

Introduction to model-fitting

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- 1. Elements on model-fitting theory
 - understand a few concepts
 - understand the assumptions
 - getting hints useful for the practice
- 2. Digression on the correlations of data
- 3. LITpro software
 - short presentation of the main features
- 4. On the adventure of model-fitting
 - examples and hints
- 5. Short introduction to the practice





Elements on model-fitting theory

- understand the concepts
- understand the assumptions
- getting hints useful for the practice





d

m(x)

x

Model fitting actors

- What we have
 - data (here OIFITS) and uncertainties on data
 - OI_VIS2 squared visibility amplitude
 - OI_VIS complex visibility (amplitude and phase)
 - OI_T3 triple product (amplitude and phase)
 - priors: all possible models of object
 - What we want
 - identity the observed object with a model
 - estimate object parameters *and* uncertainties on the parameters
 easy (•)
- What we need
 - tools for model-fitting
 - know what we are doing (*no black magic !*)



Model fitting principle









Criterion for the *best* **parameters**

• *best* parameters maximize the probability of the data (knowing the model)

$$x_{\text{best}} = \arg \max_{x} \operatorname{Pdf}(d \mid m(x))$$

• where

d	data (random quantities, known statistics)
x	parameters
m(x)	model (of data): ~ expected values of data

- number of parameters < number of data
 - difference from image reconstruction
- priors are not objective
 - we have strong prior: the model of the object!
 - fundamental difference from image reconstruction



assumption: Gaussian statistics

• data have Gaussian statistics:

$$\operatorname{Pdf}(\boldsymbol{d} \mid \boldsymbol{m}(\boldsymbol{x})) = \frac{\exp\left(-\frac{1}{2} \boldsymbol{r}^{\mathrm{T}} \cdot \boldsymbol{C}_{\boldsymbol{r}}^{-1} \cdot \boldsymbol{r}\right)}{\sqrt{(2\pi)^{N_{\text{data}}} \det\left(\boldsymbol{C}_{\boldsymbol{r}}\right)}}$$

• where

$$r = d - m(x)$$
 residuals

$$C_r = \langle r.r^{T} \rangle - \langle r \rangle \langle r \rangle^{T}$$
 covariance matrix of residuals

• maximize Pdf ⇔ minimize argument of the Gaussian

$$\boldsymbol{x}_{\text{best}} = \arg\min_{\boldsymbol{x}} \left[\boldsymbol{d} - \boldsymbol{m}(\boldsymbol{x}) \right]^{\mathrm{T}} \cdot \mathbf{C}_{r}^{-1} \cdot \left[\boldsymbol{d} - \boldsymbol{m}(\boldsymbol{x}) \right]$$





assumption: data statistically independent

• C_r is a diagonal matrix:

$$\boldsymbol{x}_{\text{best}} = \arg\min_{\boldsymbol{x}} \left[\boldsymbol{d} - \boldsymbol{m}(\boldsymbol{x}) \right]^{\text{T}} \cdot \mathbf{C}_{\boldsymbol{r}}^{-1} \cdot \left[\boldsymbol{d} - \boldsymbol{m}(\boldsymbol{x}) \right]$$
$$= \arg\min_{\boldsymbol{x}} \sum_{i=1}^{N_{\text{data}}} \left(\frac{d_i - m_i(\boldsymbol{x})}{\sigma_i} \right)^2$$



• thus we need to minimize $\chi^2(x)$:

$$\chi^{2}(\mathbf{x}) = \sum_{i=1}^{N_{\text{data}}} \left(\frac{d_{i} - m_{i}(\mathbf{x})}{\sigma_{i}} \right)^{2} = \sum_{i=1}^{N_{\text{data}}} \frac{r_{i}^{2}(\mathbf{x})}{\sigma_{i}^{2}} = \sum_{i=1}^{N_{\text{data}}} e_{i}(\mathbf{x})^{2}$$

a.k.a non-linear weighted least squares

where

 $e_i(\mathbf{x})$ normalized residual: random variable with standard normal distribution

