M. Juvela Observatory, University of Helsinki

Inverse problems in the analysis of astronomical images

Inversion methods in astronomy Helsinki University Observatory 28.2.2008

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 - Iinear methods, Bayesian framework
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- present in all observations
 - finite time resolution \rightarrow convolution of time
 - detector response, temporal sampling
 - finite spectral resolution → convolution of frequencies
 - detector bandpass, channel resolution
 - point spread function → convolution of spatial coordinates
 - telescope beam, seeing, detector geometry

• in 1D:
$$(f*g)(h) = \int_{-\infty}^{+\infty} f(x)g(h-x)dx$$

convolution of source intensity *I(f)* with the detector response curve *R(f)*

$$I_{obs}(f) = (I_{true} * R_{det})(f) = \int_{0}^{+\infty} I_{true}(f') R_{det}(f-f') df'$$

- observed intensity distribution on the sky

$$I_{obs}(\theta_{0},\phi_{0}) = \int_{0}^{2\pi} d\phi \int_{0}^{\pi} d\theta \ I_{true}(\theta,\phi) \ B(\theta_{0}-\theta,\phi_{0}-\phi)$$

 convolution can be calculated easily with Fourier transforms: convolution theorem

$$F(I_{obs}) = F(I_{true} * B) = F(I_{true}) F(B)$$

... but if the filter function *B* is known, the original signal can be recovered directly

$$I_{true} = F^{-1} \left(F(I_{obs}) / F(B) \right) \qquad \square$$

(this is the least squares solution)

De-convolution

- How would this work in practice
 - Example 1: deconvolution of a 1 D signal
 - Example 2: deconvolution of a 2D map

- the noise should be part of the model $F(I_{obs}(x, y)) = F(I_{true}) F(B) + F(n(x, y))$
 - least squares should be fine for gaussian noise

De-convolution

• conclusion:

- de-convolution is trivial in the sense of getting a function whose convolution is equal to the observation
- result is extremely sensitive to the noise (and the knowledge of the convolving function)
 - solution also tries to fit all the noise
- deconvolution becomes easily an ill-posed problem => need some regularization

- usually one works with discrete quantities $D_i = \sum_j H_{i,j} I_j + \epsilon_j$
 - D is the observed image, H elements of the point spread matrix, I the true signal, and ε the noise in the observed data elements

Naive solution

 naively one might try a least squares solution (assuming the errors were normally distributed)

$$min_{I} \frac{\|H * I - D\|^{2}}{\sigma^{2}}$$

- as the previous examples showed, this does not usually work
 - oscillatory solutions
 - might be acceptable if number of data points
 number of points in the reconstructed
 image and the noise level is small



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Inversion methods in astronomy

- in the basic regularization we require the result image to be 'smooth'
 - no rigorous definition of smoothness
- the solution is found by minimizing

$$\min_{I} \left[\frac{\|H * I - D\|^2}{\sigma^2} + \lambda \phi(I) \right]$$

- λ is a smoothing parameter
- $\boldsymbol{\phi}$ is smoothing function, for example

$$\phi(I) = \sum_{j} (I_{j} - I_{j+1})^{2}$$

 in Tikhonov regularization one minimizes function

$$J(I) = \|D(x, y) - (H * I)(x, y)\| + \lambda \|P * I\|$$

- first term is χ^2
- second term contains convolution of the result image with a high pass filter
- λ is regularization parameter that determines balance between exact fit and image smoothness
- the solution (note syntax: $F(x) = \tilde{x}$)

$$\tilde{I} = \frac{H^* \tilde{D}}{|\tilde{H}|^2 + \lambda |\tilde{P}|^2}$$

- more generally one might write the smoothing function as a quadratic form $\phi(f) = f^T C f$
- the solution of the resulting equation $\min_{I} \left[\frac{\|HI - D\|^{2}}{\sigma^{2}} + \lambda I^{T} C I \right]$ becomes $I = (H^{T} H + \lambda C)^{-1} H^{T} D = K(\lambda) D$
 - solution is found quickly with linear algebra
 - least squares solution recovered with $\lambda{=}0$
 - stable solution as soon as λ 'sufficiently' large

- the main problem is the selection of the smoothing parameter
 - often an ad hoc value what looks right
 - below we follow Thompson & Graig -92
- objectively λ could be chosen so that correct χ^2 -value is recovered $\|\hat{g}-g\|^2 = n\sigma^2$
 - g the observed data, \hat{g} reconstructed image
 - in practice this leads to too smooth solutions
- different criteria developed for finding the optimal smoothing

Smoothing parameters: EDF

• the reason the normal χ^2 criterion fails is that counts d.o.f. of the fit but ignores the d.o.f. of the observed image

 $\|\hat{g}-g\|^2 + \langle |\hat{g}-\langle \hat{g} \rangle|^2 \rangle = n \sigma^2$ (1)

- χ^2 criterion ignores the second term => fit becomes less precise => resulting image is too smooth
- the variance can be estimated if the probability distribution of the recovered image is known
 - see Thompson & Graig (1992)

Smoothing parameters: EDF

• when $I = K(\lambda) D$, the variance term becomes

$$\langle |\hat{g} - \langle \hat{g} \rangle |^2 \rangle = \sigma^2 tr(K(\lambda)) = \sigma^2 tr(H(H^T H + \lambda C)^{-1} H^T)$$

– λ is selected so that Eq. 1 holds

$$||H\hat{f}-g||^2 = \sigma^2 tr(I-K(\lambda))$$

 result can be generalized for non-quadratic smoothing functions (Thompson & Kay -92)

Smoothing parameters: CB

- Craig & Brown (1990) use the same criterion $\|\hat{g}-g\|^2 + \langle |\hat{g}-\langle \hat{g} \rangle|^2 \rangle = n\sigma^2$ but calculate the second term according to the stability of the solution
- the probability of a realization g_k is $P(g_k) \propto \exp\left(\frac{1}{2} \left\|\frac{Hf - g_k}{\sigma}\right\|^2\right) = \exp\left(\frac{1}{2} \left\|\frac{g - g_k}{\sigma}\right\|^2\right)$
 - the latter form follows when *Hf* is replaced with our best estimate, i.e., the actually observed map

