Introduction to model-fitting

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Outline

1. Elements on model-fitting theory
   - understand a few concepts
   - understand the assumptions
   - getting hints useful for the practice

2. LITpro software
   - short presentation of the main features

3. On the adventure of model-fitting
   - examples and hints

4. Short introduction to the practice

Elements on model-fitting theory

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

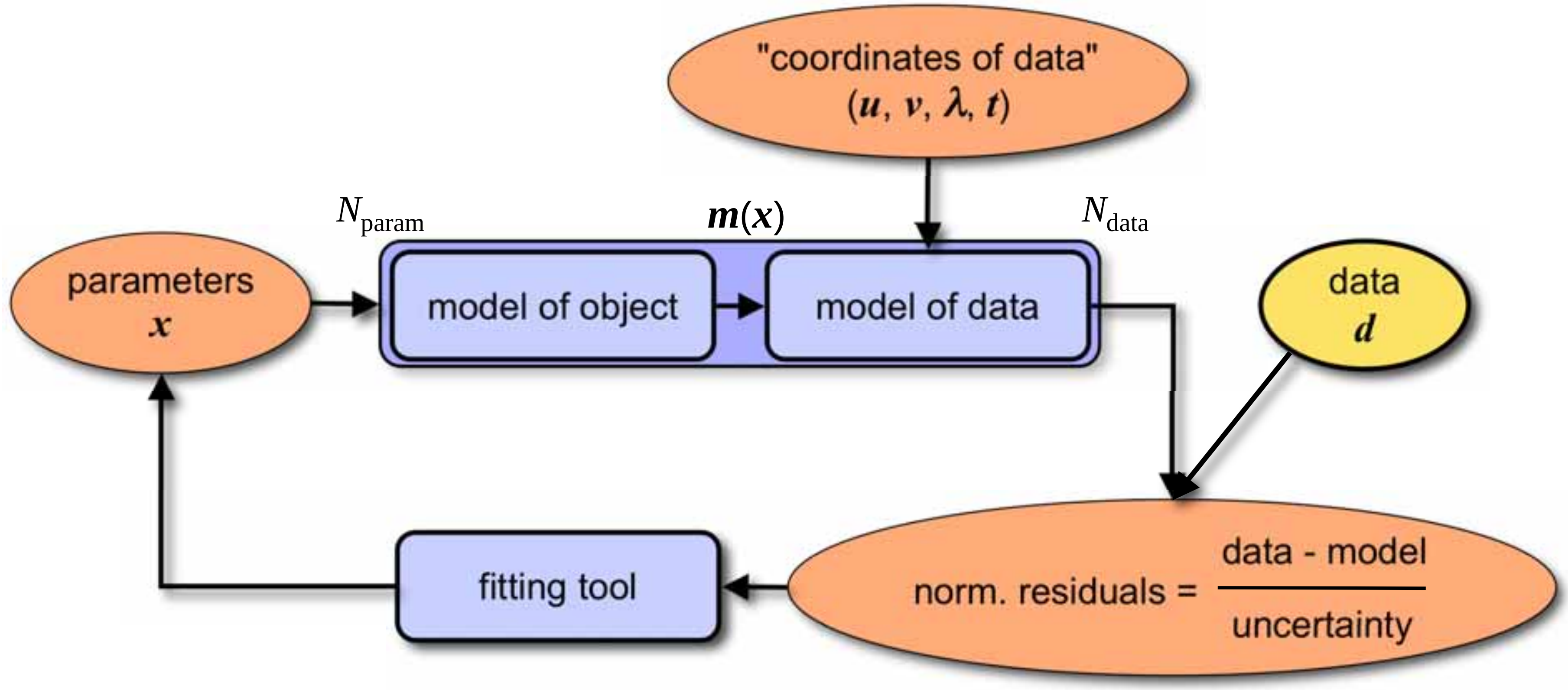
Model fitting actors

- What we have
  - ***d*** — 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
  - ***m*(*x*)** — identity the observed object with a model
  - ***x*** — 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 probabitity of the data (knowing the model)

$$\boldsymbol{x}_{\text{best}} = \arg\max_{\boldsymbol{x}} \text{Pdf}\left(\boldsymbol{d} \,\middle|\, \boldsymbol{m}(\boldsymbol{x})\right)$$

- where

$\boldsymbol{d}$	data (random quantities)
$\boldsymbol{x}$	parameters
$\boldsymbol{m}(\boldsymbol{x})$	model (of data): ~ expected values of data

- number of parameters < number of data
  - difference from image reconstruction
- no objective priors
  - we have strong prior: the model of the object!
  - fundamental difference from image reconstruction

assumption: Gaussian statistics

- data have Gaussian statistics:

$$\mathrm{Pdf}\left(\boldsymbol{d}\,\middle|\,\boldsymbol{m}(\boldsymbol{x})\right) = \frac{\exp\left(-\frac{1}{2}\,\boldsymbol{r}^{\mathrm{T}}.\mathbf{C}_{\boldsymbol{r}}^{-1}.\boldsymbol{r}\right)}{\sqrt{(2\pi)^{N_{\mathrm{data}}}\det\left(\mathbf{C}_{\boldsymbol{r}}\right)}}$$

- where

$$\boldsymbol{r} = \boldsymbol{d} - \boldsymbol{m}(\boldsymbol{x}) \qquad \text{residuals}$$

$$\mathbf{C}_{\boldsymbol{r}} = \langle \boldsymbol{r}.\boldsymbol{r}^{\mathrm{T}} \rangle - \langle \boldsymbol{r} \rangle.\langle \boldsymbol{r} \rangle^{\mathrm{T}} \qquad \text{covariance matrix of residuals}$$

