SAND2017-8667C

An Introduction to Statistical Inverse Problems and Bayesian Inference

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Livermore, CA, USA

Parametric Uncertainty Summer School & Workshop
Budapest, Hungary
Jul 3-7, 2017

Acknowledgement

B.J. Debusschere, R.D. Berry, K. Sargsyan, C. Safta,
J. Prager, K. Chowdhary, M. Khalil, T. Casey
— Sandia National Laboratories, CA

R.G. Ghanem — U. South. California, Los Angeles, CA
Y.M. Marzouk — Mass. Inst. of Tech., Cambridge, MA

This work was supported by:

- US Dept of Energy Office of Advanced Scientific Computing Research (ASCR), Scientific Discovery through Advanced Computing (SciDAC)
- US Dept of Energy ASCR Applied Mathematics program.
- US Dept of Energy Office of Basic Energy Sciences, Div. of Chem. Sci., Geosci., & Biosci.

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Outline

1. Inverse Problems
   - Least Squares Parameter Estimation
   - Regularization
   - Sparsity
2. Statistical Inverse Problems
   - Bayesian Inference
   - Examples
   - Regularization & Sparsity
3. Markov chain Monte Carlo
   - Metropolis-Hastings MCMC Algorithm
   - Examples
4. Approximate Bayesian Computation (ABC) Methods
5. Model Selection, Validation, Averaging
6. Closure

Inverse Problem Definition

Inverse problem :

$$f(x;\lambda) = y$$

Given x, y, solve for λ

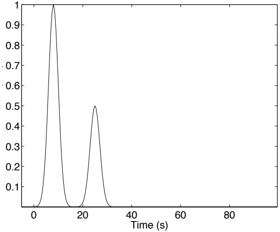
- $x \in \mathbb{R}^d$: independent coordinates, space, time, operating conditions
- $\lambda \in \mathbb{R}^n$: model parameters – objects of inference
  - Generally $\lambda(x) : \Omega \to \mathbb{R}^n$, infinite dimensional
- $f()$: forward model
  - e.g. polynomial fit model, PDE system, etc
- $y \in \mathbb{R}^m$: prediction observable, data
  - Data: $D = \{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\}$

Challenges with Inverse Problems

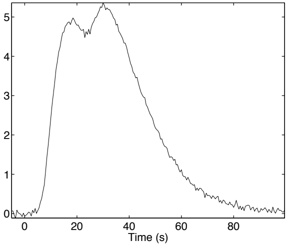
- Inverse problem solution is difficult
  - f^{-1} often non-local, non-causal
- Inverse problems are typically ill-posed:
  - No solution may match the data (existence)
  - Many solutions may match the data (uniqueness)
    - Dependence on initial guess on λ
  - Ill-conditioning or lack of stability
    - Small changes in y can lead to large changes in λ
    - Sensitivity to noise
  - Regularization

Challenges with – noise and ill-conditioning

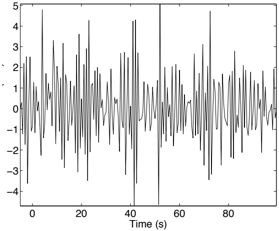
True Input



Forward Model + 5% noise



Inverse Problem Solution



Parameter Estimation and Inverse Problems
Aster, Borchers, and Thurber
Academic Press, 2004, 2012

Least-Squares Parameter Estimation

- Fit model $f()$; unknown parameters λ; measurement y
- Forward Problem:

$$f(\lambda) = y$$

- Estimate λ for best fit between $f(\lambda)$ and y :

$$\lambda_{\text{fit}} \quad = \quad f^{-1}(y)$$

- Inverse problem – solve using least-squares regression

$$\lambda_{\text{rms}} \quad = \quad \underset{\lambda}{\operatorname{argmin}}(||y - f(\lambda)||)$$

i.e. minimize the χ^2:

$$\chi^2 = \sum_{k=1}^{\mathcal{D}} \frac{((f(\lambda) - y)^2}{\sigma_k^2}$$

- Uncertainty estimation, e.g. with Support Planes method
  - χ^2 value decays with parameter variation away from optimum
  - Vary one parameter at a time away from λ_{rms}, refit, estimate stdv based on χ^2 decay below specified threshold