Smoothing parameters: CB

the previous leads to the result

$$\begin{aligned} \langle |\hat{g} - \langle \hat{g} \rangle |^2 \rangle &= \langle |\hat{g} - \langle \hat{g}_k \rangle |^2 \rangle \\ &= \int (\hat{g}_k - \langle \hat{g}_k \rangle)^T (\hat{g}_k - \langle \hat{g}_k \rangle) \exp(-\frac{1}{2} \left(\frac{g_k - g}{\sigma} \right)^2) d(g_k) \\ &= \sigma^2 tr(K(\lambda) K(\lambda)) \end{aligned}$$

- smoothin parameter is found based on $\|H\hat{f} g\|^2 = \sigma^2 tr(I K(\lambda)K(\lambda))$
- larger filter factor than EDF, asymptotical difference smaller than a factor of two

Smoothing parameters: BAS

- Bayesian derivation by Gull (1988)
 - several formulations (one method identical with EDF)
 - one particular form

$$\|H\hat{f} - g\|^2 + \lambda \hat{f}^T C\hat{f} = n\sigma$$

- *H* was the beam, *C* the constraints
- this can be evaluated without calculating the trace of matrix K => suitable for large problems

Smoothing parameters

- conclusions of Thompson & Graig
 - easy problem = low blur
 - EDF reconstruction close to the best possible
 - CB oversmooths slightly (some bias)
 - BAS worse, consistently undersmoothed
 - harder problem = large blur
 - \bullet EDF sensitive to $\sigma_{\!\!\!\!\!\!}$ sometimes grossly undersmoothed
 - CB appears slightly more robust
 - BAS undersmoothed (features produced by noise) but insensitive to the value of $\boldsymbol{\sigma}$

– the $\chi^{\scriptscriptstyle 2}$ method produces grossly oversmoothed results

Linear regularization methods

- some problems
 - Gibbs oscillations near discontinuities
 - hard to use any a priori information (even positivity constraints)
 - regularization usually through smoothing: leads to loss of resolution

Some regularization schemes

$$\|CI\| = \sum \sum I(x, y) - \frac{I(x-1, y) + I(x+1, y) + I(x, y-1) + I(x, y+1)}{4}$$

- sometimes called (simultaneous) autoregressive model
- model • equivalent to prior $\propto \exp\left(-\frac{\alpha}{2} \|CI\|\right)$
- examples of other forms
 - Charbonnier et al. (1997)
 - Moline et al. (1996, 2001, 2000)

Bayesian framework

- the Bayes formula of probabilities $P(I|D) = \frac{P(I)P(D|I)}{P(D)}$
- in this case we interpret D as the observed data and I as the true intensity
- solution found by maximizing posterior probability *P(I|D)*
 - P(I) is prior probability of given solution I
 - P(D|I) is the probability of data when model I is given (by itself would often lead to χ^2 minimization)
 - P(D) is merely a normalization factor

Bayesian framework

– the maximum likelihood estimate would be $ML(I) = max_{I} p(D|I)$

while the solution from Bayes formula is $ML(I) = max_I p(D|I) p(I)$

- MAP = maximum a posteriori solution
- denominator *P(D)* does not affect the solution
- ML = MAP with constant prior

Bayes: Gaussian noise

for gaussian (=normally distributed) noise

$$p(D|I) = (\dots) \exp\left[-\frac{1}{2}\left(\frac{D-I * H}{\sigma}\right)^2\right]$$

- in unconstrained case this leads to $\chi^{\rm 2}$ minimization

$$\max p(D|I) = \max \exp(\frac{-1}{2}x^2) \Rightarrow \min x^2$$

- in constrained case regularization can be built in the iterative optimization algorithm
 - Landweber / successive approximations / Jacobi method
 - number of iterations ~ smoothness of solution
 - include other constraints, e.g., positivity

Bayes: Gaussian noise

 in the special case that both object and noise are normally distributed with zero mean, the Bayes solution leads to Wiener filtering

$$\tilde{I} = \frac{H^* \tilde{D}}{|\tilde{H}|^2 + \sigma_N^2 / \sigma_o^2}$$

- as before, H is the beam, D the observations, and I the recovered intensity
- σ_N^2 the noise variance and σ_o^2 the object variance
- Wiener filtering is very fast to calculate and optimal in case of stationary, Gaussian signal
- ... but causes artifacts (e.g., rings around point sources) and needs noise estimates in the *frequency* space $\sigma = \sigma(v)$!

Bayes: Poisson noise

Poisson distribution is

$$p(k) = \frac{\mu^k}{k!} e^{-\mu}$$

- *k* is the discrete number of events
- $\bullet~\mu$ is the expectation value (and variance) and the probability becomes

$$p(D|I) = \prod_{x,y} \frac{\left[(H*I)(x,y) \right]^{D(x,y)} e^{-(H*I)(x,y)}}{D(x,y)!}$$

 ML estimate is found by setting derivate of In p(D|I) to zero

$$\frac{\partial \ln p(D|I)}{\partial I} = 0 \quad \Rightarrow \quad \frac{D}{H * I} * H^* = 1$$

Bayes: Poisson noise

- this leads to an iterative algorithm
 - multiply both sides with *I*, evaluate left side using an old estimate on the right hand side

$$I^{(n+1)} = I^{(n)} \left(\frac{D}{H * I^{(n)}} * H^{*} \right)$$

- this is the famous Richardson-Lucy algorithm (Lucy 1974) or the expectation maximization (EM) method
- the flux is conserved and the solution is always non-negative
- still only a maximum likelihood solution

Bayes: Poisson noise

if we denote with *M* the true solution, the probability of given model *I* becomes

$$p(I) = \frac{\prod M^{I} e^{-M}}{I!}$$

and the MAP solution is

$$I = M \exp\left\{ \left[\frac{D}{H * I} - 1 \right] * H^* \right\}$$

setting $M = I^{(n)}$ one obtains an iterative formula

$$I^{(n+1)} = I^{(n)} \exp\left\{ \left[\frac{D}{H * I^{(n)}} - 1 \right] * H^{*} \right\}$$

Inversion methods in astronomy

- let I be the recovered intensity
- constraints can be presented as a function P_c so that we require, e.g.,
 - positivity of solution
 - object belongs to spatial domain D

$$I(x, y) = \begin{cases} I(x, y), & \text{if } (x, y) \in D \\ 0, & \text{otherwise} \end{cases}$$