 $=>\chi^2$ law

- Independency in real world ?
 - calibrator
 - normalization by incoherent flux

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χ^2 law: definition

$$\chi^2(\boldsymbol{x}_{\text{best}}) = \sum_{i=1}^{N_{\text{data}}} e_i^2(\boldsymbol{x}_{\text{best}}) \quad \text{with} \quad e_i(\boldsymbol{x}) = \frac{d_i - m_i(\boldsymbol{x})}{\sigma_i}$$

 $e_i(\mathbf{x}_{\text{best}})$: standard normal distribution $\mathcal{N}(0,1)$

number of degrees of freedom: $N_{\text{free}} = N_{\text{data}} - N_{\text{param}}$ expected value: $E\{\chi^2(\mathbf{x}_{\text{best}})\} = N_{\text{free}}$ variance: $\text{Var}\{\chi^2(\mathbf{x}_{\text{best}})\} = 2 N_{\text{free}}$











reduced χ^2 : $\chi^2_r = \frac{\chi^2}{N_{\text{free}}}$

number of degrees of freedom:

expected value:

variance:

 $N_{\text{free}} = N_{\text{data}} - N_{\text{param}}$ $E \{ \chi_{\text{r}}^{2}(\boldsymbol{x}_{\text{best}}) \} = 1$ $Var \{ \chi_{\text{r}}^{2}(\boldsymbol{x}_{\text{best}}) \} = 2 / N_{\text{free}}$

Assume model is good !



- statistics is very sharp !
 - confidence level not very useful
- in practice, statistics cannot be used to accept or rule out a model
 - modeling errors may be high
 - noise level may be badly estimated
- can be used to compare two models:

 $\frac{\chi^2(\boldsymbol{m}_1)}{N} \longleftrightarrow \frac{\chi^2(\boldsymbol{m}_2)}{N}$

keep in mind var. of χ^2

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Errors on fitted parameters ?

- general theorem of Cramér-Rao lower bound
- $\mathbf{C}_{\boldsymbol{x}} \geq \left[\nabla_{\boldsymbol{x}} \nabla_{\boldsymbol{x}} \mathcal{L}(\boldsymbol{x}) \right]^{-1}$ with log-likelihood:

$$\mathcal{L}(\boldsymbol{x}) = -\log \operatorname{Pdf}(\boldsymbol{d} \mid \boldsymbol{m}(\boldsymbol{x}))$$

we come back to χ^2 using Gaussian assumption: •





Errors on fitted parameters: computation

• Computation of curvature of log-likelihood

$$C_x \ge \left[\nabla_x \nabla_x \mathcal{L}(x)\right]^{-1}$$
 with $\mathcal{L}(x) = \frac{1}{2} \left[d - m(x)\right]^{\mathrm{T}} \cdot C_r^{-1} \cdot \left[d - m(x)\right] + \mathrm{Cte}$

• Linearization of the model around the best solution

$$m(\mathbf{x}) \approx m(\mathbf{x}_{\text{best}}) + \Big[\frac{\partial m}{\partial \mathbf{x}}(\mathbf{x}_{\text{best}})\Big](\mathbf{x} - \mathbf{x}_{\text{best}})$$

• Relation between errors on data and errors on parameters

$$C_{\boldsymbol{x}} \geq \left[\left[\frac{\partial \boldsymbol{m}}{\partial \boldsymbol{x}}(\boldsymbol{x}_{\text{best}}) \right]^{\mathrm{T}} \cdot \mathbf{C}_{\boldsymbol{r}}^{-1} \cdot \left[\frac{\partial \boldsymbol{m}}{\partial \boldsymbol{x}}(\boldsymbol{x}_{\text{best}}) \right] \right]^{-1}$$

Assume fitted model is good !