Issues with Least Squares (LS) Parameter Estimation

- Choice of optimal number of fit parameters (p)
  - χ^2 decreases with increased p
  - Danger of overfitting
- No general means for handling *nuisance* parameters
  - Other uncertain parameters in the problem
  - Not objects of inference
- LS best fit is the Maximum Likelihood Estimate (MLE) assuming Gaussian noise in the data
  - What about non-Gaussian noise?
- LS Estimation of Uncertainty in inferred parameter values relies on assumed linearity of the model in the parameters
- Uncertainty estimate does not provide general probabilistic characterization of parameters

Regularization for Deterministic Inverse Problem Solution

- Regularization allows enforcement of select constraints on the inverse problem solution
  - Smoothness
  - Positivity, ...
- Example: Tikhonov-type regularization:

$$\lambda = \underset{\lambda'}{\operatorname{argmin}} \left(\|f(\lambda') - y\|_2^2 + \alpha \|L\lambda'\|_2^2 \right)$$

- How to choose regularization form, L, α ?
  - Somewhat arbitrary
- Regularization introduces bias, destroys consistency
- What about uncertainty/confidence intervals in λ ?

The choice of norm

- The use of the L2-norm

$$
\begin{aligned}
||y - g(x,\theta)||_2^2 &= \frac{1}{N}\sum_{i=1}^{N}(y_i - g(x_i,\theta))^2 \\
||J(\theta)||_2^2 &= \frac{1}{M}\sum_{k=1}^{M}(J(\theta_k))^2
\end{aligned}
$$

  is not the only option for regression fitting or regularization
- Fitting:
  - Model-data misfit, Likelihood function
  - Reflect known data noise structure; Gaussian, Poisson, etc
  - The modeler's choice of metric for measuring misfit "distance" between data and model predictions
- Regularization
  - Optimization regularization term
  - Subjective choices; Prior information
  - Previous measurement

ℓ_1 norm fitting

- The ℓ_1-norm is of particular interest

$$
\begin{aligned}
||y - g(x,\theta)||_1 &= \frac{1}{N}\sum_{i=1}^{N} |y_i - g(x_i,\theta)| \\
||J(\theta)||_1 &= \frac{1}{M}\sum_{k=1}^{M} |J(\theta_k)|
\end{aligned}
$$

- The ℓ_1-norm is useful because it *automatically* identifies **sparsity** in the model, when
  - there is underlying sparsity
  - the model is linear in the parameters

Sparsity

- A sparse model is one that provides reliable predictions with only small number of its parameters being non-zero
  - Physical models: usually **sparse** in prediction of **smooth** observables
- Consider *e.g.* a chemical model for a hydrocarbon fuel
  - thousands of reactions $\Rightarrow$ thousands of parameters
- Not **all** these parameters are important for smooth quantities of interest
  - *e.g.* laminar flame burning speed S_L
- Full dimensionality for a chemical model with N reactions

$$S_L = f\left((A,n,E)_1, \cdots, (A,n,E)_N\right), \quad N \sim 10^4 \text{ (Hydrocarbon fuel)}$$

  Intrinsic dimensionality

$$S_L = g\left((A,n,E)_1, \cdots, (A,n,E)_K\right), \quad K \sim 10 \text{ (important reactions)}$$

- For linear models, ℓ_1-norm constrained ℓ_2 fitting allows identification of the underlying sparse structure of the model

Sparse regression

Model:

$$y = f(x) \simeq \sum_{k=0}^{K-1} c_k \Psi_k(x)$$

with $x \in \mathbb{R}^n$, Ψ_k max order p, and $K = (p+n)!/p!/n!$

- N samples $(x_1, y_1), \dots, (x_N, y_N)$
- Estimate K terms $c_0, \dots, c_{K-1}$, s.t.

$$\min ||\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}||_2^2$$

$$\text{where } \boldsymbol{y} \in \mathbb{R}^N,\ \boldsymbol{c} \in \mathbb{R}^K,\ \boldsymbol{A}_{ik} = \Psi_k(x_i),\ \boldsymbol{A} \in \mathbb{R}^{N \times K}$$

With $N << K \Rightarrow$ under-determined

- Need some form of regularization

Regularization – Compressive Sensing (CS)