- solution is band limited

$$P_{C}(\tilde{I}(x, y)) = \begin{cases} \tilde{I}(x, y), & \text{if } v < v_{0} \\ 0, & \text{otherwise} \end{cases}$$

 P_{i}

- the constraints can be implemented easily in iterative schemes
 - smaller number of iterations acts also like regularization
- below are examples of regularized versions of the following algorithms
 - Jansson-Van Cittert
 - Landweber
 - Tikhonov
 - Richardson-Lucy

- the van Cittert iteration is very simply $I^{(n+1)} = I^{(n)} + \alpha (D - H * I^{(n)})$
 - convergence parameter can be set $\alpha{\sim}1$
 - may converge in a few iterations, diverges in the presence of noise
- Jansson (-70) considered constraint A<I<B

$$\alpha \to C \left[1 - 2 \frac{|I^{(n)} - (A+B)/2|}{B-A} \right]$$

- more generally $I^{(n+1)} = P_C \left\{ I^{(n)} + \alpha \left(D - H * I^{(n)} \right) \right\}$

- regularized Landweber iteration $I^{(n+1)} = P_{C} \left\{ I^{(n)} + \gamma H^{*} * (D - H * I^{(n)}) \right\}$
 - ~steepest descent minimization (Jacobi method)
 - $-H^*(x,y)=H(-x,-y)$
- regularized Richardson-Lucy

$$I^{(n+1)} = P_{C} \left\{ I^{(n)} \left[\frac{D}{H * I^{(n)}} * H^{*} \right] \right\}$$

 Tikhonov solution is obtained using gradient function

 $\nabla J = [H^* * H + \mu P^* * P] * I - H^* * D$

• P is a high pass filter

- normal iteration is

$$I^{(n+1)} = I^{(n)} - \gamma \nabla J$$

and the regularized version, not surprisingly,

$$I^{(n+1)} = P_C \left\{ I^{(n)} - \gamma \nabla J \right\}$$

Edge effects

- FFT based methods are computationally efficient in de-convolution
 - Richardson-Lucy requires 4 FFT transformations and total cost is O(N²logN)
- in the case of extended emission edges cause ripple in the solution
 - artifacts can be decreased by ×10 by using reflective or anti-reflective boundary conditions
 - changes the result what did the real beam see outside the image?

Edge effects

- the boundary pixels depend on the unknown intensity outside the FOV
- Bertero & Boccacci (2005):
 - RL is used to deconvolve a larger image, which improves the reconstruction inside FOV
 - brightness values outside measured map as free parameters
 - fast implementation using FFT:s
Edge effects



original image and the beam

convolved image with Poisson noise and RL reconstruction of full image

reconstruction of smaller area with RL and with the method of Bertero & Boccacci

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Interlude: Interferometry



VLA/NRAO

Inversion methods in astronomy

 correlation of signals observed by two or more antennas



- same wavefront is observed in antennas with a phase shift $\tau_g = \frac{1}{G} \vec{B} \cdot \vec{s}$
- the correlator calculates time average of the product of measured voltages V
- V^2 is proportional to the power of the radiation
- for a point source the cross correlation is

$$R_{xy} \propto \sqrt{w_1 w_2} e^{i 2\pi v \tau}$$

- the phase shift is set to zero at a phase center close to the object
- the corrected cross correlation is called the *visibility*
 - this depends on the source intensity and the angles between the source direction and the baseline B connecting the antennas
- usually coordinates u and v are used
 - *u* = east-west length of *B* as seen from the phase centre
 - v = corresponding length of the north-south projection

- in aperture synthesis the observed visibilities are used to derive a continous map of the sky around the phase centre
- for an intensity distribution the visibility is $V(u,v) = \int I_{v}(x,y) A_{e}(x,y) e^{i2\pi(ux+yv)} dx dy$
 - I(x,y) is the true surface brightness
 - A(x,y) is the effective collecting area of the telescopes, *including their beam pattern*
 - ... one observes a Fourier transform of the surface brightness !

 when we look at a small area surrounding the phase centre, the beam of individual telescopes is almost constant

$$V(u, v)/A_{e} = \int I_{v}(x, y)e^{i2\pi(ux+yv)}dx dy$$

 if visibilities were observed for all u and v, the intensity would be obtained by a direct Fourier transform

$$I_{v}(x, y) = \int \int V(u, v) / A_{e} e^{-i2\pi(ux+vy)} du dv$$

- in practice only a small part of the (u,v) plane is covered
 - each antenna pair gives instantaneously only one position (u,v)
 - ... and the corresponding point (-u,-v)
 - because visibilities are real, V(-u,-v)=V*(u,v)
 - as the Earth rotates, each antenna pair draws a curve in the (u,v)-plane



(u,v)-coverage in two cases





Inversion methods in astronomy

- the measured visibility can be seen as a convolution between true visibility and a mask g
 - -g=1 where we have measurements, g=0 elsewhere
 - by definition the product g(u,v)V(u,v) is known everywhere and the Fourier transforms can be performed

according to convolution theorem

 $F(g(u,v)V(u,v)) = Con(P_{syn}(l,m), M(l,m))$

- P_{syn} is the Fourier transform of g = dirty beam
- this defines the final resolution of the recovered map
- M is essentially the product of the true intensity and the beam pattern of an individual antenna
 - g is also called the grading function of the synthesized aperture

- the recovered 'dirty image' contains artifacts caused by the incomplete sampling of the (u,v) plane
 - each point source produces an image of the dirty beam
 - one must somehow fill in the missing visibilities (regularization) or *clean* the final image

• dirty image:



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- the CLEAN algorithm (Högborn 1974) models image as a sum of point sources
 - 1. find an intensity peak in the (dirty) image
 - subtract the peak = (dirty) beam multiplied with a damping factor
 - 3. repeat there are no more peaks above specified level
 - convolve point source model with idealized 'CLEAN beam' (e.g., central lobe of (dirty) beam)
 - above 'dirty image' and 'dirty beam' refer to interferometric observations