- equivalent to minimize argument of the Gaussian

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

assumption: data statistically independent

- $\mathbf{C_r}$ is a diagonal matrix:

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

covariances of data not measured…

- thus we need to minimize $\chi^2(\boldsymbol{x})$:

$$\chi^2(\boldsymbol{x}) = \sum_{i=1}^{N_{\text{data}}} \left(\frac{d_i - m_i(\boldsymbol{x})}{\sigma_i}\right)^2 = \sum_{i=1}^{N_{\text{data}}} \frac{r_i^2(\boldsymbol{x})}{\sigma_i^2} = \sum_{i=1}^{N_{\text{data}}} e_i(\boldsymbol{x})^2$$

a.k.a non-linear weighted least squares

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

=> χ^2 law

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

χ^2 law: definition

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

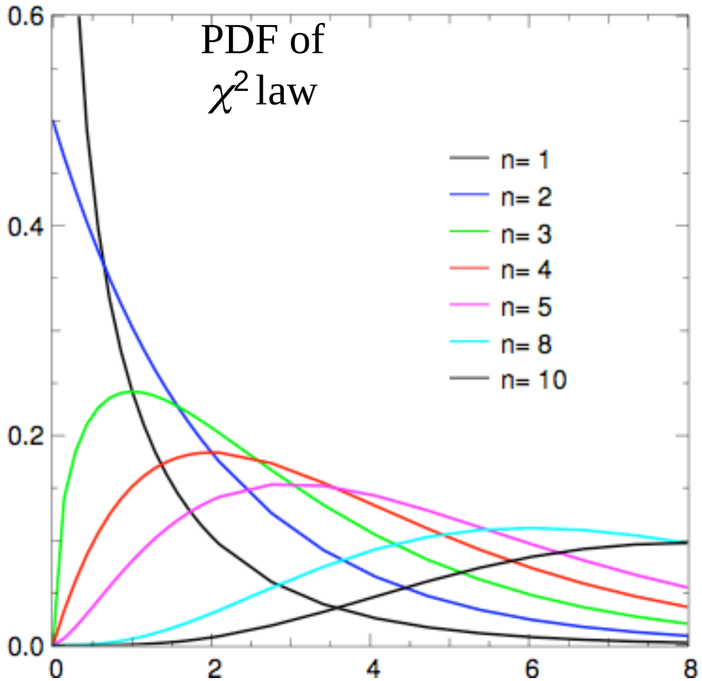
$e_i(\boldsymbol{x}_{\text{best}})$: standard normal distribution $N(0,1)$

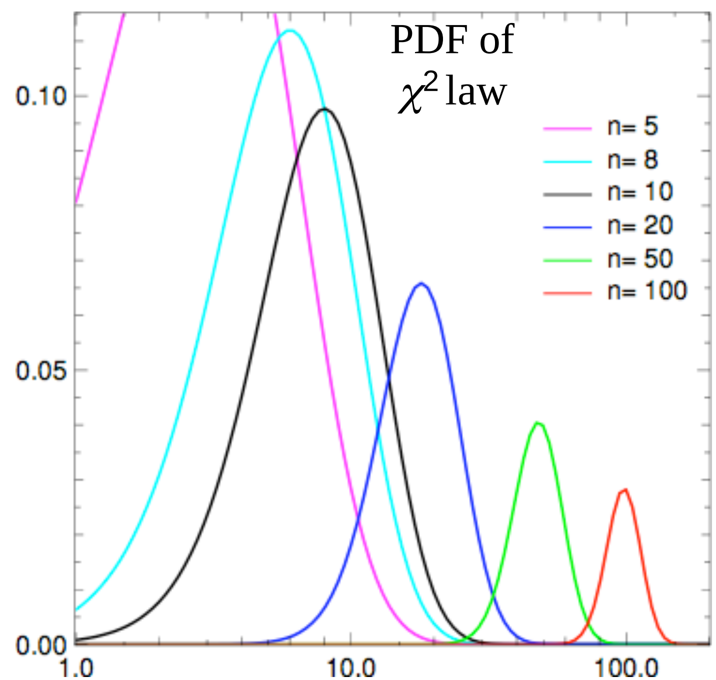
number of degrees of freedom: $N_{\text{free}} = N_{\text{data}} - N_{\text{param}}$

expected value: $E\{ \chi^2(\boldsymbol{x}_{\text{best}}) \} = N_{\text{free}}$

variance: $\text{Var}\{ \chi^2(\boldsymbol{x}_{\text{best}}) \} = 2\, N_{\text{free}}$

Assume model is good !





χ^2 law: reduced χ^2

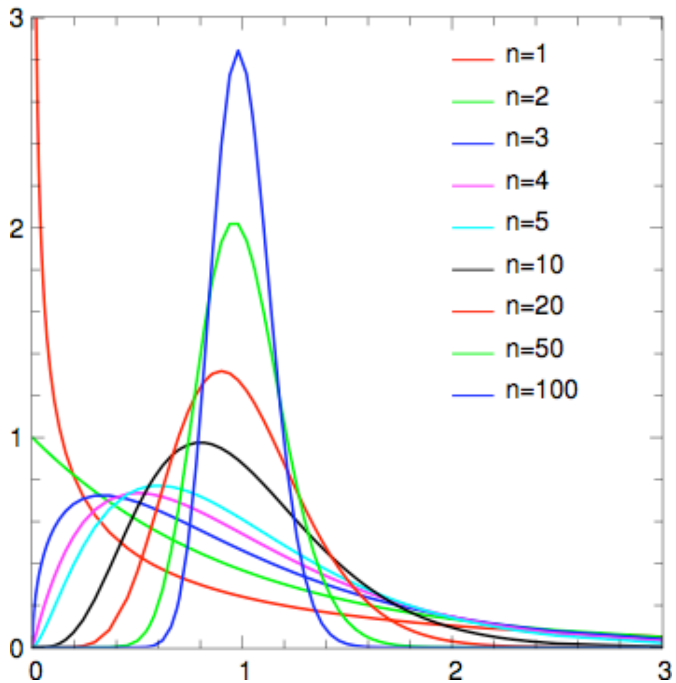
reduced χ^2 : $\chi_r^2 = \dfrac{\chi^2}{N_{\text{free}}}$