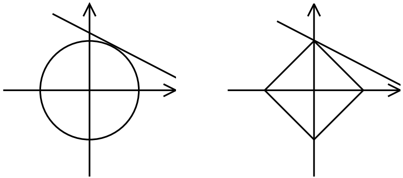
- ℓ_2-norm — Tikhonov regularization; Ridge regression:

$$\min \left\{ \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}\|_2^2 + \|\boldsymbol{c}\|_2^2 \right\}$$

- ℓ_1-norm — Compressive Sensing; LASSO; basis pursuit

$$\begin{aligned} \min \left\{ \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}\|_2^2 + \|\boldsymbol{c}\|_1 \right\} & \\ \min \left\{ \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}\|_2^2 \right\} & \quad \text{subject to } \|\boldsymbol{c}\|_1 \leq \epsilon \\ \min \left\{ \|\boldsymbol{c}\|_1 \right\} & \quad \text{subject to } \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}\|_2^2 \leq \epsilon \end{aligned}$$

$\Rightarrow$ discovery of sparse signals



Statistical Inverse Problem

Motivation

- Empirical data D generally provides noisy measurements of y
- Best fit λ is uncertain
- Seeking a single best-fit answer contributes to ill-conditioning

Recasting as a statistical inverse problem improves conditioning

- Solve for a set of solutions, rather than a best fit answer
- Statistical formulation
  - Use statistical methods to estimate confidence intervals on λ
- Formulation as a **Bayesian** inverse problem – Bayesian inference
  - Use probability to describe degree of belief about λ
  - Discrepancy between model and data represented using statistical models
  - Build a data model mapping λ to D
  - Solve for $p(\lambda|D)$

Bayes formula for Parameter Inference

- Data Model (fit model with noise)
- Introduce random variable (field) $\epsilon(\omega)$ to model data misfit

$$y = f(\lambda, \epsilon)$$

- Bayes Formula:

$$p(\lambda, y) = p(\lambda|y)p(y) = p(y|\lambda)p(\lambda)$$

$$\underbrace{p(\lambda|y)}_{\text{Posterior}} = \frac{\overbrace{p(y|\lambda)}^{\text{Likelihood}}\;\overbrace{p(\lambda)}^{\text{Prior}}}{\underbrace{p(y)}_{\text{Evidence}}}$$

- Prior: knowledge of λ prior to data
- Likelihood: forward model and measurement noise
- Posterior: combines information from prior and data
- Evidence: normalizing constant for present context

Advantages of Bayesian Methods

- Formal means of logical inference and machine learning
- Means of incorporation of prior knowledge/measurements and heterogeneous data
- Full probabilistic description of uncertain parameters
- General means of handling nuisance parameters through marginalization
- Means of identification of *optimal* model complexity
  - Ockham's razor
  - Only as much complexity as is required by the physics, and no more
  - Avoid fitting to noise

The Prior

- Prior $p(\lambda)$ comes from
  - Physical constraints, prior data, Prior knowledge
- The prior can be **uninformative**
- It can be chosen to impose **regularization**
- Unknown aspects of the prior can be added to the rest of the parameters as hyperparameters

Examples:

- $\lambda \sim U(1,5)$ – Uniform distribution between 1 and 5
- $\lambda \sim N(\mu, \sigma^2)$
  - Normal distribution with mean μ and standard deviation σ
  - (μ, σ) hyper/nuisance parameters to be inferred from data

Note:

- The prior can be crucial when there is little information in the data
- When there is sufficient information in the data, the data can overrule the prior

Construction of the Likelihood $p(y|\lambda)$

- Where does probability enter the mapping $\lambda \to y$ in $p(y|\lambda)$?
- Through a presumed error model:
- Example:
  - Model:

$$y_m = f(\lambda)$$

  - Data: y
  - Error between data and model prediction: ϵ

$$y = f(\lambda) + \epsilon$$

- Model this error as a random variable
- Example
  - Error is due to instrument measurement noise
  - Instrument has Gaussian errors, with no bias

$$\epsilon \sim N(0, \sigma^2)$$

Construction of the Likelihood $p(y|\lambda)$ – cont'd

For any given λ, this implies

$$y|\lambda, \sigma \sim N(f(\lambda), \sigma^2)$$

or

$$p(y|\lambda, \sigma) = \frac{1}{\sqrt{2\pi}\,\sigma} \exp\left(-\frac{(y - f(\lambda))^2}{2\sigma^2}\right)$$