- the residual image may be added to CLEAN image (as a check)
- instead of the real space image one can work in Fourier space using FFTs (Cark 1980) or, in the case of interferometry, directly with visibilities
- solution is unique
 - ... if there is no noise and if the number of visibility measurements is larger than the number of image elements
 - in principle superresolution should be possible
 - in practice (because of the noise and other factors) CLEAN performs badly in this respect

dirty image cleaned and restored image

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Inversion methods in astronomy

- some negative aspects
 - slow for large images
 - no handle on the image statistics
 - spurious peaks caused by the noise
 - depression in surface brightness around strong sources
 - fluctuations in extended emission
 - final convolution with 'CLEAN beam' is basically an ad hoc procedure to produce nice images
 - this affects also the relative scaling between CLEAN image and residuals!
 - if there is a good source model for extended emission, that should be subtracted before CLEANing the image

- entropy is a measure of disorder
- in image reconstruction one would like to obtain an image that contains all information available from the observations – but no additional structure
- maximation of image entropy should guarantee this
 - 'maximally noncommittal'
 - 'as featureless as the data allow'

the problem is still the inversion of eq.

$$D_i = \sum_{j} H_{i,j} I_i + N_i$$

- D is the observed quantity, in images usually the intensity
- *H* is the point spread function
- N (additive) noise
- the entropy of the recovered image is $S = \int \int f[I(x, y)] dx dy$ $S = \sum_{i,j} f[I_{i,j}]$
 - *f* is some function (not quite a unique definition!)

- entropy is related to the probability of a state
 - entropy measures the number of ways a given state can be realize
 - entropy is additive while probabilities are combined multiplicatively => entropy should be proportional to the logarithm of probability
 - if there are W ways to realize a state, each with probability $p_w = 1/W$, entropy is $S = \ln W = -\ln p_w$
 - when alternatives have probabilities p_i the average becomes

$$S = -\langle \ln p_i \rangle = -\sum_i p_i \ln p_i$$

• if original variable X is transformed to Y $S = -\int p(X) \ln[p(X)] dx = -\int q(Y) \ln[q(Y)/J(Y)] dY$

- J is the Jacobian of the transformation, J=dX/dY

this suggests that entropy should be written in form

$$S = -\int p(X) \ln[p(X)/p_0(X)] dX$$

 $-p_o(X)$ is 'prior', which is analogous with the state degeneracy g in the discrete case

$$S = -\sum_{i} p_{i} \ln(p_{i}/g_{i})$$

- the prior makes entropy independent of the scaling
- when prior is constant (flat image), entropy is maximum when p_i is constant
 - more generally, maximum corresponds to state where p is proportional to its prior
- in practice different forms of entropy are used

$$f(I) = -\ln I$$
$$f(I) = -I \ln I$$

Bayesian derivation

the Bayes equation of probabilities says

$$P(I|D) = \frac{P(I)P(D|I)}{P(D)}$$

- P(I) is the prior probability $P(I) \propto \exp[S(I)]$
- P(D|I) is the probability of observations when image I is given; in case of gaussian white noise [

$$P(D|I) \propto \prod_{r} \exp\left[-\frac{1}{2} \sum_{i} \left(\frac{H_{ri}I_{i} - D_{r}}{\sigma}\right)^{2}\right]$$

 note that the denominator P(D) does not depend on the solution and is merely a normalization factor

Bayesian derivation

when we take a logarithm we obtain probability

$$\ln P(I|D) = S(I_i) - \frac{1}{2} \sum_r \left(\frac{\sum_i H_{ri} I_i - D_r}{\sigma_r} \right)$$

- this is a sum of entropy and the χ^2 value
- our solution would correspond to the maximum of this probability
- conversely, we could minimize $\chi^2 S$
- note: assumes uncorrelated errors and normal error distribution!

- in the framework of power spectrum estimation Burg (1967) came up with the formula corresponding to $S_1 = \int \ln I$
 - there I corresponded to terms of power spectrum that can be seen as independent Gaussian random variables
 - probability is product of normal probabilities and the entropy is proportional to logarithm of variance
 - same form can be derived for images in the limit of high photon numbers

- consider an image with pixel intensities I_i
- with total flux of the image $D_0 = sum(I_i)$, we can define fractional intensity $f_i = I_i / D_0$
 - the image can be constructed in W=exp(S) different ways, which leads to

 $S_2 \approx -N \sum_i f_i \ln f_i = -(N/D_0) \sum_i \ln I_i (+constant)$

- the same formula can also be derived from thermodynamic entropy in the limit of low photon numbers
 - valid for high frequencies while S₁ might be more appropriate at radio frequencies?

- the two formulations are not necessarily contradictory
 - correspond to different probability distributions one can attribute to the same image ?
 - both go to infinity when intensity goes to zero: forces results to be positive
 - there are generalizations for cases with negative intensities
 - both have negative second derivative which suppresses rapid variations

- still another formula (Gull & Skilling 1991)

$$S = \sum_{x} \sum_{y} \left\{ I(x, y) - M(x, y) - I(x, y) \ln \frac{I}{M} \right\}$$

- *M* prior image, *I* our solution
- entropy reaches maximum (value zero) when image is equal to the prior

ME-approach to interferometry

- intensity *I(x,y)* is to be reconstructed based on measured function *F(D)(u,v)*
 - D is in real space and F(D) is its Fourier transform in the (u,v)-space so that F(I) (u,v)=F(D)(u,v) for all measured u and v

- ignoring the noise we can maximize

 $\int \int f(I) dx dy + \sum_{u,v} \lambda_{u,v} \Big(\int \int I \exp[-i 2\pi (u x + v y)] dx dy - \tilde{D}(u,v) \Big)$