number of degrees of freedom: $N_{\text{free}} = N_{\text{data}} - N_{\text{param}}$

expected value: $E\{\chi_r^2(\boldsymbol{x}_{\text{best}})\} = 1$

variance: $\text{Var}\{\chi_r^2(\boldsymbol{x}_{\text{best}})\} = 2 / N_{\text{free}}$

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:

$$\frac{\chi^2(\boldsymbol{m}_1)}{N_1} \longleftrightarrow \frac{\chi^2(\boldsymbol{m}_2)}{N_2}$$

keep in mind var. of χ^2

Errors on fitted parameters ?

- general theorem of Cramér-Rao lower bound

$$\mathbf{C}_x \geq \left[\nabla_x \nabla_x \mathcal{L}(\boldsymbol{x})\right]^{-1}$$

with log-likelihood: $\mathcal{L}(\boldsymbol{x}) = -\log \mathrm{Pdf}\left(\boldsymbol{d} \,\middle|\, \boldsymbol{m}(\boldsymbol{x})\right)$

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

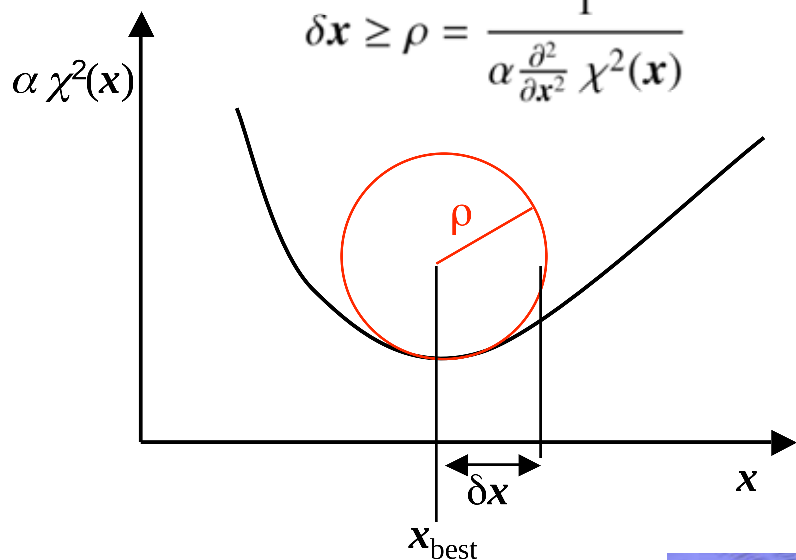
$$\mathrm{Pdf}\left(\boldsymbol{d} \,\middle|\, \boldsymbol{m}(\boldsymbol{x})\right) = \frac{\exp\left(-\frac{1}{2}\, \boldsymbol{r}^{\mathrm{T}}.\mathbf{C}_r{}^{-1}.\boldsymbol{r}\right)}{\sqrt{(2\pi)^{N_{\mathrm{data}}} \det\left(\mathbf{C}_r\right)}}$$

$$\mathcal{L}(\boldsymbol{x}) = \frac{1}{2}\left[\boldsymbol{d} - \boldsymbol{m}(\boldsymbol{x})\right]^{\mathrm{T}}.\mathbf{C}_r{}^{-1}.\left[\boldsymbol{d} - \boldsymbol{m}(\boldsymbol{x})\right] + \mathrm{Cte}$$

$$= \frac{1}{2}\chi^2(\boldsymbol{x}) + \mathrm{Cte}$$

To get the idea, in 1 dimension:

$$\delta \boldsymbol{x} \geq \rho = \frac{1}{\alpha \frac{\partial^2}{\partial \boldsymbol{x}^2} \chi^2(\boldsymbol{x})}$$



Errors on fitted parameters: computation

- Computation of curvature of log-likelihood

$$\mathbf{C}_x \geq \left[\nabla_x \nabla_x \mathcal{L}(\boldsymbol{x})\right]^{-1} \qquad \text{with} \qquad \mathcal{L}(\boldsymbol{x}) = \frac{1}{2}\left[\boldsymbol{d} - \boldsymbol{m}(\boldsymbol{x})\right]^{\mathrm{T}}.\mathbf{C}_r^{-1}.\left[\boldsymbol{d} - \boldsymbol{m}(\boldsymbol{x})\right] + \mathrm{Cte}$$

- Linearization of the model around the best solution

$$\boldsymbol{m}(\boldsymbol{x}) \approx \boldsymbol{m}(\boldsymbol{x}_{\mathrm{best}}) + \left[\frac{\partial \boldsymbol{m}}{\partial \boldsymbol{x}}(\boldsymbol{x}_{\mathrm{best}})\right](\boldsymbol{x} - \boldsymbol{x}_{\mathrm{best}})$$

