principle of maximum likelihood and nonlinear fitting

statistics and data analysis (chapter 8)

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outline

repetition

- fitting problem, linear and nonlinear models
- principle of maximum likelihood (and minimum χ^2)

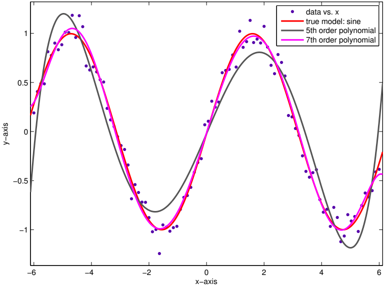
$$\mathcal{L} \propto \exp(-\chi^2/2) \quad \text{with} \quad \chi^2 = \sum_i \frac{(y_i - y)^2}{\sigma_i^2}$$

- Gauss-Markov theorem: correspondence of fits and statistical tests
- Γ-distribution for χ^2 for repeated experiments
- combination of likelihoods from different experiments

numerical exercise

assume n data points (x_i, y_i) as samples from a linear model $y(x) = ax + b$ with constant Gaussian error $\sigma_i = \sigma$. derive numerically the distribution $p(a, b)\mathrm{d}a\mathrm{d}b$ and from that the correlation coefficient r_{ab}. what's the transformation that diagonalises $p(a, b)$?

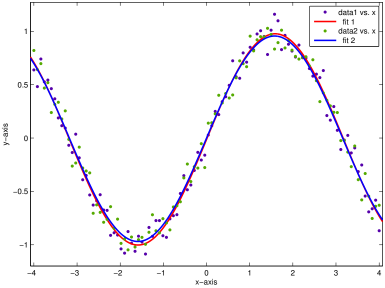
selecting the model...



fitting polynomials to a sine-wave

- choice of the model → lecture about Bayesian model selection
- in this lecture, we will assume that we fit data with the **correct** model

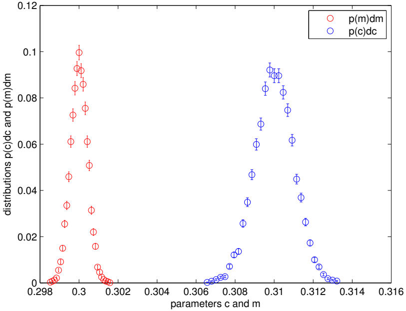
statistical properties of the likelihood



2 fits to the same model with new noise realisations

- 2 realisations of the noise → differences in the inferred parameters
- **what are the statistical properties of the likelihood, if the measurement is repeated?**

statistical properties of the likelihood



distribution of parameters

- fit of a **linear** model ($y(x) = mx + c$) → Gaussian likelihood
- uncertainty of parameters (width of likelihood) reflect noise
- on average, estimated parameters = true parameters (unbiased)

width of a Gaussian likelihood $\mathcal{L}$

- all information from a measurement about a model is contained in the likelihood $\mathcal{L}$
- for **simply shaped** likelihoods it should be sufficient to characterise our knowledge by stating the most probable estimates and their errors and covariances
- best estimate on μ: $\partial\mathcal{L}/\partial\mu = 0$ defines maximum μ^*
- error: width of the likelihood around μ^*, corresponds to curvature!
- Taylor-expansion of $L = \ln\mathcal{L} \rightarrow$ approximation with a Gaussian

$$L(\mu) = L(\mu^0) + \frac{\partial L}{\partial\mu}(\mu^0)(\mu - \mu^0) + \frac{1}{2}\frac{\partial^2 L}{\partial\mu^2}(\mu^0)(\mu - \mu^0)^2 + \dots$$