• Lagrange multipliers λ enforce the constraints

derivation wrt *l(x,y)* gives

 $f'[I(x,y)] = -\sum_{u,v} \lambda(u,v) \exp[-i2\pi(ux+vy)] \equiv J(x,y)$

 the ME image is found by formally solving this equation

$$I(x, y) = f'^{-1}[J(x, y)] \equiv g[J(x, y)]$$

 depending on the selected form of entropy we have either

$$S = \ln I \implies S' = 1/I \implies g(J) = 1/J$$

or

$$S = -I \ln I \Rightarrow S' = -\ln I + 1 \Rightarrow g(J) = \exp(-1 - J)$$

- the result has the following properties
 - in J(x,y) are only Fourier components corresponding to measured (u,v)
 - in the restored image missing values must be created by the non-linearity of the f'
 - the degree of the non-linearity depends on absolute value of I
 - if we add an offset in the intensities, the recovered map will be different
 - the slope of f ' is small at large values of I => peaks will be narrow ('superresolution')
 - the slope is large at small *I* => small scale variations are suppressed

 around extreme points Taylor expansion gives for *f=-ln I*

$$I(x, y) = \frac{1}{a(x - x_0)^2 + 2b(x - x_0)(y - y_0) + c(y - y_0)^2 + d}$$

and for $f = -I \ln I$

 $I(x, y) = \exp\left[-a(x-x_0)^2 - 2b(x-x_0)(y-y_0) - c(y-y_0)^2 - (d+1)\right]$

 in other words, in details the first definition of entropy leads to Loretzian peaks, the latter to Gaussian peaks

- the resolution depends on the intensity level: it is largest for the highest peaks
 - peak height is less reliable than the values of integrated flux
- suppression of small scale variation is best at low intensities
 - the sidelobes of a point source are not well suppressed if the source is located on an elevated plateau
- there can be spurious peaks around absorption features

ME-approach, noisy data

• in ME analysis one can resort to the old scheme: smooth until one gets expected value of $\chi^2 = \Omega \approx$ number of independent data points

- the constraint
$$\chi^2 = \sum_{u,v} \left[\frac{\tilde{I}(u,v) - \tilde{D}(u,v)}{\sigma(u,v)} \right]^2 = \Omega$$

is again forced with the help of Lagrange multipliers when maximizing

$$\int \int f(I) dx dy - \lambda(\chi^2 - \Omega)$$

'least squares MEM'

e

ME-approach, noisy data

- the function J is still band limited
 - fourier coefficients of F(J) are zero except for the measured (u,v) coordinates
- the model predictions differ from the data

$$\tilde{J}(u,v) - \lambda \frac{\tilde{I}(u,v) - \tilde{D}(u,v)}{\tilde{\sigma}^2(u,v)} = 0$$

- in the fourier space the residuals F(I)-F(D) are not random
 - highly correlated, negative at peaks and in regions of low intensity mostly positive, smoothing out variations of I
ME-approach, noisy data

- flux is transferred from peaks to background
 - the relative effect is largest for small peaks
 - at large S/N the residuals are larger than for the original data by a factor of sqrt(2) !
 - the solution is always biased towards the prior (usually flat distribution)
- additional constraints can be added for flux conservation of the whole image
- resolution depends on the S/N ratio
 - MEM is capable of superresolution
 - but how to tell, whether all the structures are real?
 - final MEM image can be convolved with a gaussian to get a more uniform resolution

ME-approach, noisy data

comparison with CLEAN

- MEM is biased, CLEAN is not; bias results from the fact that data (including he noise) is not modelled exactly
- bias is acceptable as a trade-off with smaller variance and can be decreased by convolving the original data
- MEM minimizes pixel variance so that the images are smoother than CLEAN images
- CLEAN is poor for extended emission, MEM has problems with point sources on extended emission
- in MEM a priori information can be introduced easily through prior image

ME-approach, single aperture

- here a single aperture means that we have *full coverage* of all spatial frequencies, but the S/N ratio drops at scales below the size of the psf H
- the maximized function is identical to the previous case except for the inclusion of the point spread function

$$S = \int \int f(I) dx dy$$

- $\lambda \left(\sum_{u,v} \left\{ \frac{|\tilde{H}(u,v)\tilde{I}(u,v) - \tilde{D}(u,v)|}{\tilde{\sigma}(u,v)} \right\}^2 - \Omega \right)$

Inversion methods in astronomy

- the MEM image is result of optimization
 - optimize $max\{S-\lambda C\}$
 - unknowns are image values I_{i,j} based on which entropy is defined, e.g.,

$$S = -\sum_{i,j} p_{i,j} \log p_{i,j}, \quad p_{i,j} = I_{i,j} / \sum_{i,j} I_{i,j}$$

- one can include condition for flux preservation $max\{S-\lambda C-\mu\sum I_{i,j}\}$
 - μ can be selected to fit given value of total flux
 - more simply, use corresponding value A directly as the prior

$$S = -\sum_{i,j} I_{i,j} \left[\log(I_{i,j}/A) - 1 \right]$$

- constrained optimization: maximize S subject to constraints on goodness-of-fit C
 - and possible other constraints on flux etc.
- solution is always iterative
- could be found with general optimization algorithms
- there are a number of specialized algorithms

- Gull & Daniel (1978) maximize $Q = S - \lambda C$ $I_{j}^{(n+1)} = A \exp[-\lambda \frac{\partial C(I^{(n)})}{\partial I_{j}}]$

- image remains positive on all iterations
- *unstable*, even if successive iterates are smoothed
- normal steepest ascent

$$I_{j}^{(n+1)} = I_{j}^{(n)} + x \frac{\partial Q(I^{(n)})}{\partial I_{j}}$$

- develops negative values, unless x is extremely small
- negative values must be reset and even then there will be convergence problems

- conjugate gradient algorithms
 - instead of direction ∇Q one uses only part that is conjugate to some previous directions (~attempts to estimate the Hessian based on previous steps)
 - considerably better than steepest ascent although problem of negative values persists
- search of unconstrained optimization (λ =const)
 - main expense is in the image data transformations needed for estimates of ∇Q
 - instead of a single line, it may be more efficient to search full subspace
 - some (<10) vectors are used to span the subspace

- search directions of constrained problem
 - in previous case a separate iteration is needed on λ so that C becomes correct
 - the search directions e can be selected to enforce the constraints directly
 - e.g. see Skilling & Bryan (1984)

- Cornwell & Evans (1985; AIPS task 'VM')
 - maximize $J = S \alpha \chi^2 \beta I$
 - Lagrange multipliers α and β selected so that χ^2 and total flux F both get their expected values
 - condition $\nabla J=0$ leads to the implicit formula

$$I_i = m_i \exp\left(-\alpha \left(\frac{\partial X^2}{\partial I_i}\right) - \beta\right)$$

- *m* is the prior image
- iterative substitution leads to unstable
 algorithm and slow convergence (see above)
 => better to optimize directly the J