- Relation between errors on data and errors on parameters

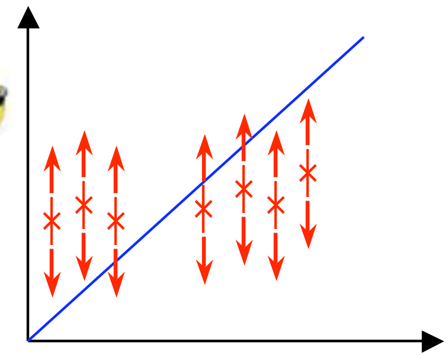
$$\mathbf{C}_x \geq \left[\left[\frac{\partial \boldsymbol{m}}{\partial \boldsymbol{x}}(\boldsymbol{x}_{\mathrm{best}})\right]^{\mathrm{T}}.\mathbf{C}_r^{-1}.\left[\frac{\partial \boldsymbol{m}}{\partial \boldsymbol{x}}(\boldsymbol{x}_{\mathrm{best}})\right]\right]^{-1}$$

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

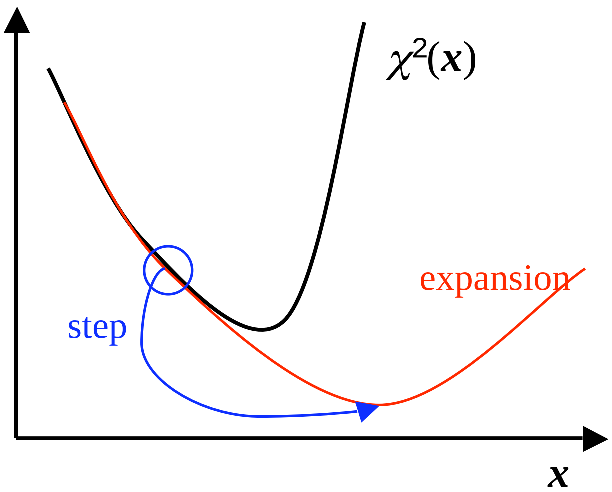
$$\Rightarrow \qquad \alpha = \sqrt{\frac{\chi^2(\boldsymbol{x}_{\text{best}})}{N_{\text{free}}}} = \sqrt{\chi_r^2(\boldsymbol{x}_{\text{best}})}$$

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

Outline of the optimization

- Needs
  - Minimize $\chi^2(\boldsymbol{x})$ (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 ↔ 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

LITpro model fitting software for optical interferometry

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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

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)—› 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 ($\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{\lambda}, \boldsymbol{t}$)

Leading requirements ⇒ implementation

- Accessible to astronomers + flexible for advanced users
  - flexible ⇒ high level language (*Yorick*)
    - easy modifications and adds in the software
    - "expert layer"
  - accessible ⇒ 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

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

fit altogether

- Associate data with a model…
  - data files, …
  - + function 1: parameter1 = "p1", …
  - + function 2: parameter1 = "p2", …
  - + …
- As many groups as you want …
  - other data files, …
  - + function 1: parameter1 = "p3", …
  - + function 3: parameter1 = "p4", …
  - + …
- As many groups as you want…
  - other data files, …
  - + disk: diameter = "d1", x="x", y="y" …
  - + disk: diameter = "d2", x="x", y="y" …
  - + …

Configuration of parameters

- "p1" —› starting value, bounds, fixed or fitted, units
- "p2" —› starting value, bounds, fixed or fitted, units
- …
- "r1" —› starting value, bounds, fixed or fitted, units
- …

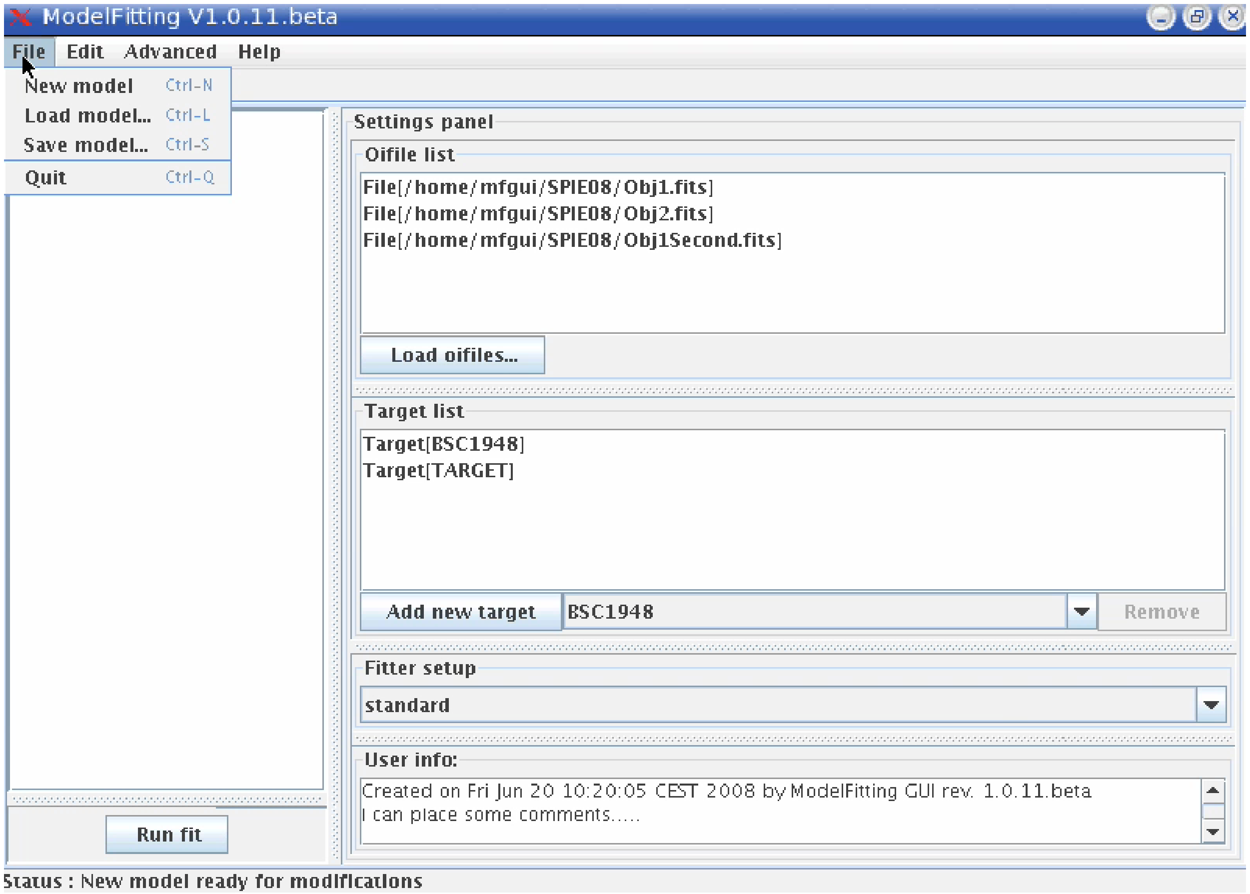
- Through the GUI
  or through a form (file editor)

