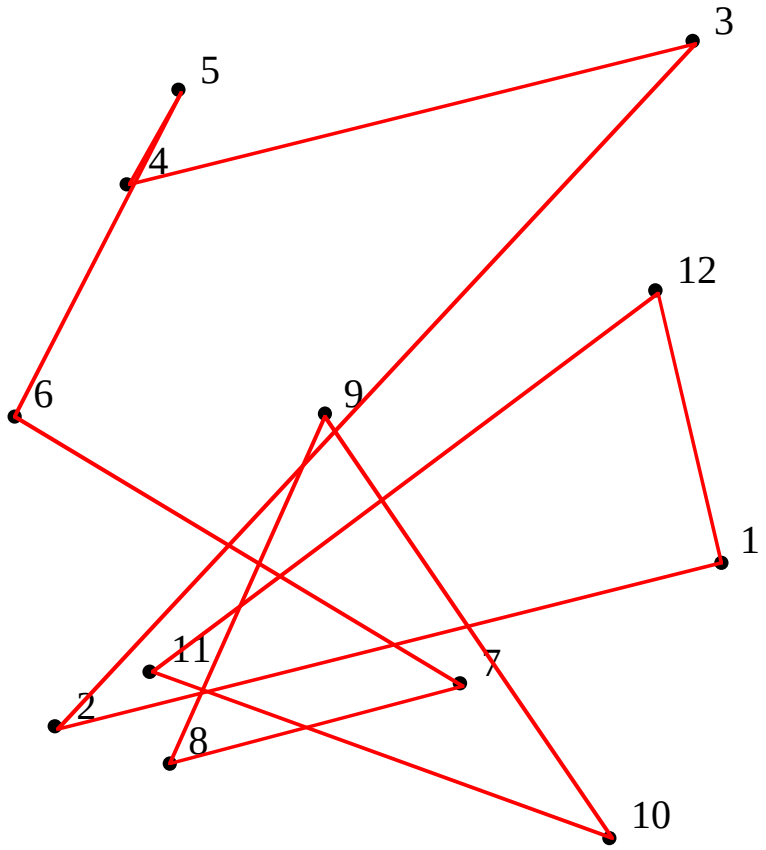
# *9. The Traveling Salesman Problem and Simulated Annealing*

To introduce the method, we consider the *Traveling Salesman Problem* (TSP), where we want to find the shortest closed path that connects N cities.

The problem was first stated by the Viennese mathematician Karl Menger in 1930 and is one of the most studied problems in combinatorial optimization.

For many up-to-date links, see
http://www.math.uwaterloo.ca/tsp/index.html

See also the history page
http://www.math.uwaterloo.ca/tsp/history/index.html




12 “cities” randomly distributed in the (0,1) square: the path corresponds to a random permutation of the sequence of cities.

(path length L=1.93834)

Paths are enumerated by permutations of “city names”, e.g., {9, 2, 7, 8, 1, 12, 4, 5, 3, 10, 11, 6} (start at 9, step to 2, and so on until you reach 6 and then return to 9).

The total number of configurations (undirected paths) is

$$\frac{1}{2}(n-1)!$$

The problem belongs to the class of NP-complete problems (Non-Polynomial complexity, a class of particularly hard problems)

*In such cases there is only one known exact solution: the full enumeration of all paths.*

13 May 1983, Volume 220, Number 4598

SCIENCE

# Optimization by Simulated Annealing

S. Kirkpatrick, C. D. Gelatt, Jr., M. P. Vecchi

*Summary.* There is a deep and useful connection between statistical mechanics (the behavior of systems with many degrees of freedom in thermal equilibrium at a finite temperature) and multivariate or combinatorial optimization (finding the minimum of a given function depending on many parameters). A detailed analogy with annealing in solids provides a framework for optimization of the properties of very large and complex systems. This connection to statistical mechanics exposes new information and provides an unfamiliar perspective on traditional optimization problems and methods.

*Approximate solution of the TSP with the Simulated Annealing algorithm*

**path length** → **energy of the system**

exploration of the configuration space with the *Metropolis algorithm* (51909 citations to date, April 10, 2024)
(Metropolis, Rosenbluth Rosenbluth ,Teller and Teller, 1953)

THE JOURNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUNE, 1953

## Equation of State Calculations by Fast Computing Machines

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
*Los Alamos Scientific Laboratory, Los Alamos, New Mexico*

AND

EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*

(Received March 6, 1953)