Given N measurements $(y_1, \dots, y_N)$, and presuming independent identically distributed (*iid*) noise

$$\begin{aligned} y_i &= f(\lambda) + \epsilon_i \\ \epsilon_i &\sim N(0, \sigma^2) \\ L(\lambda) = p(y_1, \dots, y_N|\lambda, \sigma) &= \prod_{i=1}^{N} p(y_i|\lambda, \sigma) \end{aligned}$$

Construction of the Likelihood $p(y|\lambda)$ – cont'd

It is useful to use the log-Likelihood

$$\ln L(\lambda) = -\frac{1}{2} N \ln \sigma^2 - \frac{N}{2} \ln(2\pi) - \frac{1}{2} \sum_{i=1}^{N} \left[\frac{y_i - f(\lambda)}{\sigma} \right]^2$$

Frequently, signal noise amplitude is not constant
e.g. σ varies with signal amplitude
then

$$\ln L(\lambda) = -\frac{1}{2} \sum_{i=1}^{N} \ln \sigma_i^2 - \frac{N}{2} \ln(2\pi) - \frac{1}{2} \sum_{i=1}^{N} \left[\frac{y_i - f(\lambda)}{\sigma_i} \right]^2$$

Construction of the Likelihood $p(y|\lambda)$ – cont'd

Recall that the weighted least-squares data mis-fit is given by

$$\chi^2 = \sum_{i=1}^{N} \left[\frac{y_i - f(\lambda)}{\sigma_i} \right]^2$$

and the best-fit estimate of λ is

$$\lambda_{\mathrm{rms}} = \underset{\lambda}{\operatorname{argmin}}(\chi^2(\lambda))$$

Minimizing χ^2 is equivalent to maximizing the likelihood
Maximum Likelihood Estimate (MLE):

$$\lambda_{\mathrm{MLE}} \equiv \lambda_{\mathrm{rms}}$$

Exploration of the likelihood provides for a more general examination of quality of fit than χ^2

Likelihood Modeling

- This is frequently the *core* modeling challenge
  - Error model: a statistical model for the discrepancy between the forward model and the data
  - composition of the error model with the forward model
- Error model composed of discrepancy between
  - data and the truth – (data error)
  - model prediction and the truth – (model error)
- Mean bias and correlated/uncorrelated noise structure
- Hierarchical Bayes modeling, and dependence trees

$$p(\phi, \theta | D) = p(\phi | \theta, D) p(\theta | D)$$

- Choice of observable – constraint on Quantity of Interest?

Experimental Data

- Empirical data error model structure can be informed based on knowledge of the experimental apparatus
- Both bias and noise models are typically available from instrument calibration
- Noise PDF structure
  - A counting instrument would exhibit Poisson noise
  - A measurement combining many noise sources would exhibit Gaussian noise
- Noise correlation structure
  - Point measurement
  - Field measurement

Posterior

$$p(\lambda|y) \propto p(y|\lambda)p(\lambda)$$

Continuing the above *iid* Gaussian likelihood example, consider also an *iid* Gaussian prior on λ with

$$\lambda \sim N(m, s^2)$$

$$p(\lambda) = \frac{1}{\sqrt{2\pi}\, s} \exp\left(-\frac{(\lambda - m)^2}{2s^2}\right)$$

Posterior cont'd

Then the posterior is

$$p(\lambda|y) \propto_\lambda \; e^{-||y-f(\lambda)||} \; e^{-||\lambda-m||}$$

and the log posterior is

$$\ln p(\lambda|y) \;\; = \;\; -||y - f(\lambda)|| - ||\lambda - m|| + C_\lambda$$

Thus, the maximum a-posteriori (MAP) estimate of λ is equivalent to the solution of the regularized least-squares problem

$$\underset{\lambda}{\operatorname{argmin}}(||y - f(\lambda)|| + ||\lambda - m||)$$

The prior plays the role of a regularizer

Line fitting example

Consider the fitting of a straight line

$$y_m = ax + b$$

to data $D = \{(x_i, y_i),\ i = 1, \dots, N\}$.
Consider an (improper) uninformative prior

$$\pi(a, b) = \mathrm{Const}$$

providing no prior information on (a, b).
Assume *iid* additive unbiased Gaussian noise in y with a given constant noise variance σ^2, thus the data model is:

$$y = ax + b + \epsilon, \qquad \epsilon \sim N(0, \sigma^2)$$

with no noise in the independent variable x.