- quadratic approximation of entropy is valid but only very close to solution => need to use second order methods
- direct Newton-Raphson gives

ΔI	=	$(-\nabla \nabla J)^{-1} \nabla J$
∇J	=	$\nabla S - \alpha \nabla \chi^2 - \beta I$
$\nabla \nabla J$	=	$\nabla \nabla S - 2 \alpha H$

- Hessian of J is diagonal apart from the contribution from beam profile H
- approximation: neglect non-diagonal part of the Hessian = sidelobes of the beam

 beam H is replaced with a scaled identity matrix

 $\nabla \nabla J = \nabla \nabla S - 2 \alpha q I$

- q is a scaling factor that depends on the beam solid angle (conversion from flux in the beam to flux within a pixel) – exact value is not important
- previous equations give the search direction Δb along which a line search is performed
 - two convolutions are required for the calculation of residuals but also these can be interpolated

- convergence criterion $\|\nabla J \cdot \nabla J\| < \epsilon \|1 \cdot 1\|$
- update of lagrange multipliers

$$\Delta \alpha = -\Delta X^2 / \|\nabla X^2 \cdot \nabla X^2\|$$

$$\Delta \beta = -\Delta F / \|\nabla F \cdot \nabla F\|$$

- these updates interfere with update of J so that step size must be limited
- one must correct for negative values
 - small values are cut, lower limit decreased during the iterations
- for large images VM is generally faster than CLEAN

Problems in deconvolution

- Starck & Pantin (2002)
 - fourier based methods give band-limited solutions (Wiener filtering, Tikhonov method, ...)
 - CLEAN cannot restore extended emission (and is slow for large images)
 - MEM cannot recover both compact and entended sources
 - results depend on the background level
 - poor results for features below the background level
 - spatial correlations ignored
 - iterative methods cause noise amplification
 - van Cittert, Richardson-Lucy, Landweber, ...

Problems in deconvolution

- two images with identical entropy



Starck et al. 2001

- Fourier-based methods perform poorly when signal contains point sources or edges
 - base functions extend over the whole space
- wavelet transform promises to be a good alternative
 - base functions are wavelets that are localized in both real and frequency space
 - data is presented as a sum of wavelets that are scaled and translated
 - presentation is hierarchical, each level describing the structures at one particular scale

- original signal s is decomposed in to a coarse image c_j and wavelet bands w_j , j=1,...,J
 - *J* is the number of scales used
- the coarse image corresponds to frequencies $<(1/2)^{J}$ and each wavelet band to frequencies [$(1/2)^{J+1}$, $(1/2)^{J}$]
- the decomposition is calculated using lowand high pass filters h and g

$$c_{j+1,l} = \sum_{k} h(k-21) c_{j,k}$$

$$w_{j+1,l} = \sum_{k} g(k-21) c_{j,k}$$

filters are derived from the wavelet function

- for 2D images there are three wavelets, one horizontal, one vertical, and one diagonal
 - three wavelet images on each resolution level
 - total number of pixels same as in the original data

f ⁽²⁾ f ⁽²⁾ V.D. j=2	H.D. j=2 D.D. j=2	Horiz. Det. j = 1	Horizontal Details
Vert. Det. j = 1		Diag. Det. j = 1	j = 0
Vertical Details j = 0		Details	Diagonal Details j = 0

• NGC 2997



Starck, Pantin, Murtagh (2002)

 deconvolution can be done by first applying inverse filter H⁻¹

$$H^{-1}(u, v) = 1/\tilde{H}(u, v)$$

 $F = H^{-1}*D+H^{-1}*N = I+Z$

- in F the noise Z is still normally distributed, and may be **amplified**
- the wavelet transformation of F is thresholded and inverse transformation provides the result
 - thresholding sets small wavelet coefficients (=noise) to zero
- wavelet-vaguelette method (Donoho -95)

- Neelamani (1999, 2001) hybrid scheme
 - regularization still done in Fourier domain through a window function W $\tilde{W} = \frac{|\tilde{H}|^2}{|\tilde{H}|^2 + \lambda \sigma^2 / \tilde{S}}$
 - S is the noise power spectrum !
 - the windowed function F is

 $F = W * H^{-1} * D + W * H^{-1} * N$

- parameter λ should be small
- remaining noise eliminated with wavelet transform (eliminates Gibbs oscillations)
- positivity constraint not used

- some problems of the previous approach
 - determination of the regularization parameter $\boldsymbol{\lambda}$ is not trivial
 - positivity constraint is not used at all
 - the power spectrum of noise is usually unknown
 - restricted to the case of Gaussian noise

 in iterative deconvolution the residual at a particular iteration is

$$R^{(n)}(x, y) = D(x, y) - (H * I^{(n)})(x, y)$$

 using a wavelet algorithm the residuals can be written as sum of last smooth array and wavelets at J scales

$$R^{(n)}(x, y) = c_J(x, y) + \sum_{j=1}^J w_{j, x, y}$$

... but a large part of $w_{j, x, y}$ may be just noise

- need to separate *significant* structures from noise
- define **multiresolution support** *M* as

$$M(j, x, y) = \begin{cases} 1, & \text{if } w_j(x, y) \text{ significant} \\ 0, & \text{if } w_j(x, y) \text{ insignificant} \end{cases}$$

- coefficient is significant if $P(|w > w_{j,x,y}| < \varepsilon$
- for Gaussian noise, e.g., $w > 3\sigma_i$
- one can include a source mask in M
- one can write 'noiseless' residual $\overline{R}^{(n)}(x, y) = c_J(x, y) + \sum_{j=1}^J M(j, x, y) w_{j, x, y}$

 with the previous definition one can transform a simple iteration (van Cittert)

$$I^{(n+1)}(x, y) = I^{(n)}(x, y) + \alpha R^{(n)}(x, y)$$

into a more stable scheme

$$I^{(n+1)}(x, y) = I^{(n)}(x, y) + \alpha \overline{R}^{(n)}(x, y)$$

- only statistically significant structures are carried over to the reconstructed image
- final result is the restored image and residuals that are pure noise (R=N)