A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

# *10. The Metropolis algorithm and its application to the TSP*

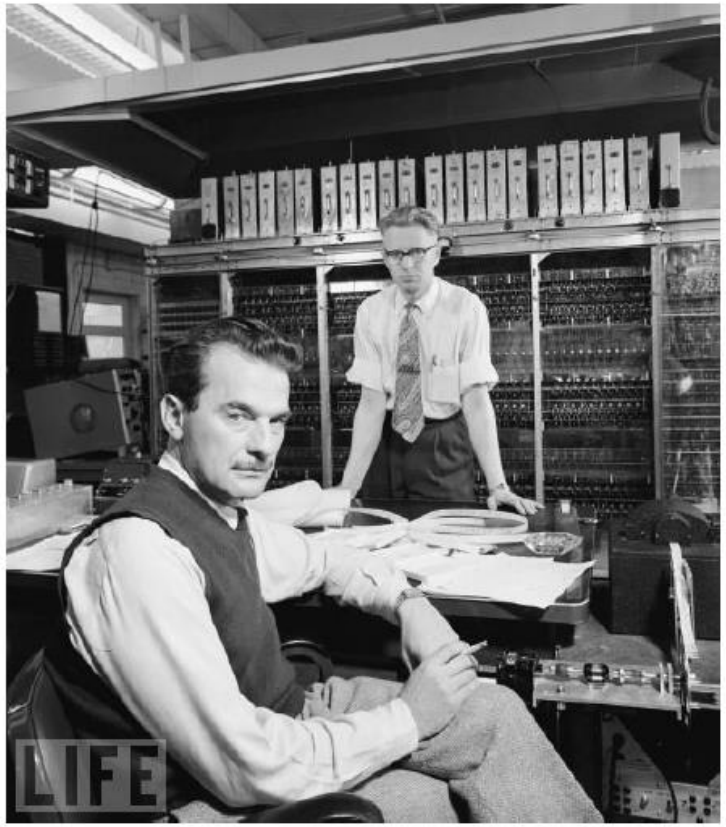


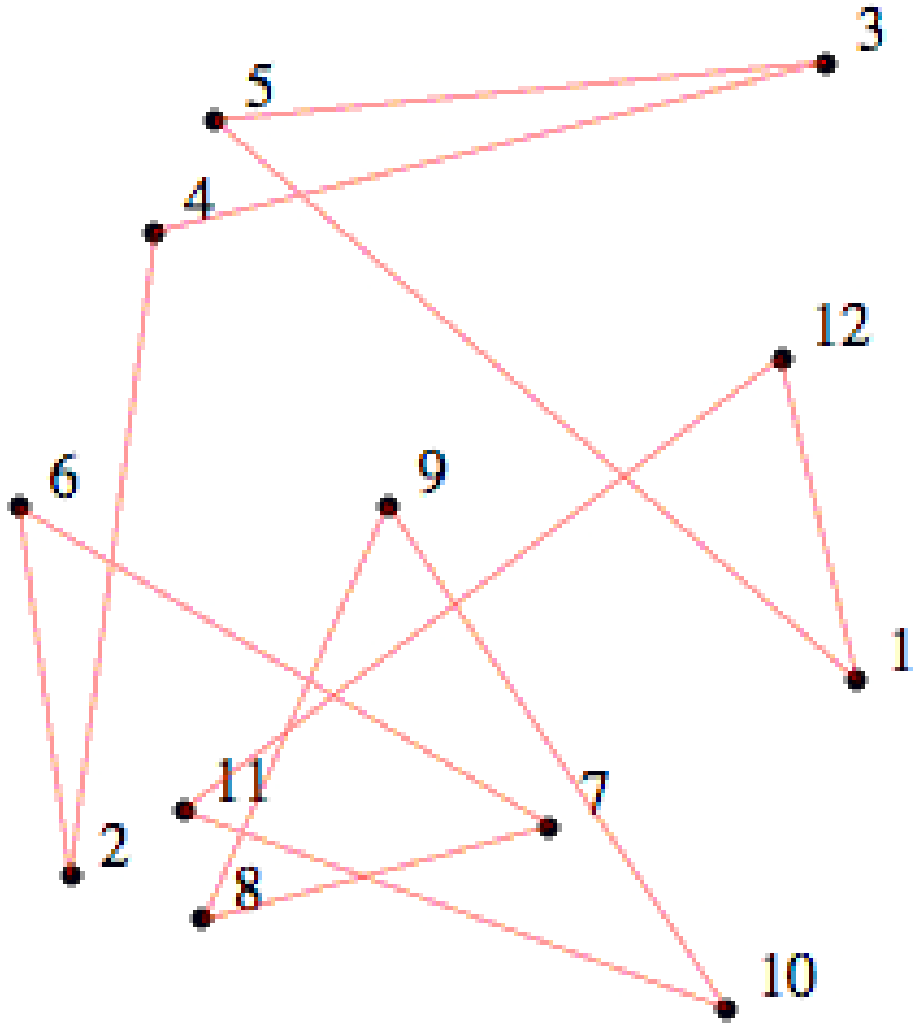

Figure 8.14: Portrait of American computer scientists Nicholas Metropolis (1915 - 1999) (seated) and James Henry Richardson (1918 - 1996) at Los Alamos National Laboratory, Los Alamos, New Mexico, November 1953 (from `http://www.life.com`).