- But:
 - assume modeled data are the expected value of data (i.e. the fitted model is good)
 - this only translates the statistical errors from data to the parameters
 - ... and we are optimistic: we consider the equality





Errors on fitted parameters: rescaling

- The model is good (assumption), but:
 - χ^2 is bad (>> N_{free})
 - errors on parameters may be good (only statistics) !

$$\chi^2(\boldsymbol{x}_{\text{best}}) = \sum_{i=1}^{N_{\text{data}}} \frac{r_i^2(\boldsymbol{x}_{\text{best}})}{\sigma_i^2} \gg N_{\text{free}}$$

we look for α such that:

$$\sum_{i=1}^{N_{\text{data}}} \frac{r_i^2(\boldsymbol{x}_{\text{best}})}{(\alpha \ \sigma_i)^2} = N_{\text{free}}$$

$$\Rightarrow \qquad \alpha = \sqrt{\frac{\chi^2(\boldsymbol{x}_{\text{best}})}{N_{\text{free}}}} = \sqrt{\chi_r^2(\boldsymbol{x}_{\text{best}})}$$

$$\Rightarrow \mathbf{C}_{\mathbf{x}} = \alpha^{2} \left[\left[\frac{\partial \mathbf{m}}{\partial \mathbf{x}} (\mathbf{x}_{\text{best}}) \right]^{\mathrm{T}} \cdot \mathbf{C}_{\mathbf{r}}^{-1} \cdot \left[\frac{\partial \mathbf{m}}{\partial \mathbf{x}} (\mathbf{x}_{\text{best}}) \right] \right]^{-1}$$





Outline of the optimization

- Needs
 - Minimize $\chi^2(x)$ (sum of squares)
 - Non-linear, non-convex
- Local optimization with Newton method
 - step from a local expansion at second order
 - need of gradients (Jacobian matrix)
 - need of second derivatives (Hessian matrix)
 - but step may be too long
 - outside region where quadratic approximation is valid
- Control of the length of the step
 - add a constrain that deforms the cost function
- Levenberg-Marquardt algorithm
 - we minimize a sum of squares
 - we only need gradients
 - finite differences are ok
 - Hessian is approximated
 - we only keep product of derivatives

Newton step may be too long



=> We are currently looking for a local minimum





Summary on theory

- OI-FITS data
 - with errors on data, but no covariance
- model of object \Leftrightarrow model of data
- assumption of Gaussian statistics of residuals
- assumption of statistical independency of data
 - no really true in real world
- χ^2 law
 - assume fitted model is good
 - sharp statistics
 - use reduced χ^2 for comparing two models on same data
- errors on parameters
 - Cramér-Rao, gaussian statistics
 - estimated from data errors, rescaled for systematic errors
 - correlations of parameters are estimated
- Optimization
 - Local minimization
 - Need of gradients only





Digression on correlations of data





Appearance of independence



- simulated data
- model is perfect
- model is outside the error bars (1 sigma) for 32% of the data



- easier to compare data with various error bars
- show the true weight of data

Beware : only one realization here !





Data with adjacent correlations: 50%

×



- 50% correlation coefficient, only between adjacent points.
- Similar effect as spectral correlations in real data
- more alignments of successive points
- less dispersion of residuals

Beware : only one realization !





Data with adjacent correlations: 70%

××



- correlation coefficient:
 - 70% between adjacent points.
 - -25% with next points
- Similar effect as (more) spectral correlations in real data
- yet more alignments of successive points
- less dispersion of residuals

Beware : only one realization !





Data with global correlations: 70%



- 70% correlation between any points => more correlations
- Similar effect as noise on normalization (incoherent flux, calibrator)
- less dispersion of residuals

Beware : only one realization !





Examples on real data





Summary on correlation

- Several ways to get correlated data
- When assuming independent data, correlations make χ^2 smaller
- Thus don't trust χ^2 , confidence level, etc.
 - can be used to compare different models (reduced χ^2) or assess the progress of the fit.
 - cannot be used to accept or rule out a model.





LITpro model fitting software for optical interferometry

CRAL: I. Tallon-Bosc, P. Berlioz-Arthaud, M. Tallon
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What is LITpro ?