- regularization by significant structures

 the same can be applied similarly to the Richardson-Lucy algorithm

$$I^{(n+1)} = I^{(n)} \left(\frac{D}{H * I^{(n)}} * H^{*} \right)$$

- setting $D^{(n)}$ as noiseless data $D(x, y) = D^{(n)}(x, y) + R^{(n)}(x, y) \quad D^{(n)}(x, y) = (H * I^{(n)})(x, y)$ the regularized version becomes $I^{(n+1)} = I^{(n)} \left(\frac{D^{(n)} + \overline{R}^{-(n)}}{D^{(n)}} * H^{*} \right)$

- the basic idea of the Pixon method is somewhat similar to the 'regularization using significant structures'
 - not based on wavelets; see Dixon et al. 1996
 - data modelled as a sum of pseudo-images that are smoothed with spatially varying scale
 - final image consists of a dictionary of features
 - +weak regularization for strong features
 - if feature cannot be detected directly from data, it is strongly regularized as part of the background

 simulation of galaxy cluster observed with Hubble Wide Field Camera

original: no noise, no aberration



'observed': aberrated and noisy



Starck, Pantin, Murtagh (2002)

Inversion methods in astronomy

Richardson-Lucy



Pixon method



original: no noise, no aberration



'observed': aberrated and noisy



wavelette-vaguelette



wavelet-Lucy



- conclusions from the previous test
 - Richardson-Lucy amplifies the noise; some of the fainter objects disappear
 - in Pixon method the pixon features are identified from noisy (partially deconvolved data): strong sources are weakly regularized (=good), weak sources suppressed (=bad)
 - wavelet-vaguelette is very fast; results better than with the previous methods
 - wavelet-Lucy produced best results (fewer spurious sources)

Wavelet CLEAN

CLEANing

- consisted of repeated subtraction of strongest *point* sources
- results were not good for diffuse emission
- MRC CLEAN (Walker & Schwartz 1988)
 - build a smoothed image and the difference between original and the smoothed image
 - apply CLEAN separately to both images
 - result is the sum of processed maps

Wavelet CLEAN

- in wavelet CLEAN the procedure is generalized to many scales (Starck 1998)
 - calculate wavelet transformations of the image, the PSF and the CLEAN beam
 - on each level, apply CLEAN using scale j of image and PSF transformations
 - construct result image using the wavelet transformation of the CLEAN beam

Multiscale entropy

- image *I(x,y)* is decomposed into a smooth image *c_{np}(x,y)* and a set of wavelet coefficients *w_i(x,y)*
 - index j refers to the scale, $j=1, ..., n_p$
 - original image is $I(x, y) = c_{np}(x, y) + \sum_{j=1}^{np} w_j(x, y)$
 - *w_j* are calculated as the difference between the last smoothed plane and an image obtained with a low pass filter

$$c_{j}(k) = \sum_{l} h(l) c_{j-1}(k+2^{j-1}l)$$

$$w_{j}(k) = c_{j-1}(k) - c_{j}(k)$$

Multiscale entropy

- entropy is related to the sum of information on each scale
- in wavelet transformation information is related to the probability that individual wavelet coefficients are caused by noise

$$S = -\sum_{j=1}^{J} \sum_{k=1}^{N_{j}} \ln p(w_{j,k})$$

- minimize

$$J = \frac{1}{2} \sum_{k=1}^{N} \left[\frac{D_k - (H * I)_k}{\sigma} \right]^2 \pm \alpha S$$

Inversion methods in astronomy
- for Gaussian noise

$$S = \sum_{j=1}^{J} \sum_{k=1}^{N_{j}} s(w_{j,k})$$

where

$$s(w_{j,k}) = \frac{w_{j,k}^2}{2\sigma_j^2} + constant$$

- *s_j* is again the noise in the wavelet coefficients at the level *j*
- the constant term does not affect the maximization
- entropy ~ information => with the above definition smooth solution requires minimization of entropy

 in Starck & Pantin (1996) multiscale entropy is defined

$$S_{m} = \frac{1}{\sigma_{I}} \sum_{scales j} \sum_{pixels} \sigma_{j} \left[w_{j}(x, y) - m_{j} - |w_{j}(x, y)| \ln \frac{|w_{j}(x, y)|}{m_{j}} \right]$$

- in the absence of signal the wavelet coefficients at level *j* approach m_j – this should be small compared with any real signal, i.e., a small fraction of the noise
- the noise $\sigma_{\!_j}$ acts as a weighting factor of the different scales
- entropy maximized

- multiresolution support
 - images at all wavelets scales, with pixel value TRUE if some information is present at given scale and location (hard threshold, 'hard weighting')
 - 1. calculate wavelet transform of image *I(x,y)*
 - 2. estimate σ of the scale and set a threshold value for the significance (e.g. 3σ)
 - 3. multiresolution support M(j,x,y) is

$$M(j, x, y) = \begin{cases} 1, & \text{if } w_j(x, y) \ge k \sigma_j \\ 0, & \text{if } w_j(x, y) < k \sigma_j \end{cases}$$

- the aim
 - to reconstruct significant structures (where we have enough signal) without strong regularization
 - to eliminate noise (strong regularization)
- new definition for multiscale entropy

$$S_{m} = \frac{1}{\sigma_{I}} \sum_{scales \, j} \sum_{pixels} \left[1 - M(j, x, y) \right] \sigma_{j} \left[w_{j}(x, y) - m_{j} - |w_{j}(x, y)| \ln \frac{|w_{j}(x, y)|}{m_{j}} \right]$$

 entropy is calculated only for scales and regions with low signal-to-noise ratio

- previous M can be replaced with a continuous function going from 0 to 1
 - *M*~1 => weak regularization
 - *M*~0 => strong regularization
- the values σ_j can be obtained from simulations
 - create noise image with $\sigma{=}1$ and do wavelet transform
 - calculate standard deviations of wavelet coefficients at each scale, $\sigma_{\!_{i}}^{\,e}$
 - $\sigma_j = \sigma_l \sigma_j^e$

- image noise σ_{I}
 - estimated from the difference of the image and average filtered image
 - e.g. in the case of CCD images one should disregard the high noise borders
 - look at the intensity histogram
 - estimate can be improved iteratively, using the wavelet transformation
 - calculate multiresolution support and re-estimate noise from pixels $M \sim 0$

for minimization of

$$J = \sum_{pixels} \frac{1}{2} \left(\frac{D - H * I}{\sigma_I} \right)^2 - \alpha S_{ms}(I)$$