1. We generate a new configuration $C'$ from the present configuration $C$
2. We compute the energy of the new configuration, $E'$
3. We compute the energy difference $\Delta E = E' - E$
4. The new configuration is accepted with probability $p$

$$\begin{cases} p = 1 & \Delta E < 0 \\ p = \exp\left(-\frac{\Delta E}{kT}\right) & \Delta E \geq 0 \end{cases}$$

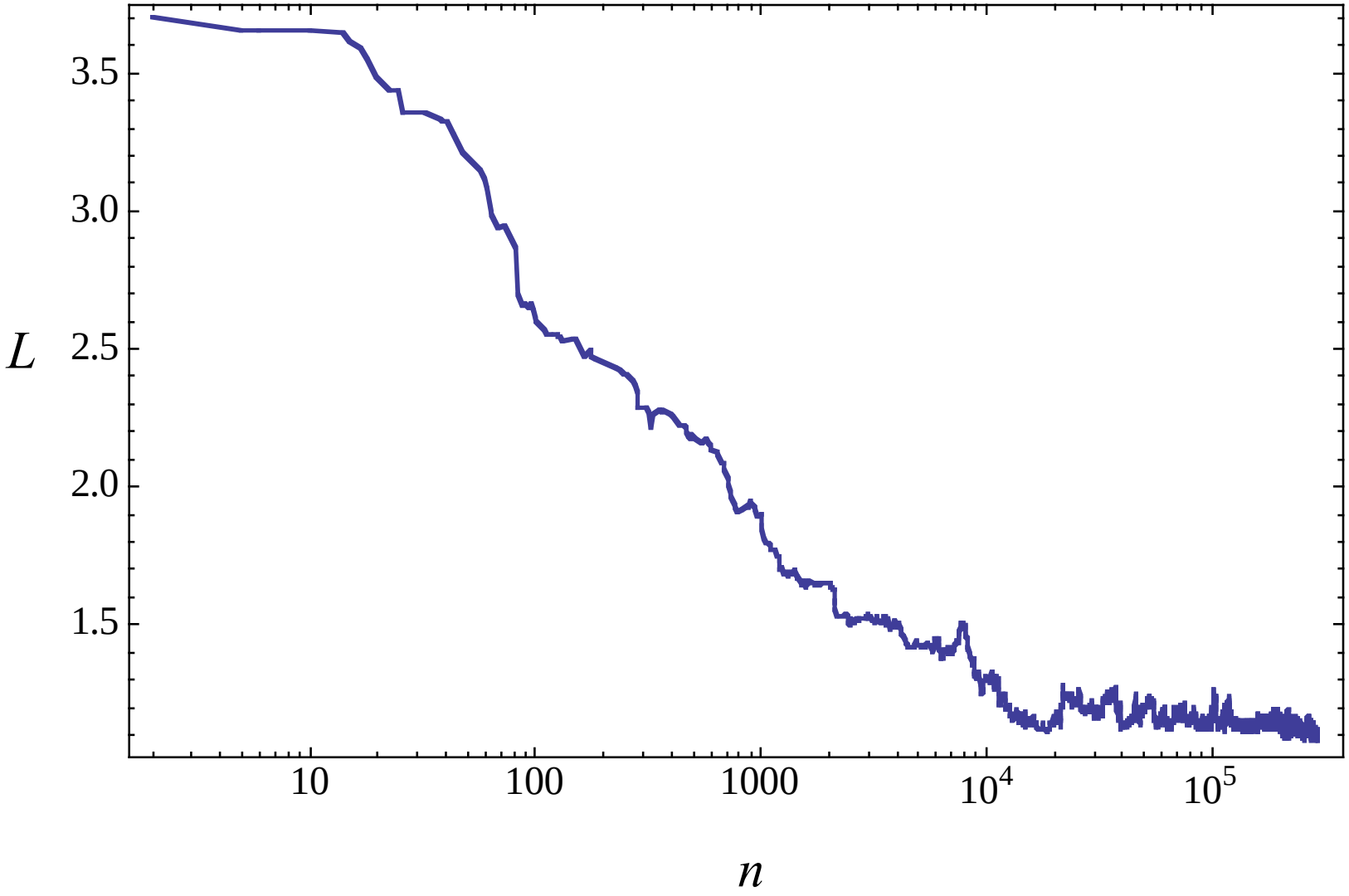
Additional details

- the algorithm needs a slow cooling (it is common to choose an exponential cooling schedule)
- if cooling is not gradual, the system can get stuck into a local minimum
- simple exchanges of pairs of cities are the individual moves in the SA solution of the TSP
- the individual steps from one configuration to the next can be described by a Markov chain




k = 1
T = 0.05
L = 1.84655

Decrease of total path length in a realization of the SA solution of a 50-cities problem