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



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

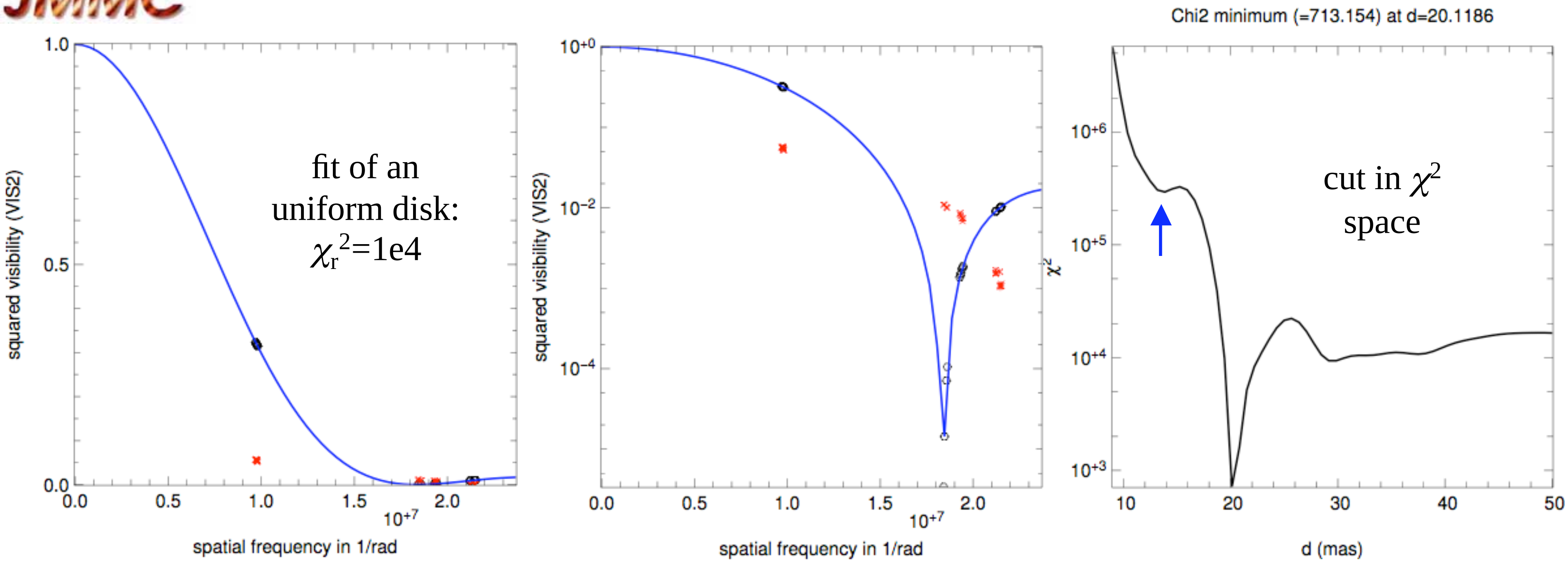
Work in progress

- 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

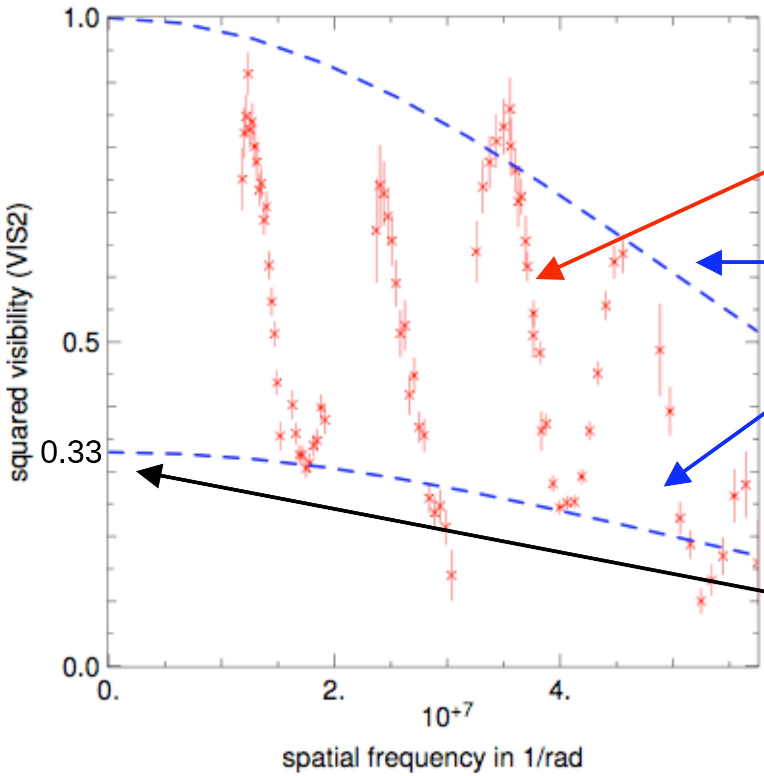
- Local minimum
  - example of an uniform disk
- Observe your data… the Guru way
  - useful for the initial guess (local minimum)
- Degeneracies
  - on the total energy
- Example of a "heterogeneous" model-fitting

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 !



$$V^2_{\min} = 0.33 \Rightarrow r = 0.27$$

Modulation = binary (or >2 components)

Attenuation = components resolved

- binary convolved by an extended function

  ⇓

  Fourier transform multiplied by a window

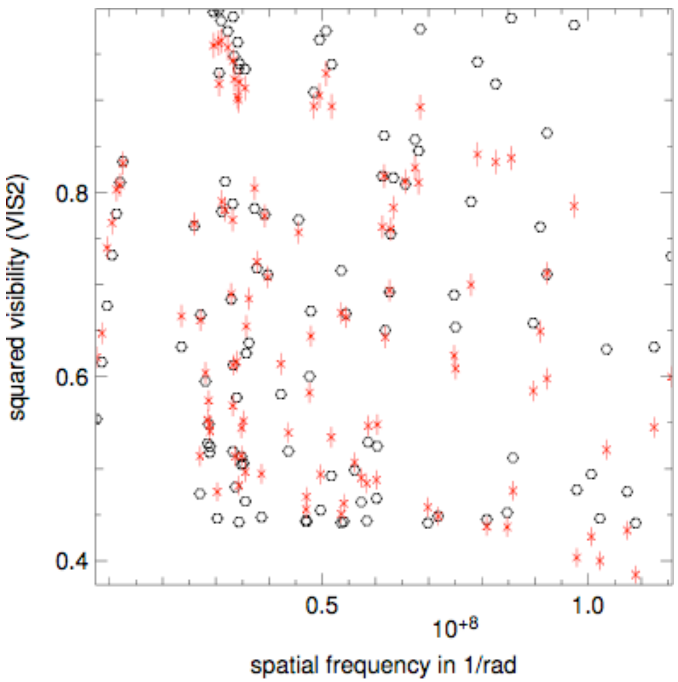
Minimum of modulation gives intensity ratio of the components:

$$r = \frac{1 - \sqrt{V^2_{\min}}}{1 + \sqrt{V^2_{\min}}}$$

— Starting from a good first guess may be decisive —