Line fitting example

Presuming σ known, we have the likelihood,

$$L(a,b) = p(D|a,b) = \prod_{i=1}^{N} p(y_i|a,b)$$

where

$$p(y_i|a,b) = \frac{1}{\sqrt{2\pi}\,\sigma} \exp\left(-\frac{(y_i - ax_i - b)^2}{2\sigma^2}\right)$$

and, per Bayes formula, the posterior density $p(a,b|D)$ is

$$p(a,b|D) \quad = \quad \frac{p(D|a,b)\pi(a,b)}{p(D)} \propto p(D|a,b)\pi(a,b)$$

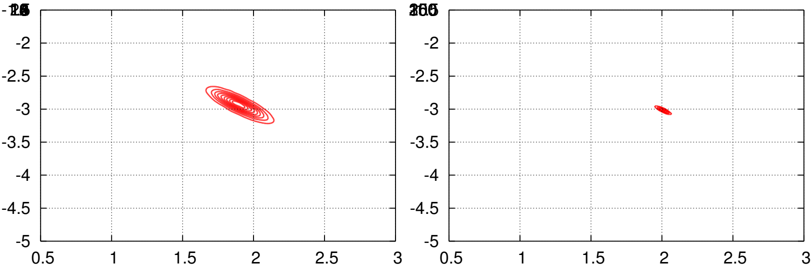
Line fitting example – cont'd

The posterior on (a, b) is the two-dimensional Multivariate Normal (MVN) distribution

$$
\begin{aligned}
p(a, b|D) &\propto (2\pi\sigma^2)^{-N/2} \prod_{i=1}^{N} \exp\left(-\frac{(y_i - ax_i - b)^2}{2\sigma^2}\right) \\
&\propto (2\pi\sigma^2)^{-N/2} \exp\left(-\sum_{i=1}^{N} \frac{(y_i - ax_i - b)^2}{2\sigma^2}\right)
\end{aligned}
$$

Linear model, Gaussian noise, σ-given, and a Gaussian or constant-uninformative prior.

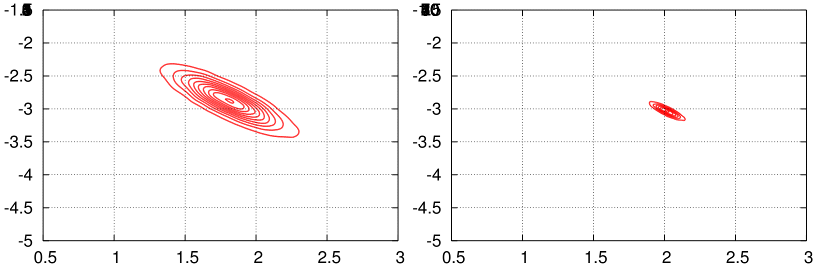
Line fitting example – Effect of data size on $p(a, b|D)$ Low data noise: $\sigma = 0.25$



$N = 20$ $N = 200$

- More data $\Rightarrow$ more accurate parameter estimates

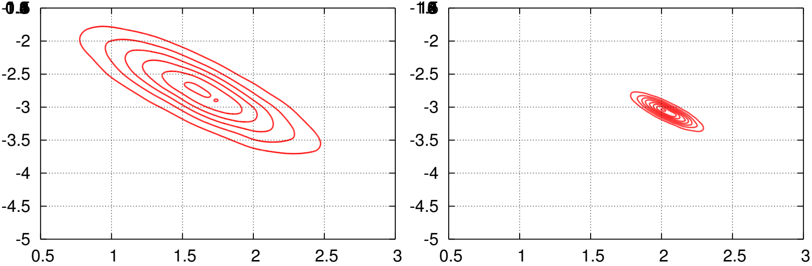
Line fitting example – Effect of data size on $p(a,b|D)$ Medium data noise: $\sigma = 0.5$