Here we note that the transition probability can be written as follows

$$T(C \to C') = \min\left[1, \exp\left(-\frac{(E' - E)}{kT}\right)\right]$$

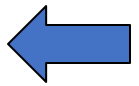
Moreover, it is easy to show that the algorithm preserves detailed balance

$$T(C \to C')P(C) = T(C' \to C)P(C')$$

where P(C) is the stationary probability of configuration C. Indeed, at equilibrium we find that, if E' > E,

$$P(C)\exp\left(-\frac{(E' - E)}{kT}\right) = P(C')$$

$$\frac{P(C')}{P(C)} = \exp\left(-\frac{(E' - E)}{kT}\right)$$



Boltzmann's distribution is the equilibrium distribution

# *11. Image restoration and Markov Random Fields (MRF)*

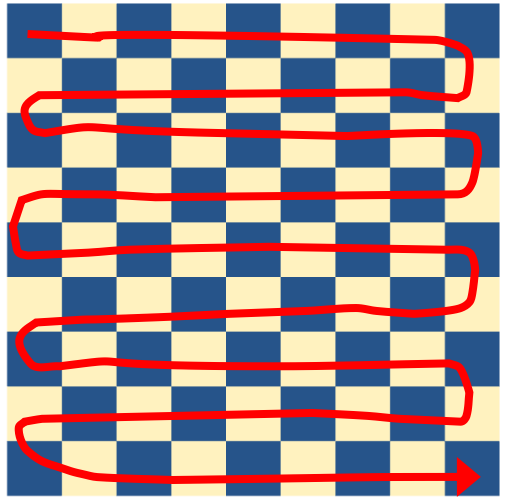
The optimization problem.

When dealing with signals, we usually assume that data are corrupted by noise

$$d = x + w$$

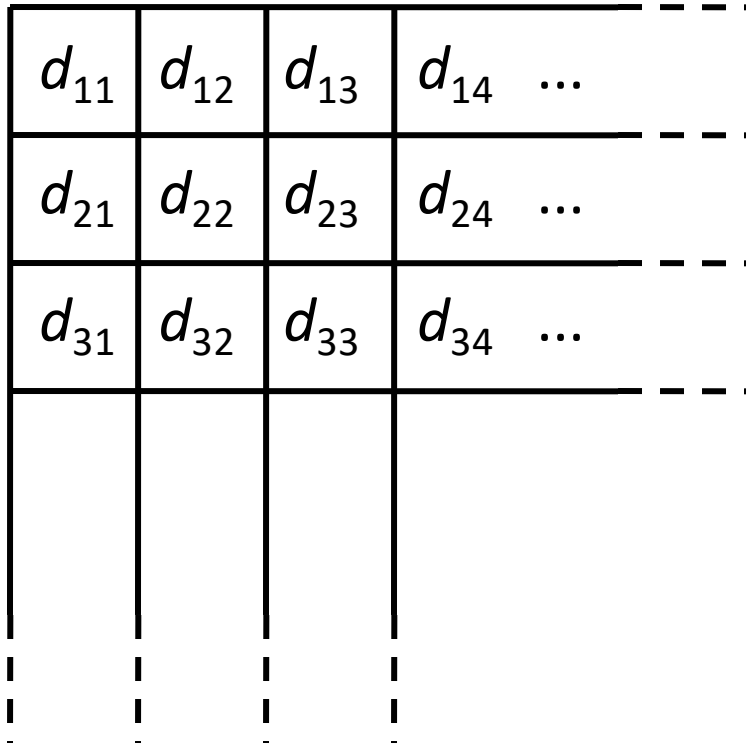
data vector — signal vector — (vector) noise process

An image can be viewed as a vector, for instance unfolding the sequence of pixels as shown on the right, we obtain the equivalent of a long signal vector.



If there are $n$ pixels on each side, there are in all $n^2$ pixels, and if there are L gray levels, then the number of possible configurations that define an image is

$$N = L^{n^2}$$




pixel map

true pixel vector

$\mathbf{x}$

*posterior* pixel distribution

*likelihood*

*prior* pixel distribution

$$P(\mathbf{x}|\mathbf{d}) = \frac{P(\mathbf{d}|\mathbf{x})}{P(\mathbf{d})} P(\mathbf{x}) \propto P(\mathbf{d}|\mathbf{x}) P(\mathbf{d})$$

Bayesian estimate of true pixel vector from observed pixel vector

Given the number of possible configurations

$$N = L^{n^2}$$

we see that even for small image sizes, say $n = 100$, with binary levels, $L = 2$, we find

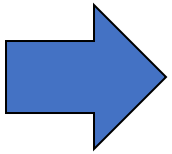
$$N = 2^{10^4}$$

therefore, the problem of finding the MAP estimate in a Bayesian context is a hard computational task.

The MAP estimate depends on the prior distribution

Possible priors:

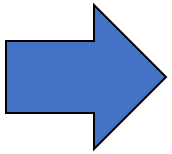
$P(\mathbf{x})$ flat prior



Maximum Likelihood Estimate (MLE)

$$P(\mathbf{x}|\mathbf{d}) \propto P(\mathbf{d}|\mathbf{x})P(\mathbf{d}) \propto P(\mathbf{d}|\mathbf{x})$$

$P(\mathbf{x})$ entropic prior



Maximum Entropy Method (MEM)

Notice also that

$$\ln P(\mathbf{x}|\mathbf{d}) \approx \ln P(\mathbf{d}|\mathbf{x}) - [-\ln P(\mathbf{d})]$$

therefore, the MAP estimate is equivalent to maximizing the likelihood with a *penalty function*

$$-\ln P(\mathbf{d})$$

Experiments have been tried with many different penalties, many of them barely justified on probabilistic grounds (or not at all!)