- exponentiate:

$$\mathcal{L} = \exp(L) \simeq \mathcal{L}_0 \exp\left(-\frac{1}{2}\frac{\partial^2 L}{\partial\mu^2}(\mu^0)(\mu - \mu^0)^2\right)$$

and identify $\sigma^2 \sim (-\partial^2 L/\partial\mu^2)^{-1}$, evaluated at μ^0

multivariate likelihoods

- more than one parameter: relation between the curvature and the inverse covariance
- Taylor-expansion of a multidimensional function:

$$L = L(\mu^0) + \sum_\alpha \frac{\partial L}{\partial \mu_\alpha}(\mu^0) + \frac{1}{2}\sum_{\alpha\beta}\frac{\partial^2 L}{\partial\mu_\alpha\partial\mu_\beta}(\mu-\mu^0)_\alpha(\mu-\mu^0)_\beta$$

  where the gradient vanishes due to the extremum
- we will see (shortly), that $C^{-1} = F$: the inverse covariance is the Fisher-matrix:

$$\mathcal{L}(\mu) = \frac{1}{(2\pi)^{N/2}\sqrt{\det C}}\exp\left(-\frac{1}{2}(\mu-\mu^0)_\alpha(C^{-1})_{\alpha\beta}(\mu-\mu^0)_\beta\right)$$

- curvature of the likelihood: Fisher-matrix

$$F_{\alpha\beta} = \left\langle\frac{\partial^2 L}{\partial\mu_\alpha\partial\mu_\beta}\right\rangle$$

  width σ is given by $\sigma^2 \sim F^{-1}$

quadratic estimates: find the best parameters

- principle of maximum likelihood: find most **plausible** model parameters μ^*, which extremise the likelihood

$$\left.\frac{\partial\mathcal{L}}{\partial\mu_\alpha}\right|_{\mu=\mu^*} = 0$$

- remember: likelihood $\mathcal{L}(y_i|\mu)$ depends on data, it varies from measurement to measurement!
- finding the minimum: Taylor-expand $\mathcal{L}$ or $L = \ln\mathcal{L}$ around μ^0, which is a guessed value for the minimum μ^*

$$\left.\frac{\partial L}{\partial\mu_\alpha}\right|_{\mu} = \left.\frac{\partial L}{\partial\mu_\alpha}\right|_{\mu^0} + \sum_\beta \frac{\partial^2 L}{\partial\mu_\alpha\partial\mu_\beta}(\mu-\mu^0)_\beta + \ldots = 0$$

- apply iteratve Newton-Raphson scheme for finding the minimum:

$$(\mu-\mu^0)_\beta \simeq \sum_\alpha \left(\frac{\partial^2 L}{\partial\mu_\alpha\partial\mu_\beta}\right)^{-1}\frac{\partial L}{\partial\mu_\alpha} \rightarrow \mu_\beta = \mu_\beta^0 - \sum_\alpha \left(\frac{\partial^2 L}{\partial\mu_\alpha\partial\mu_\beta}\right)^{-1}\frac{\partial L}{\partial\mu_\alpha}$$

likelihood of a nonlinear fit

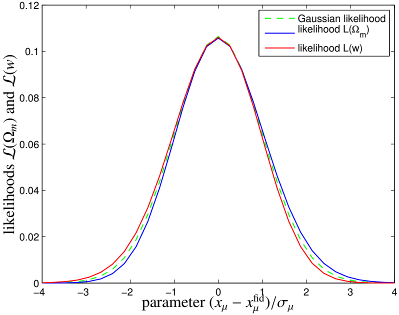
- nonlinear models $\rightarrow y = g(x)$ with a nonlinear function including parameters μ
  - χ^2 is not quadratic in the parameters μ
  - $\mathcal{L} \propto \exp(-\chi^2/2)$ is not Gaussian in μ
- **but:** strong measurements have very peaked liklihoods, and in the vicinity of μ^*, the model can be Taylor-expanded

$$\chi^2 = \sum_i \frac{1}{\sigma_i^2}(y_i - g(x_i,\mu))^2 \simeq \sum_i \frac{1}{\sigma_i^2}\left(y_i - \sum_\alpha \left.\frac{\partial g}{\partial \mu_\alpha}\right|_{\mu^*}(\mu-\mu^*)_\alpha \pm \ldots\right)^2$$