Degeneracy on total energy

fit of a binary



Model of the binary

- main component at (0,0) with intensity i1
- secondary at (x,y) with intensity i2

```
Final values for fitted parameters and standard deviation:
      i1 =       0.20152 +/- 9.95e+04
      i2 =        0.9982 +/- 4.93e+05
       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
.
--- Correlation matrix ---
              i1        i2         x        y
  i1           1         1    0.0011  -0.0015
  i2           1         1    0.0011  -0.0015
   x      0.0011    0.0011         1    -0.44
   y     -0.0015   -0.0015     -0.44        1
```

- this degeneracy does not change χ^2
- huge errors because of no curvature of $\chi^2(\boldsymbol{x}_{best})$ 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

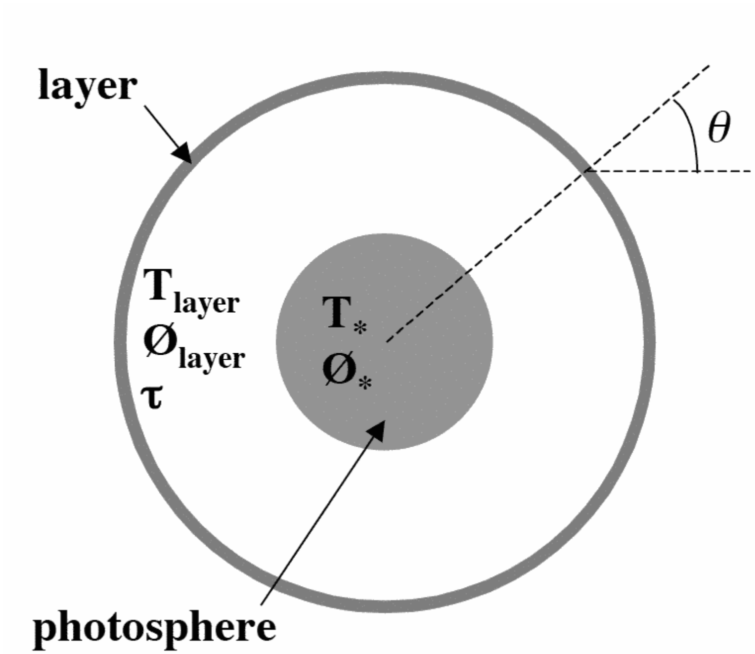
- But the added term MUST BE ZERO at the end of the fit !
  - If not: χ^2 is changed and quantities are wrong !