Now, let $\boldsymbol{x}$ be the vector of "true values" (uncorrupted intensities of an image, a spectrum, etc. ...), and translate these values into counts

$$n_i = \lfloor \alpha d_i \rfloor$$

($i$ = 1, ..., $M$). The least informative prior corresponds to a structureless image, and pixelwise it is once again the uniform prior. Then, the probability of one count at the $i$-th position is just $1/M$.

Likewise, the probability of a given vector of values where the total number of counts is $N$, is given by the multinomial probability

$$P(\mathbf{n}) = \frac{N!}{n_1! n_2! \ldots n_M!} \left(\frac{1}{M}\right)^N ; \quad \sum_k n_k = N$$

Using Stirling's approximation

$$n! \approx n^n e^{-n}; \quad \ln n! \approx n \ln n - n$$

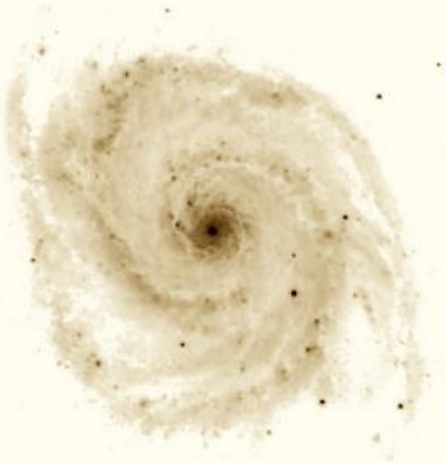
we find, with the definition $p_i = \dfrac{d_i}{\sum_{k=1}^{M} d_k}$

$$\begin{aligned}
\ln P(\mathbf{n}) &\approx (N \ln N - N) - \sum_k (n_k \ln n_k - n_k) \\
&= N \ln N - \sum_k n_k \ln n_k \\
&\approx -\alpha \sum_k d_k \ln d_k + \text{const.}
\end{aligned}$$

*entropic prior*

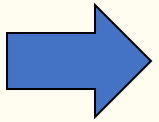
$$P(\mathbf{n}) \sim \exp\left(-\alpha \sum_k d_k \ln d_k\right) \sim \exp\left(-\alpha' \sum_k p_k \ln p_k\right) = \exp\left[\alpha' S(\mathbf{d})\right]$$

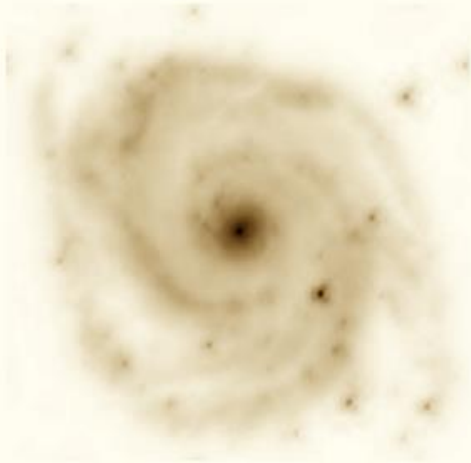
# Image likelihood: 1. the observation model