and χ^2 becomes then quadratic in μ

- close to the likelihood peak, everything looks Gaussian

example of a non-Gaussian likelihood



non-Gaussian and Gaussian likelihoods

- non-linearities in the model cause non-Gaussian shapes

Gaussian likelihoods: curvature

- make things easy: **Gaussian likelihood**

$$\mathcal{L}(y_i|\mu_\alpha) = \frac{1}{(2\pi)^{N/2}\sqrt{\det C}}\exp\left(-\frac{1}{2}\sum_{ij} y_i (C^{-1})_{ij} y_j\right)$$

with covariance matrix C

- logarithmic likelihood L

$$L = \ln\mathcal{L} = \mathrm{const} - \frac{1}{2}\mathrm{tr}\ln C - \frac{1}{2}\sum_{ij} y_i (C^{1})_{ij} y_j$$

using $\ln\det C = \mathrm{tr}\ln C$

question

show that $\ln\det C = \mathrm{tr}\ln C$! (hint: principal axis transformation)

Gaussian likelihoods: curvature

- build first derivative of L wrt parameter μ_α

$$\frac{\partial L}{\partial \mu_\alpha} = -\frac{1}{2}\mathrm{tr}C^{-1}\frac{\partial C}{\partial \mu_\alpha} + \frac{1}{2}\vec{y}^t C^{-1}\frac{\partial C}{\partial \mu_\alpha}C^{-1}\vec{y}$$

with $\partial_\mu \ln C = C^{-1}\partial_\mu C$

- build second derivative of L wrt parameters μ_α and μ_β

$$\frac{\partial^2 L}{\partial \mu_\alpha \partial \mu_\beta} = \frac{1}{2}\mathrm{tr}C^{-1}\frac{\partial C}{\partial \mu_\alpha}C^{-1}\frac{\partial C}{\partial \mu_\beta} - \frac{1}{2}\mathrm{tr}C^{-1}\frac{\partial^2 C}{\partial \mu_\alpha \partial \mu_\beta} +$$

$$\frac{1}{2}\vec{y}^t C^{-1}\frac{\partial^2 C}{\partial \mu_\alpha \partial \mu_\beta}C^{-1}\vec{y} - \vec{y}^t C^{-1}\frac{\partial C}{\partial \mu_\alpha}C^{-1}\frac{\partial C}{\partial \mu_\beta}C^{-1}\vec{y}$$

- average $\langle\ldots\rangle$ over many measurements: for any matrix A

$$\langle \vec{y}^t A \vec{y}\rangle = \left\langle \sum_{ij} y_i A_{ij} y_j \right\rangle = \sum_{ij} A_{ij}\langle y_i y_j\rangle = \mathrm{tr}(AC)$$

Gaussian likelihoods: curvature

- average over many measurements replaces data y_i with the covariance matrix C
- Fisher matrix $F_{\alpha\beta}$: curvature of the likelihood surface

$$F_{\alpha\beta} = -\left\langle \frac{\partial \ln \mathcal{L}}{\partial\mu_\alpha\partial\mu_\beta} \right\rangle$$

- statistical errors (statistical uncertainties) σ_α^2 on the parameters μ_α follow from the inverse Fisher matrix
- **keep in mind**: large entries in F are good, they give small errors σ
- naturally, F is a positive definite and symmetric matrix, with real, positive eigenvalues

question

show that $\partial_\mu \ln C = C^{-1}\partial_\mu C$ and $\partial_\mu C^{-1} = -C^{-1}\partial_\mu C C^{-1}$!

Fisher-matrix $F_{\alpha\beta}$

- quantification of the **statistical errors** and **independence of parameters** of a fit
  - Gaussian noise σ_i
  - linear model $y(x)$
- Fisher matrix $F_{\alpha\beta}$: curvature of the likelihood surface

$$F_{\alpha\beta} = -\left\langle \frac{\partial \ln \mathcal{L}}{\partial\mu_\alpha \partial\mu_\beta} \right\rangle$$

- substitution of the second derivatives:

$$F_{\alpha\beta} = \frac{1}{2}\mathrm{tr}\left(C^{-1}\frac{\partial C}{\partial\mu_\alpha}C^{-1}\frac{\partial C}{\partial\mu_\beta}\right)$$

question

show that if data from two independent experiments are combined, the Fisher-matrices add!