- Parametric model fitting software for interferometry
 - LITpro: Lyon Interferometric Tool prototype
 - Conceived and developed up-to-now at CRAL in Lyon
 - Graphical User Interface developed at JMMC (Jean-Marie Mariotti Center)
 - Maintained and improved by the "model-fitting" group at JMMC (several labs in France)
- Aim: "exploit the scientific potential of existing interferometers", e.g. VLTI
- Complementary to image reconstruction
 - Sparse (u,v) coverage
 - Reconstructed images identify models
 - Model fitting extracts measured quantities

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Leading requirements of LITpro

- Accessible to "general users" + flexible for "advanced users"
 - Opposite needs:
 - General users want simplicity (stepping stone)
 - Advanced users want a powerful tool (pioneering work)
 - Exchanges:
 - general users $-(needs) \rightarrow advanced users$
 - general users <---(training)--- advanced users
 - Progress must benefit to everybody (share experiences)
- Concentrate on the model of the object
 - Easy implementation of new models.
 - Only need to compute the Fourier transform of the object specific intensity on given coordinates (u, v, λ, t)





Leading requirements ⇒ implementation

- Accessible to astronomers + flexible for advanced users
 - flexible \Rightarrow high level language (*Yorick*)
 - easy modifications and adds in the software
 - "expert layer"
 - accessible \Rightarrow GUI
 - new abilities exposed once they are validated in the "expert" layer
- Concentrate on the model of the object
 - From Fourier transform of the object:
 - Modeled data (interferometric, spectroscopic, photometry, ...)
 - Images
 - LITpro also provides
 - Modeling builder (with GUI or filling a form)
 - Fitter "engine"
 - Tools for analysis

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Types of data

- OIFITS
 - Squared visibilities (VIS2)
 - Complex visibilities (VISAMP, VISPHI)
 - Bispectrum (T3AMP, T3PHI)
- Others
 - Spectral Energy Distribution (dispersed fringes mode)
 - Photometry (see example)

- ...









Setting up the fitting process / principle



• Through the GUI or through a form (file editor)





Fitting process

- Levenberg-Marquardt algorithm (modified)
 - Combined with a Trust Region method
 - Bounds on the parameters
 - Partial derivatives of the model by finite differences
- More latter...
 - Search of global minimum





Implementation of the GUI

🗙 ModelFitting V1.0.11.b	eta 🕒 🕒 🕲 🖉				
File Edit Advanced Help					
New model Ctrl-N					
Load model Ctrl-L	Settings panel				
Save model Ctrl-S	Oifile list				
Quit Ctrl-Q	File[/home/mfgui/SPIE08/Obj1.fits]				
	File[/home/mfgui/SPIE08/Obj2.fits]				
	File[/home/mfgui/SPIE08/Obj1Second.fits]				
	Load oifiles				
	Target list				
	Target[BSC1948]				
	Target(TARGET)				
	Add new target BSC1948				
	Fitter setup				
	standard 🗸				
	User info:				
	Created on Fri Jun 20 10:20:05 CEST 2008 by ModelFitting GUI rev. 1.0.11.beta				
Run fit					

- Implemented in JAVA
 - Web service
 - Links with other services (JMMC)
 - Virtual Observatory
 - Data explorer
 - User feedback
 - ...
- GUI just tells "expert layer" (*Yorick*) what to do
- First public release: October 2009



Status : New model ready for modifications



Work in progress

- LITpro
 - First public release Octobre 2009
- High in the list for near future
 - Search for global minimum of χ^2
 - Tools for multichromatic modeling (e.g. dynamics)
 - Cooperation between Image reconstruction and Model fitting





On the adventure of model fitting

- Local minimum
 - example of an uniform disk
- Observe your data... the Guru way
 - useful for the initial guess (local minimum)
- Degeneracies
 - on the total energy
- Example of a "heterogeneous" model-fitting





Beware of local minima !



- local minima exists even for a uniform disk, depending on data
- what to do ?
 - change first guess
 - cuts in χ^2 sub-spaces
 - use bounds
 - do not forget the low frequencies (or just confirm what we already know...)





Observe your data !



- Starting from a good first guess may be decisive -





Binary with what ?



Degeneracy on total energy



- this degeneracy does not change χ^2
- huge errors because of no curvature of $\chi^2(\mathbf{x}_{best})$ for i1+i2
- this prevents reading the values of i1 and i2





Degeneracy on total energy: solution

- FAQ:
 - We could construct a normalized model !
 - Yes, but we want to combine all sorts of functions...
 - We could combine normalized functions !
 - Not always possible ! Ex: disk with constant amplitude (spot on a star)
- When total energy is not fixed by the data, we add this constraint:

$$\chi^2_{\star}(\boldsymbol{x}) = \chi^2(\boldsymbol{x}) + N_d \left(\frac{\sum_i \Delta \lambda_i \ m_i(\boldsymbol{x}, \boldsymbol{u} = 0)}{\sum_i \Delta \lambda_i} - 1\right)^2$$

This drives total energy to unity

- But the added term MUST BE ZERO at the end of the fit !
 - If not: χ^2 is changed and quantities are wrong !
- Other degeneracies in practice
 - translation of the map (unless phase reference)
 - symmetries if no phase

- ...