$N = 20$ $N = 200$

- More data $\Rightarrow$ more accurate parameter estimates
- Higher noise amplitude $\Rightarrow$ higher uncertainty

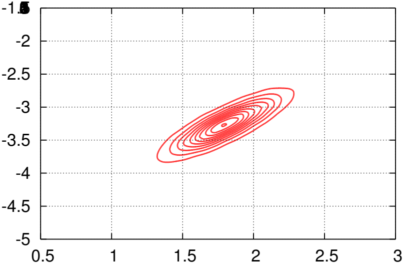
Line fitting example – Effect of data size on $p(a,b|D)$ High data noise: $\sigma = 1.0$



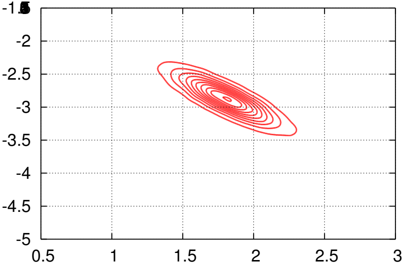
$N = 20$ $N = 200$

- More data $\Rightarrow$ more accurate parameter estimates
- Higher noise amplitude $\Rightarrow$ higher uncertainty

Line fitting example – Effect of data range on $p(a, b|D)$ Medium data noise: $\sigma = 0.5$



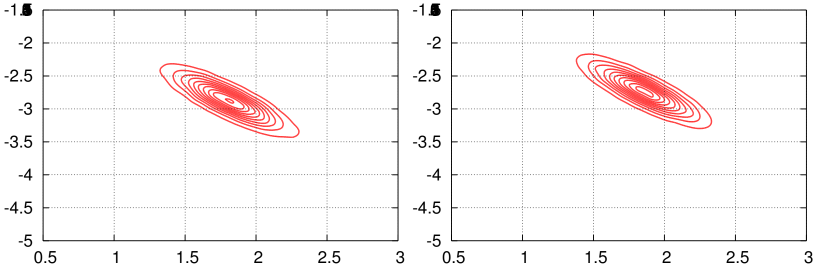
$x \in [-2, 0]$



$x \in [0, 2]$

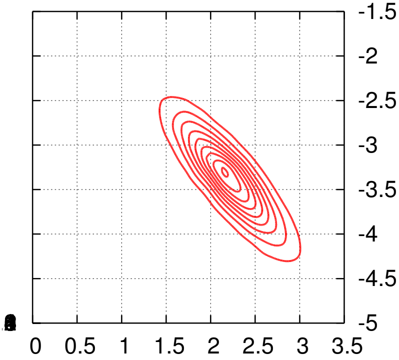
- Posterior correlation structure depends on subjective details of the experiment

Line fitting – Effect of data realization on $p(a, b|D)$
Medium data noise: $\sigma = 0.5$

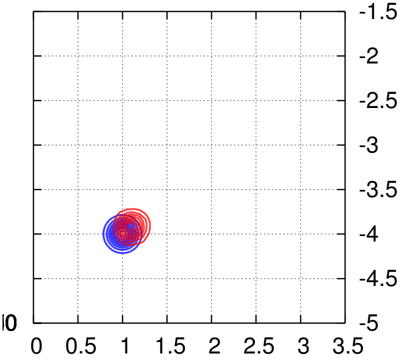


- Posterior depends on specific measured data set
- Two data sets, each with $N = 20$