Fisher-matrix: unbiased estimates

- if we estimate the best fit parameters: do they correspond to the **true** values used by Nature? at least for a Gaussian likelihood, with estimates following from a quadratic estimator, the answer is **yes!**
- estimates are **unbiased**: $\langle\mu\rangle = \mu^*$ (great news!)
- substitute Fisher matrix into the quadratic estimator

$$\langle\mu_\beta\rangle = \mu_\beta^0 + \frac{1}{2}(F^{-1})_{\alpha\beta}\left(\vec{y}^t C^{-1}\frac{\partial C}{\partial\mu_\alpha}C^{-1}\vec{y} - \mathrm{tr}C^{-1}\frac{\partial C}{\partial\mu_\alpha}\right)$$

- expand covariance C at initial guess μ^0

$$C(\mu) = C(\mu^0) + \frac{\partial C}{\partial\mu_\alpha}(\mu-\mu^0)_\alpha$$

- use $\langle y_i y_j\rangle = C_{ij}$

$$\langle\mu_\beta\rangle = \mu_\beta^0 + (\mu^* - \mu^0)_\gamma\underbrace{(F^{-1})_{\alpha\beta}F_{\alpha\gamma}}_{=\delta_{\beta\gamma}} = \mu_\beta^*$$

Cramer-Rao bounds σ_α

- on average, the estimate μ corresponds to the true value μ^*
- but what is the uncertainty when infering μ from data y_i?
- variance (just a single parameter!)

$$\sigma^2 \equiv \langle(\mu - \mu^*)^2\rangle = \langle\mu^2\rangle - (\mu^*)^2$$

use:

  - $\langle\vec{y}^t A\vec{y}\rangle = \mathrm{tr}AC$
  - Wick-theorem: $\langle y_i y_j y_k y_l\rangle = C_{ij}C_{kl} + C_{ik}C_{jl} + C_{il}C_{jk}$
  - $\langle\vec{y}^t C^{-1}\partial_\mu C C^{-1}\vec{y} = \mathrm{tr}(C^{-1}\partial_\mu C)$

- finally: statistical error corresponds to the curvature of $\mathcal{L}$

$$\sigma_\alpha^2 = \langle(\mu - \mu^*)^2\rangle = \frac{1}{2}F^{-2}\mathrm{tr}\left(\frac{\partial \ln C}{\partial\mu}\frac{\partial \ln C}{\partial\mu}\right) = (F^{-1}) = \frac{1}{F}$$

Cramer-Rao bounds σ_α and correlations $r_{\alpha\beta}$

- for a multivariate likelihood, one distinguishes two types of error
    - marginalised errors: $\sigma_\alpha^2 = (F^{-1})_{\alpha\alpha}$ contains uncertainty in all other parameters
    - conditional errors: $\sigma_\alpha^2 = 1/F_{\alpha\alpha}$ assumes that all other parameters are perfectly known
- furthermore, the parameter might not independent: there might be compensating effects, and the parameters might show some degree of **degeneracy**
- quantified with the correlation coefficient $r_{\alpha\beta}$:

$$r_{\alpha\beta} = \frac{(F^{-1})_{\alpha\beta}}{\sqrt{(F^{-1})_{\alpha\alpha}(F^{-1})_{\beta\beta}}}$$

    - r close to $+1$: positively correlated
    - r very small: uncorrelated
    - r close to -1: anticorrelated

sensitivity

- what is important in an experiment to give small errors?
- obviously, large entries in $F_{\alpha\beta}$ give small uncertainties σ_α
- look at contributions to the Fisher matrix

$$F_{\alpha\beta} = \frac{1}{2}\mathrm{tr}\left(C^{-1}\frac{\partial C}{\partial\mu_\alpha}C^{-1}\frac{\partial C}{\partial\mu_\beta}\right) = \frac{1}{2}\mathrm{tr}\left(\frac{\partial\ln C}{\partial\mu_\alpha}\frac{\partial\ln C}{\partial\mu_\beta}\right) = \frac{1}{2}\mathrm{tr}\left(Q_\alpha Q_\beta\right)$$