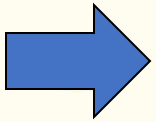
true image
of a galaxy

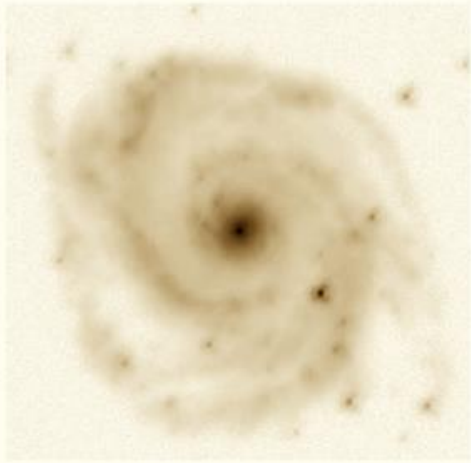
PSF
(Point Spread
Function





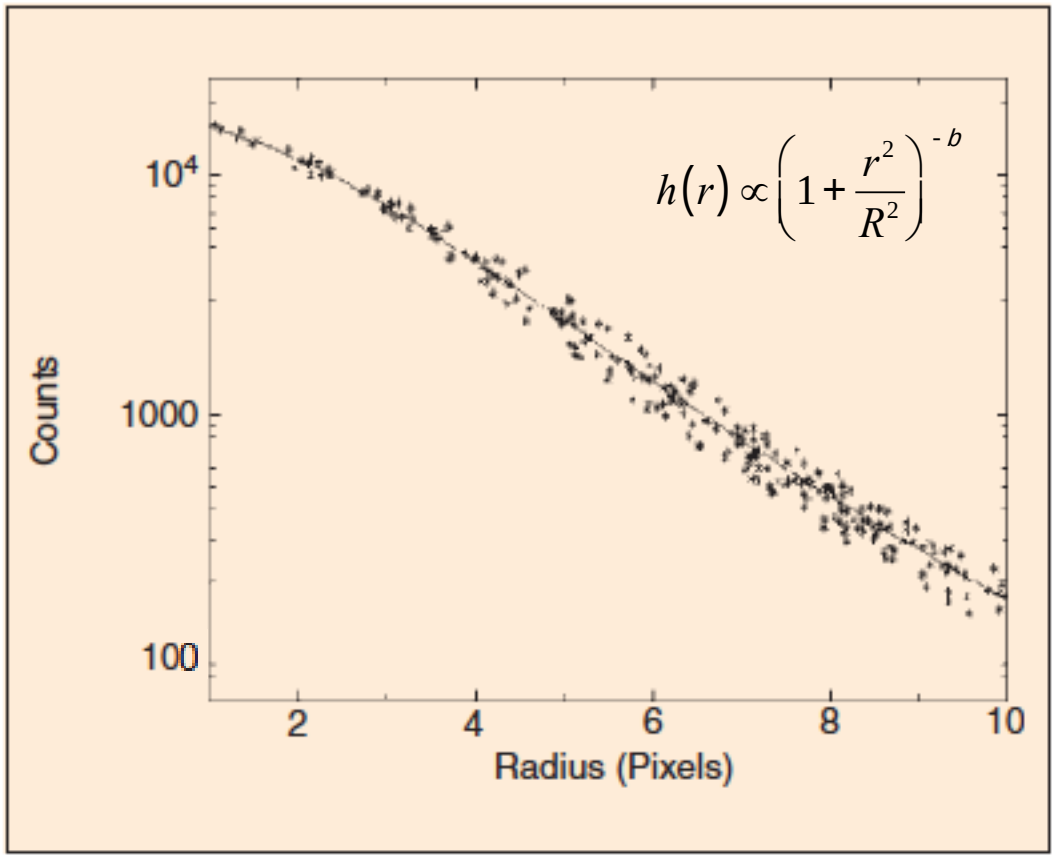
Noise





(example from Eric Thiebaut)

“dirty image”




PSF from atmospheric turbulence

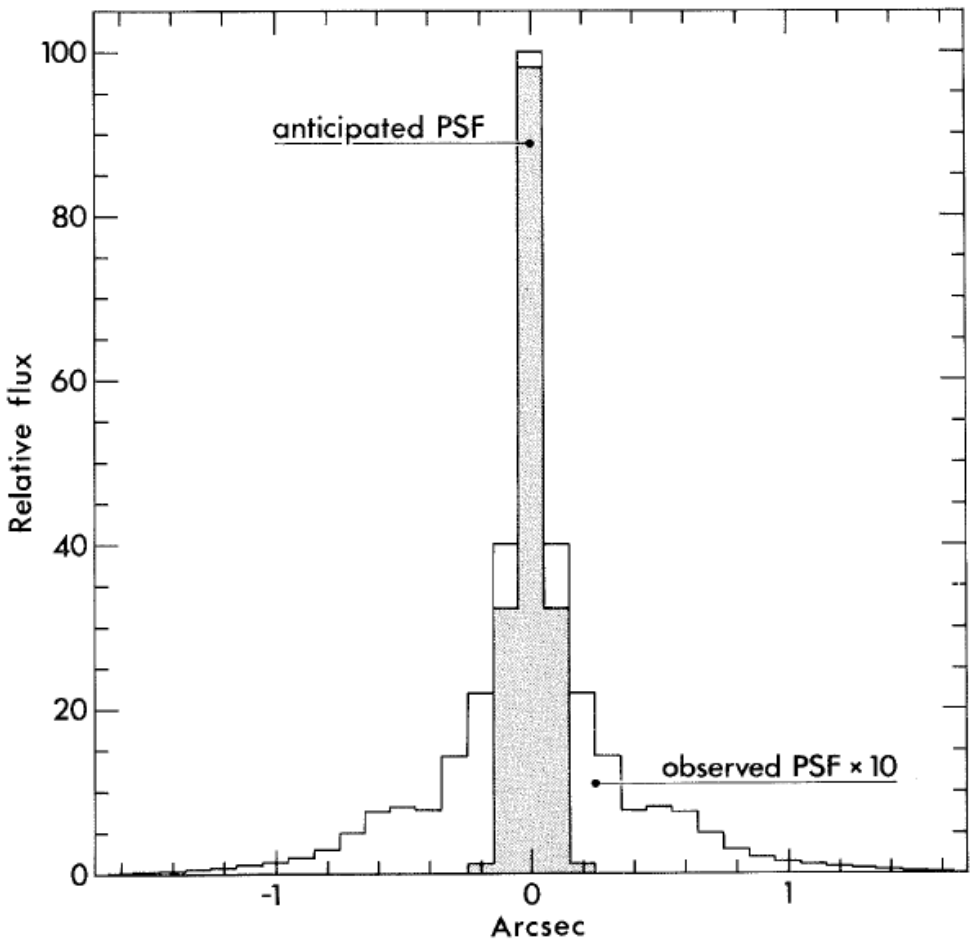
In general, the effect of the PSF is modeled by a linear operator