Line fitting example – prior vs. data-size
20 data points

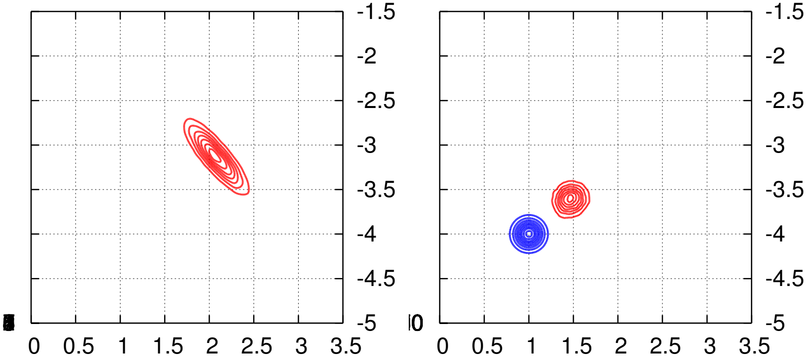


Constant uninformative prior



Gaussian prior

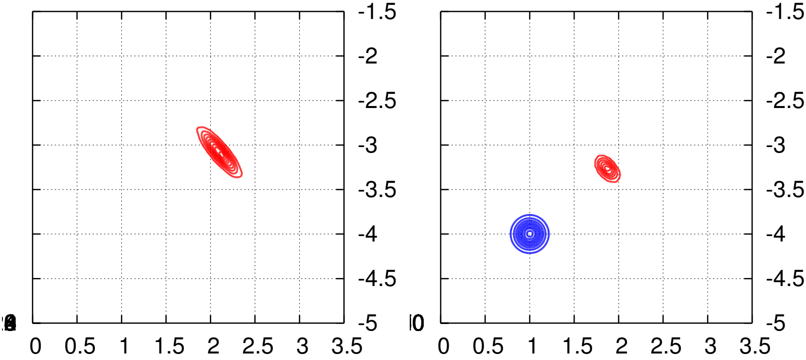
Line fitting example – prior vs. data-size 80 data points



Constant uninformative prior

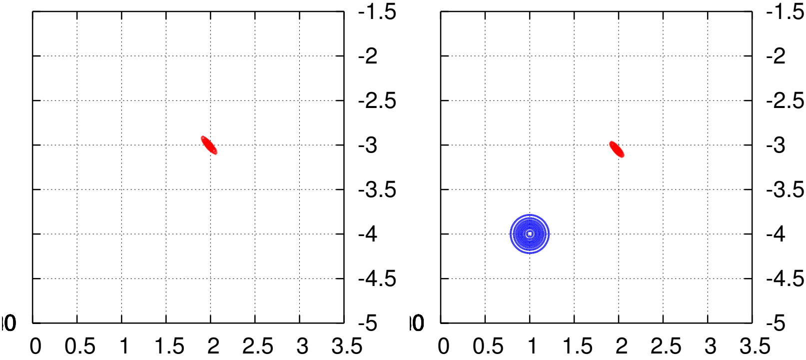
Gaussian prior

Line fitting example – prior vs. data-size
200 data points



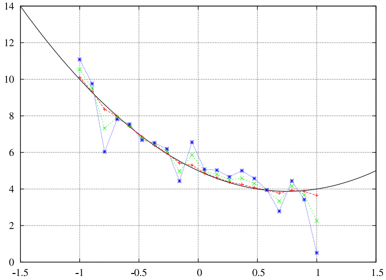
Constant uninformative prior   Gaussian prior

Line fitting example – prior vs. data-size
2000 data points



Constant uninformative prior | Gaussian prior

Bayesian inference illustration: noise↑ ⇒ uncertainty↑



- data: $y = 2x^2 - 3x + 5 + \epsilon$
- $\epsilon \sim \mathcal{N}(0, \sigma^2)$, $\sigma = \{0.1, 0.5, 1.0\}$
- Fit model $y = ax^2 + bx + c$

Marginal posterior density $p(a, c)$:

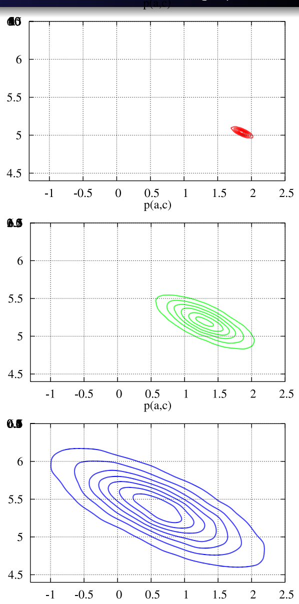
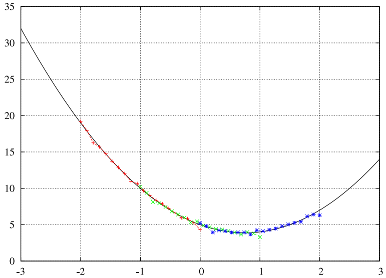
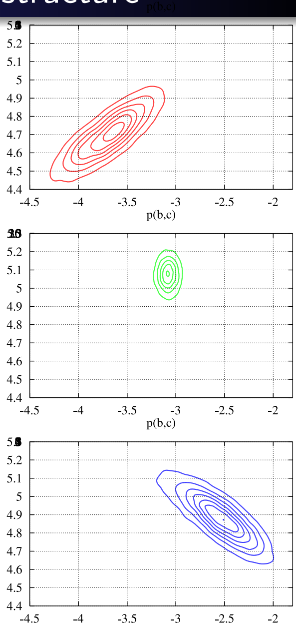