- Other degeneracies in practice
  - translation of the map (unless phase reference)
  - symmetries if no phase
  - …

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
.
--- Correlation matrix ---
             i1        i2         x         y
  i1          1         1   0.00021   0.00058
  i2          1         1   -0.0011   -0.0029
   x    0.00021   -0.0011         1     -0.44
   y    0.00058   -0.0029     -0.44         1
```

Example: chromatic model + heterogeneous data / 1



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

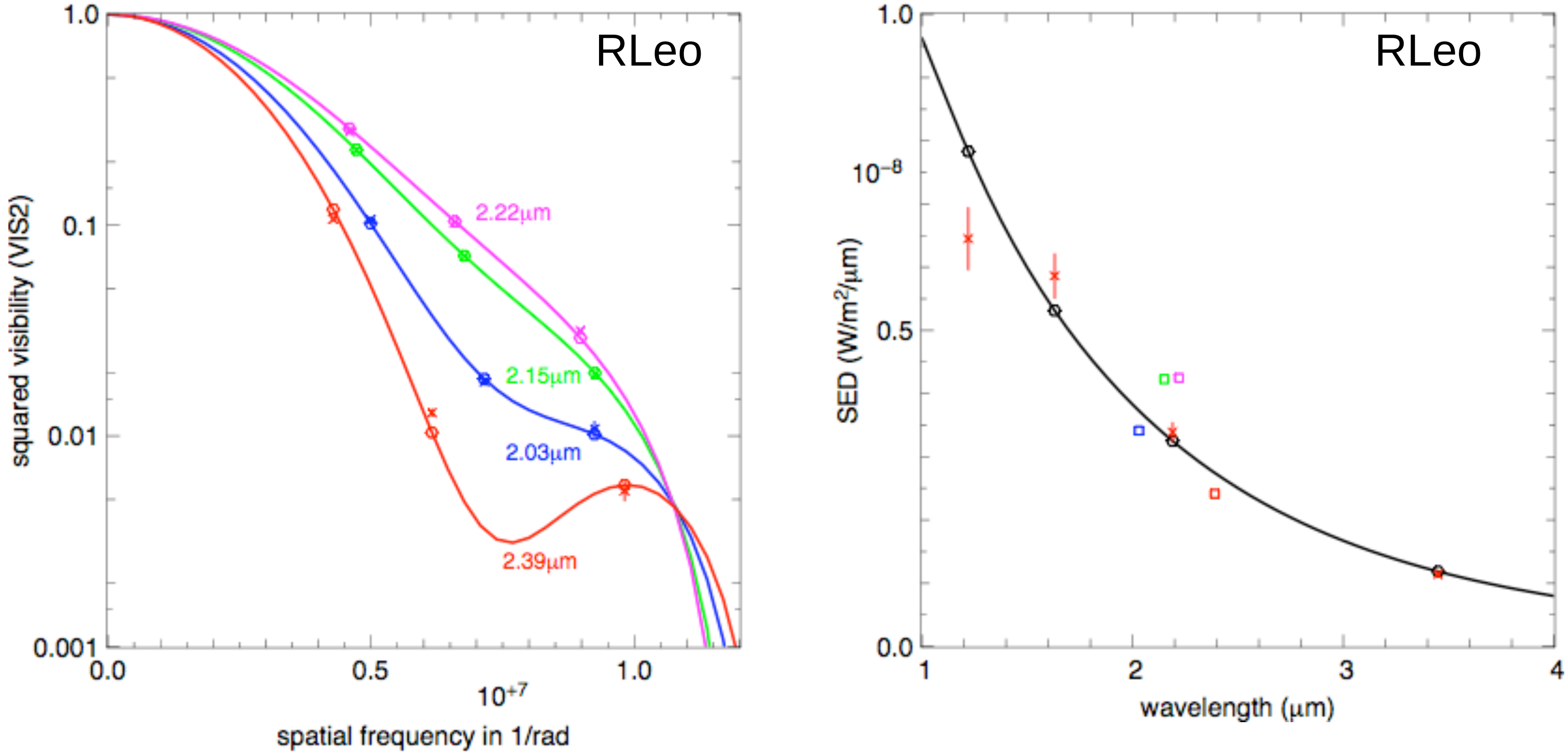
$$I(\lambda,\theta) = B(\lambda, T_\star)\exp(-\tau(\lambda)/\cos(\theta)) + B(\lambda, T_{\rm layer})\,[1 - \exp(-\tau(\lambda)/\cos(\theta))]$$

for $\sin(\theta) \le \O_\star/\O_{\rm layer}$ and:

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

- 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

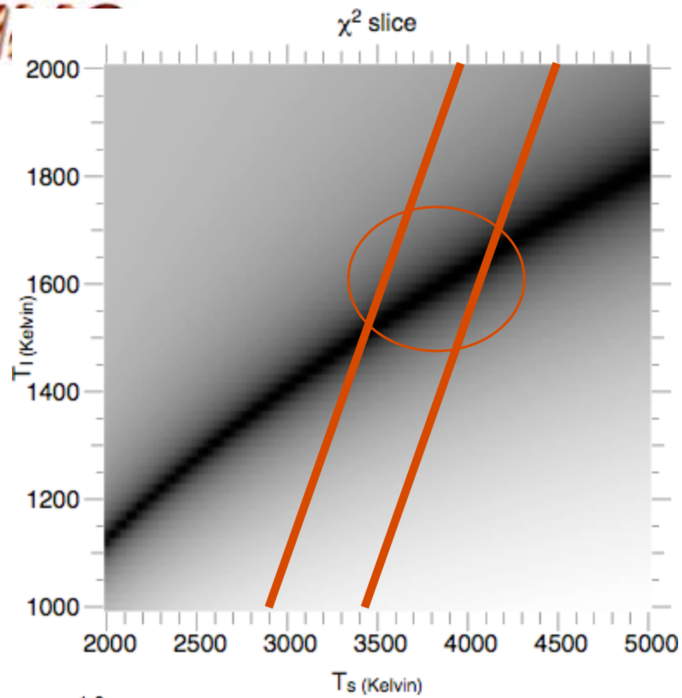
Example: chromatic model + heterogeneous data / 2

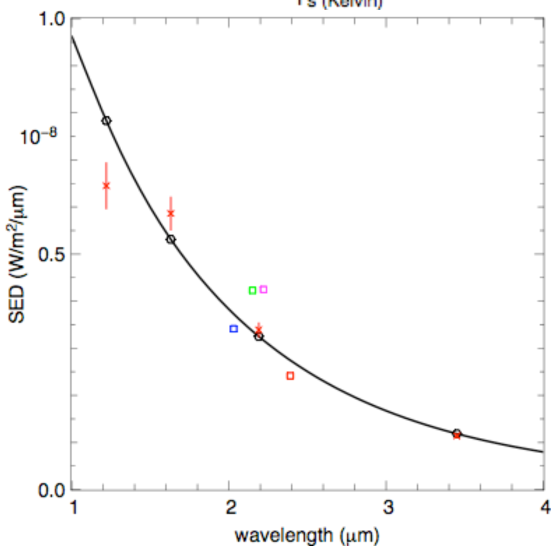


Perrin et al, A&A 426, 279, 2004

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

Perrin et al. fitting procedure





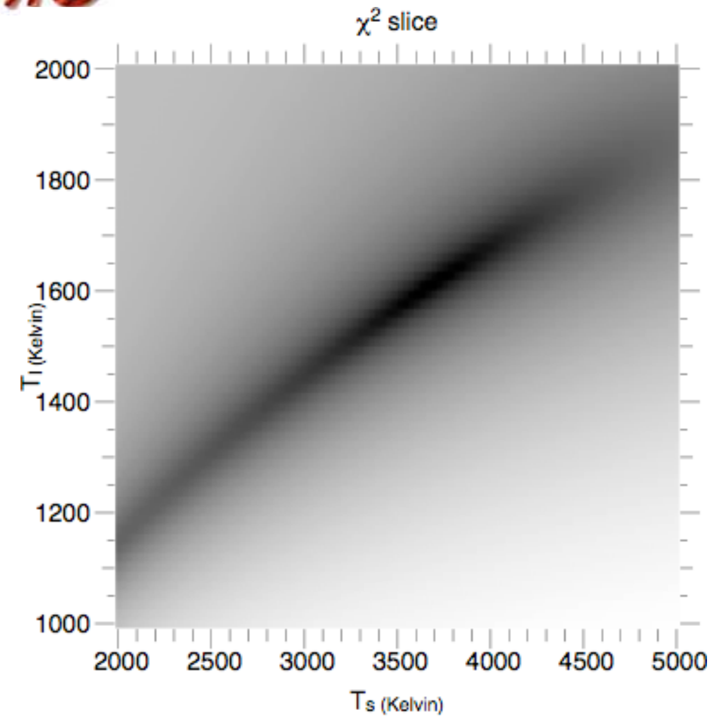
1) (R_*,R_L) from gridding
   - fit all other parameters from fixed sampled values (R_*,R_L)
   - arbitrary initial values of other parameters