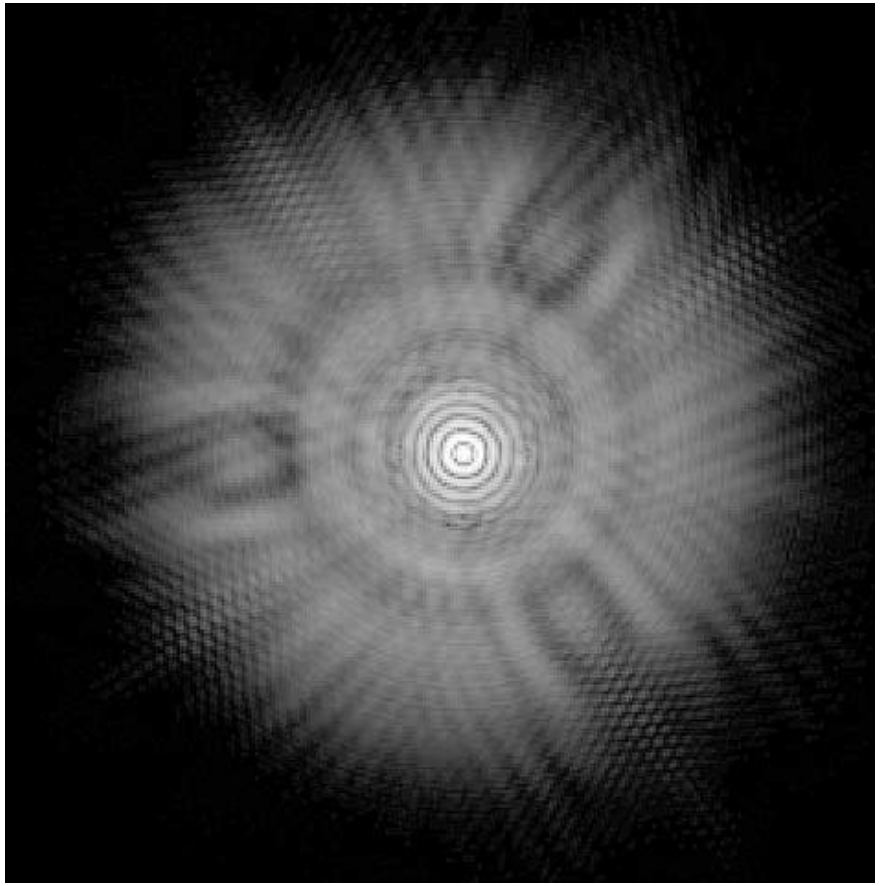
$$\mathbf{x} \rightarrow \mathbf{Hx}$$

"true" pixel vector

the action of the optical system on the "true image" is modeled by the matrix **H**

# The Hubble PSF before the first servicing mission



# Image likelihood: 2. the noise model (degradation model)

Gaussian noise model

$$P(\mathbf{x}|\mathbf{d}) \propto \exp\left[-\frac{(\mathbf{x}-\mathbf{Hd})^2}{2\sigma^2}\right]$$

Poisson noise model

$$P(\mathbf{x}|\mathbf{d}) \propto \prod_n \frac{(\mathbf{Hd})_n^{d_n}}{d_n!} \exp\left[-(\mathbf{Hd})_n\right]$$

Poisson noise mostly from detection process, Gaussian noise mostly from electronics or from approximation of Poisson noise. Sometimes we can use the Gaussian approximation of Poisson noise

$$P(\mathbf{d}|\mathbf{x}) \propto \prod_n \frac{(\mathbf{Hx})_n^{d_n}}{d_n!} \exp\left[-(\mathbf{Hx})_n\right] \approx \prod_n \exp\left[-\frac{(d_n-(\mathbf{Hx})_n)^2}{2(\mathbf{Hx})_n}\right] = \exp\left[-\sum_n \frac{(d_n-(\mathbf{Hx})_n)^2}{2(\mathbf{Hx})_n}\right]$$

# Stochastic Relaxation, Gibbs Distributions, and the Bayesian Restoration of Images

STUART GEMAN AND DONALD GEMAN

*Abstract*—We make an analogy between images and statistical mechanics systems. Pixel gray levels and the presence and orientation of edges are viewed as states of atoms or molecules in a lattice-like physical system. The assignment of an energy function in the physical system determines its Gibbs distribution. Because of the Gibbs distribution, Markov random field (MRF) equivalence, this assignment also determines an MRF image model. The energy function is a more convenient and natural mechanism for embodying picture attributes than are the local characteristics of the MRF. For a range of degradation mechanisms, including blurring, nonlinear deformations, and multiplicative or additive noise, the posterior distribution is an MRF with a structure akin to the image model. By the analogy, the posterior distribution defines another (imaginary) physical system. Gradual temperature reduction in the physical system isolates low energy states ("annealing"), or what is the same thing, the most probable states under the Gibbs distribution. The analogous operation under the posterior distribution yields the maximum *a posteriori* (MAP) estimate of the image given the degraded observations. The result is a highly parallel "relaxation" algorithm for MAP estimation. We establish convergence properties of the algorithm and we experiment with some simple pictures, for which good restorations are obtained at low signal-to-noise ratios.