- define **sensitivity** $Q_\alpha = \frac{\partial\ln C}{\partial\mu_\alpha}$
- good measurements have high Q_α:
  - small noise, C is small
  - depend strongly on a parameter, $\partial C/\partial\mu_\alpha$ is large
  - combine many measurements, sum over i

reparameterisation of the Fisher-matrix

- Fisher-matrix describes errors on parameters μ in a model $y(x)$
- what if you want to reexpress the errors in a different parameterisation for $y(x)$ with parameters τ?
- assume: there is an **invertible** mapping between μ and τ
- new Fisher matrix $F'_{\alpha\beta}$:

$$F'_{\alpha\beta} = \left\langle \frac{\partial^2}{\partial\tau_\alpha\partial\tau_\beta} \ln\mathcal{L} \right\rangle = \frac{\partial\mu_a}{\partial\tau_\alpha}\frac{\partial\mu_b}{\partial\tau_\beta} \left\langle \frac{\partial^2}{\partial\mu_a\partial\mu_b} \ln\mathcal{L} \right\rangle = J_{\alpha a}J_{\beta b}F_{ab}$$

with Jacobian matrices

$$J_{\alpha a} \equiv \frac{\partial\mu_a}{\partial\tau_\alpha}$$

fitting with the wrong model

- if there are systematic deviations present, the true model provides a bad fit!
- conversely, a fit would not correspond to the true model μ_t, and there are systematical errors in the infered parameters
- systematic bias $\delta \equiv \mu_w - \mu_t$
- write down χ^2-functionals

$$\chi_t^2 = \sum_i (y_i - y_t)^2 \quad \text{and} \quad \chi_w^2 = \sum_i (y_i - y_w)^2$$

- expand wrong χ_w^2 around the **true** best fitting model μ_t:

$$\chi_w^2 = \chi_w^2(\mu_t) + \sum_\alpha \frac{\partial \chi_w^2}{\partial \mu_\alpha}(\mu_t)\delta_\alpha + \frac{1}{2}\sum_{\alpha\beta} \frac{\partial^2 \chi_w^2}{\partial \mu_\alpha \partial \mu_\beta}(\mu_t)\delta_\alpha\delta_\beta$$

biases due to systematics

- average and find μ_w by extremisation

$$\underbrace{\left\langle\frac{\partial\chi_w^2}{\partial\mu_\alpha}\right\rangle_{\mu_t}}_{=a_\alpha} = -\underbrace{\sum_\beta\left\langle\frac{\partial^2\chi_w^2}{\partial\mu_\alpha\partial\mu_\beta}\right\rangle_{\mu_t}}_{G_{\alpha\beta}}\delta_\beta$$

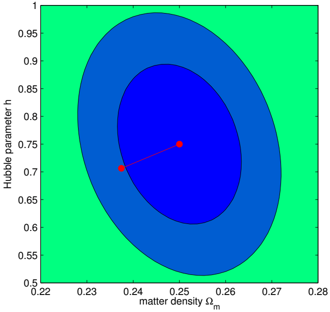
- solve for δ_β

$$\sum_\beta G_{\alpha\beta}\delta_\beta = a_\alpha \quad\rightarrow\quad \delta_\alpha = \sum_\beta (G^{-1})_{\alpha\beta}a_\beta$$

- systematic can be reduced if a strong prior is used

$$G_{\alpha\beta} \rightarrow G_{\alpha\beta} + F_{\alpha\beta}^{\mathrm{prior}}$$

example from cosmology: gravitational lensing



systematical and statistical errors

- uncorrected systematics bias the estimates

summary

- linear models and Gaussian noise provide Gaussian parameter likelihoods
- likelihood can be optimised using a quadratic estimator, e.g. Newton-Raphson
- estimates are unbiased
- variances are the smallest possible, Cramer-Rao errors
- systematics: model is incomplete, and parameter estimates are biased