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.

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

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

Comparison of results

Parameter	Perrin et al.	Simultaneous fit	Fit with relative photometry
$R_\star$ (mas)	10.94 ± 0.85	11 ± 0.13	11 ± 0.19
R_L (mas)	25.00 ± 0.17	25.4 ± 0.16	25.4 ± 0.18
$T_\star$ (K)	3856 ± 119	3694 ± 113	3778 ± 163
T_L (K)	1598 ± 24	1613 ± 35	1681 ± 174
$\tau_{2.03}$	1.19 ± 0.01	1 ± 0.14	0.9 ± 0.35
$\tau_{2.15}$	0.51 ± 0.01	0.42 ± 0.08	0.36 ± 0.17
$\tau_{2.22}$	0.33 ± 0.01	0.27 ± 0.05	0.23 ± 0.11
$\tau_{2.39}$	1.37 ± 0.01	1.2 ± 0.13	1.08 ± 0.32
γ	–	–	0.9 ± 0.2

Fit with only relative photometry, like the SED given by an optical interferometer

Correlation matrix

	R_l	Rs_ratio	T_l	T_s	tau1	tau2	tau3	tau4
R_l	1	-0.66	-0.36	0.14	0.21	0.17	0.16	0.13
Rs_ratio	-0.66	1	0.71	-0.6	-0.67	-0.67	-0.66	-0.62
T_l	-0.36	0.71	1	-0.74	-0.94	-0.93	-0.93	-0.92
T_s	0.14	-0.6	-0.74	1	0.91	0.91	0.92	0.92
tau1	0.21	-0.67	-0.94	0.91	1	0.99	0.99	0.99
tau2	0.17	-0.67	-0.93	0.91	0.99	1	0.99	0.99
tau3	0.16	-0.66	-0.93	0.92	0.99	0.99	1	0.99
tau4	0.13	-0.62	-0.92	0.92	0.99	0.99	0.99	1

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
  - chi2
  - understand errors *and correlations* on parameters
  - various plots

Ready for the practice ?

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)