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Degeneracy on total energy: solved

Final values for fitted parameters and standard deviation: i1 = 0.83203 + - 0.0812 i2 = 0.16797 + - 0.0164 x = -6.6657 + - 0.00441 mas y = 20.08 + - 0.00631 mas

Chi2: initial= 7.376e+04 - final= 1983 - sigma= 14.2127 reduced Chi2: initial= 730.3 - final= 19.63 - sigma= 0.14072 Number of degrees of freedom = 101

C	orrelation	matrix		
	i1	i2	x	у
i1	1	1	0.00021	0.00058
i2	1	1	-0.0011	-0.0029
х	0.00021	-0.0011	1	-0.44
у	0.00058	-0.0029	-0.44	1





Example: chromatic model + heterogeneous data / 1

Perrin et al, A&A 426, 279, 2004

 $I(\lambda, \theta) = B(\lambda, T_{\star}) \exp(-\tau(\lambda)/\cos(\theta)) + B(\lambda, T_{\text{layer}}) \left[1 - \exp(-\tau(\lambda)/\cos(\theta))\right]$ for $\sin(\theta) \le \emptyset_{\star}/\emptyset_{\text{layer}}$ and: $I(\lambda, \theta) = B(\lambda, T_{\star}) \left[1 - \exp(-2\tau(\lambda)/\cos(\theta))\right]$

 $I(\lambda, \theta) = B(\lambda, T_{\text{layer}}) \left[1 - \exp(-2\tau(\lambda)/\cos(\theta)) \right]$

- Why this example in particular ?
 - Fitting procedure is difficult
 - Need to improve procedures for "general users" (accessible ?)
 - How LITpro performs ?
 - Fitting interferometric + photometric data
 - Assess how it can help the fitting process



Example: chromatic model + heterogeneous data / 2





Perrin et al, A&A 426, 279, 2004

- squared visibilities : 4 sub-bands in K band (IOTA)
- magnitudes : J, H, K, L bands (Whitelock et al 2000)

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Perrin et al. fitting procedure



- 1) (R_*,R_L) from gridding
 - fit all other parameters from fixed sampled values (R_{*},R_L)
 - arbitrary initial values of other parameters
- 2) (T_*, T_L) from gridding + intersection with K photometry
 - Difficult to use the other bandwidths
- 3) Fit 4 optical depths from fixed other parameters
- 4) Compare photometry with other bandwidths: J, H, L.



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Simultaneous fitting of all the data



- 1) Overall size of the object ?
 - Radius of uniform disk: 18 mas
- 2) Overall temperature ?
 - For an uniform disk: 1540K
- 3) Fit from this initial values
 - Initial values of optical depths set to zero => uniform disk

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May be useful (and reassuring) to use physical arguments for the first guess...





Comparison of results





Conclusions on the adventure

- Local minima even with uniform disk
 - cuts in χ^2 space
 - change first guess
 - check χ_r^2 if variations are significant
- Model-fitting algorithm has no brain
 - use yours: look carefully at the data: (u,v) coverage, baselines
- Degeneracies may appear
 - check covariances of parameters
 - check ON/OFF normalization of total energy
- Quality of the fit / model
 - $-\chi^2$
 - understand errors *and correlations* on parameters
 - various plots





Ready for the practice tomorrow ?





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Your road map: 4 exercises

- 1. Fit of a simple model on one file (Arcturus)
 - easy fits, easy problem
 - explore the software
- 2. Fit with parameter sharing on several files (Arcturus)
 - more evolved model
- 3. Fit with degeneracies (binary)
 - explain them !
- 4. Fit on AMBER data
 - you are alone (almost)
- 5. Subsidiary data for fun (and to check your expertise)