# The Ising model as an example of Markov Random Field

The model describes a system of spins that point only in the +*z* or -*z* direction, so that their value can only be ±1.

The Hamiltonian includes only the interaction with the external magnetic field and the interaction between neighboring spins

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - B \sum_i \sigma_i$$

The corresponding lattice magnetization is

$$M = \langle \sigma_i \rangle$$

a quantity that ranges between -1 and +1

# The Bragg-Williams approximation

This is a simple mean–field approximation

$$\langle \sigma_i \sigma_j \rangle \approx \langle \sigma_i \rangle \langle \sigma_j \rangle$$

correlations are ignored

so that the Hamiltonian can be restated in terms of an effective magnetic field

$$H \approx -J \sum_i \sigma_i \sum_{\langle j \rangle_i} \sigma_j - B \sum_i \sigma_i \approx (-Jz\langle \sigma_i \rangle - B) \sum_i \sigma_i = -B_{\text{eff}} \sum_i \sigma_i$$

Then, the partition function is

$$Z = \sum_{\text{configurations}} \exp\left( \frac{B_{\text{eff}} \sum_i \sigma_i}{kT} \right) = \prod_i \left( e^{B_{\text{eff}}/kT} + e^{-B_{\text{eff}}/kT} \right)$$

$$= \left[ 2 \cosh\left( B_{\text{eff}}/kT \right) \right]^N = \left[ 2 \cosh\left( \beta B_{\text{eff}} \right) \right]^N$$

Therefore, the magnetization can be obtained as follows

$$M = \frac{1}{NZ} \sum_{\text{configurations}} \sigma_i e^{\beta B_{\text{eff}} \sigma_i} = \frac{1}{NZ} kT \frac{\partial}{\partial B_{\text{eff}}} \sum_{\text{configurations}} e^{\beta B_{\text{eff}} \sigma_i}$$

$$= kT \frac{\partial}{\partial B_{\text{eff}}} \ln Z = \tanh\left(\beta B_{\text{eff}}\right)$$

$$= \tanh\left[\beta\left(B + JzM\right)\right]$$

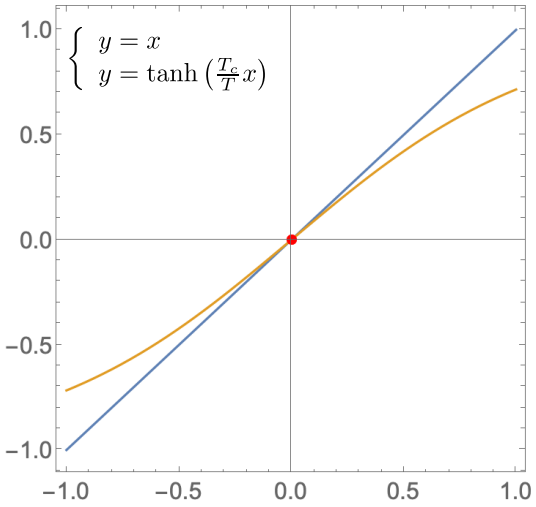
i.e., the magnetization is the solution of the nonlinear equation

with B field

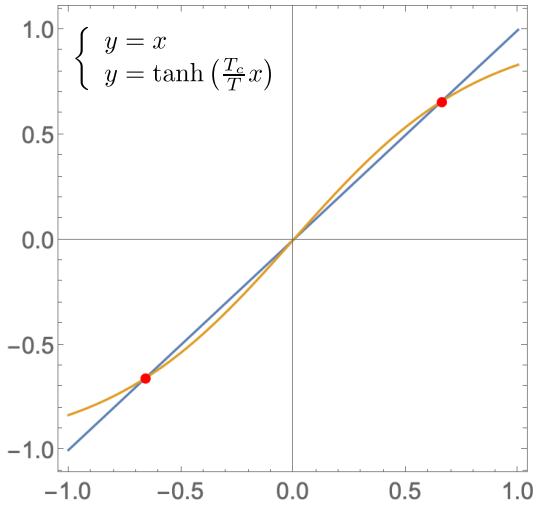
$$M = \tanh\left[\beta\left(B + JzM\right)\right]$$

no B field

$$M = \tanh\left(\beta z J M\right)$$




above critical temperature




below critical temperature

$$M = \tanh\left(\beta z J M\right)$$

Critical temperature $$T_c = \frac{zJ}{k}$$