Starck & Pantin (1996) used the gradient

$$\nabla J = -H^* * \frac{D - H * I}{\sigma_i^2} + \frac{\alpha}{\sigma_i} \sum_{scale j} \left[\left[1 - M(j) \right] \sigma_j sgn(w_j^{(0)}) \ln \left(\frac{|w_j^{(0)}|}{m_j} \right) \right] * \Psi_j^*$$

and steepest descent $I^{n+1} = I^n - \gamma \nabla J(I^n)$

– above Ψ_i is the wavelet at scale *j*

Inversion methods in astronomy

- the parameter α is fixed by the noise behaviour of the wavelet transform
 - determination far from straightforward
 - depends on the requirement of smoothness

- Starck et al. (2001)
 - the coefficient w is partly due to signal (S_s) , partly due to noise (S_N)
 - small coefficients are noise and contribute to S_N
 - large coefficients contribute mostly to S_s
 - one might want to minize

$$J = \frac{1}{2} \sum_{k=1}^{N} \left[\frac{D_{k} - (P * I)_{k}}{\sigma} \right]^{2} + \alpha S_{N}(I)$$

 in the solution minimize the information that is *due to* the noise

- the minimized function can be generalized as

$$J = S_{S}(D - P * I) + \alpha S_{N}(I)$$

- minimize signal contribution to the information in the residuals
- minimize the noise contribution to the information in the solution
- both hard and soft weighting were studied, with and without the regularizing term



- a) original
- b) blurred and with Gaussian noise
- c) de-convolved image
- d) residuals

Starck et al. (2001)

Inversion methods in astronomy

- multiscale entropy can be used to test presence of undetected sources
 - with $h(w_{j,k}) = -\ln[p(w_{j,k})]$, calculate mean entropy of each scale j

$$E(j) = \frac{1}{N} \sum_{k=1}^{N_j} s(w_{j,k})$$

for assumed noise model, calculate normalized mean entropy

$$E_n(j) = \frac{E(j)}{E^{(noise)}(j)}$$

- $E^{(noise)}$ can be calculated ... at least with simulations

- plot normalized entropy as the function of scale
- weak sources increse entropy at small scales, even when individual objects cannot be detected
- simulation (Starck 2001):
 - 0, 50, 100, 200, or 400 sources with maximum equal to noise σ and source standard deviation 2



Fig. 9. Mean entropy versus the scale of 5 simulated images containing undetectable sources and noise. Each curve corresponds to the multiscale transform of one image. From top to bottom, the image contains respectively 400, 200, 100, 50 and 0 sources

Fig. 10. Region of a simulated image containing an undetectable source at the center

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- superresolution means resolution better than the beam size (diffraction limit)
- two conditions
 - space-bandwidth product (SBP) is no more than ~ 1
 - SBP is approximately the ratio between source diameter and the diffraction limit
 - => source must be small
 - good signal to noise ratio (SNR)

- method requires *some* information about the source model
 - flux of the reconstructed object is concentrated within a smaller area
 - restoration is stable, if the total flux of the object is constrained
 - even non-negativity of the MEM can produce superresolution (of 'nearly black objects')
 - Richardson-Lucy implements both nonnegativity and flux conservation

- data is kept at original resolution
- model and the PSF are sampled at higher resolution
- for example, in the case of MAP Poisson algorithm

$$I^{(n+1)} = I^{(n)} \exp\left\{ \left(\frac{D}{(H * I^{(n)})_{\downarrow}} - 1 \right)_{\uparrow} * H^{*} \right\}$$

• oversampling = ' \uparrow ', down-sampling = ' \downarrow '

- PSF undersampled but observations are made with small shifts => deconvolved image can be reconstructed on finer grid
 - co-adding of frames on fine grid: operator L_{\uparrow}
 - estimation of k^{th} observation from $L_{\uparrow}D$: operator L^{-1}_{\downarrow}
 - Landweber iteration becomes $I^{(n+1)} = I^{(n)} + \alpha H^* \left[L_{\uparrow} (D - L_{\downarrow}^{-1} (H * I^{(n)})) \right]$
 - PSF function *H* is needed at the fine resolution

- example: Anconelli (2005)
 - 1. apply Richardson-Lucy
 - 2. if stars are resolved, go to step 3. Otherwise
 - 1. define domain D where source intensity above threshold
 - 2. apply RL to that domain
 - 3. if stars are separated, positions are obtained as the feature centroids
 - 3. fit a least squares model (sum of psf's)
 - ... in case feature still contains several stars



Fig. 1. Upper-left panel: the object; upper-right: the reconstruction after 1000 OS-EM iterations (first step); lower-left: the mask obtained with a thresholding of the previous reconstruction (50% of the maximum value); lower-right: the restoration after 1000 OS-EM iterations, initialized with the previous mask (second step). The diameter of the circle shown in each picture is λ/B .

Inversion methods in astronomy



Inversion methods in astronomy

- IRAF/STSDAS
 - Lucy (PLucy?); lucy
 - maximum entropy: mem
- Starlink, package Kappa
 - Wiener filtering
 - Richardson-Lucy
 - maximum entropy

- MIDAS
 - core commands
 - DECONVOLVE/IMAGE frame psf result [no_iter] [cont_flag]
 - package surfphot
 - REBIN/DECONVOLVE frame psf result, zoom_x, zoom_y, n_iter

- Midas ctd.
 - package wavelet
 - FILTER/WAVE
 - thresholding, multiresolution Wiener filtering
 - GRAD/WAVE
 - deconvolution by regularized one step algorithm
 - LUCY/WAVE
 - wavelet Lucy
 - DIRECT/WAVE
 - multiresolution Tikhonov, regularization term $\boldsymbol{\gamma}_{i} \|\boldsymbol{w}_{i}\|^{2}$
 - CITTERT/WAVE

- van Cittert + multiresolution support

- MR/1-2 by Starck & Murtagh
 - commercial program (www.multiresolution.com)
 - free version restricted to max 256x256 images
 - standard deconvolution methods (MEM, Lucy, Landweber, MAP, ...)
 - wavelet based methods
 - including multiresolution MEM

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