Illustration: Data range ⇒ correlation structure

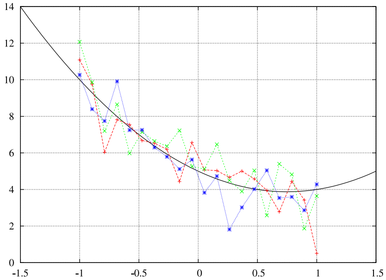


- data: $y = 2x^2 - 3x + 5 + \epsilon$
- $\epsilon \sim \mathcal{N}(0, 0.04)$
- ranges: $x \in \{[-2,0],[-1,1],[0,2]\}$
- Fit model $y = ax^2 + bx + c$

Marginal posterior density $p(b,c)$:

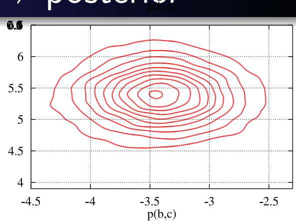


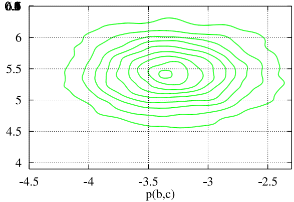
Bayesian illustration: Data realization ⇒ posterior

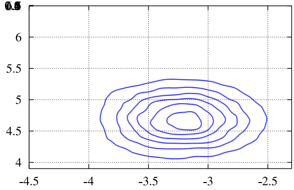


- data: $y = 2x^2 - 3x + 5 + \epsilon$
- $\epsilon \sim \mathcal{N}(0,1)$
  - 3 different random seeds
- Fit model $y = ax^2 + bx + c$

Marginal posterior density $p(b,c)$:







Bayesian Regression

- Bayes formula

$$p(\boldsymbol{c}|D) \propto p(D|\boldsymbol{c})\pi(\boldsymbol{c})$$

- Bayesian regression: prior as a regularizer, *e.g.*
  - Log Likelihood $\Leftrightarrow$ $\|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}\|_2^2$
  - Log Prior $\Leftrightarrow$ $\|\boldsymbol{c}\|_p^p$
- Laplace sparsity priors $\pi(c_k|\alpha) = \frac{1}{2\alpha} e^{-|c_k|/\alpha}$
- LASSO (Tibshirani 1996) ... formally:

$$\min \left\{ \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{c}\|_2^2 + \lambda\|\boldsymbol{c}\|_1 \right\}$$

Solution $\sim$ the posterior mode of $\boldsymbol{c}$ in the Bayesian model

$$y \sim \mathcal{N}(\boldsymbol{A}\boldsymbol{c}, I_N), \qquad c_k \sim \frac{1}{2\alpha} e^{-|c_k|/\alpha}$$

- Bayesian LASSO (Park & Casella 2008)

Bayesian Compressive Sensing (BCS)

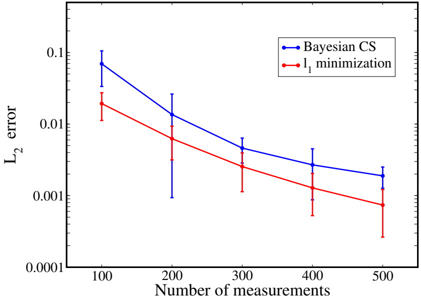
- BCS (Ji 2008; Babacan 2010)— hierarchical priors:
  - Gaussian priors $\mathcal{N}(0, \sigma_k^2)$ on the c_k
  - Gamma priors on the σ_k^2

  $\Rightarrow$ Laplace sparsity priors on the c_k
- Evidence maximization establishes ML estimates of the σ_k
  - many of which are found $\approx 0 \quad \Rightarrow \quad c_k \approx 0$
  - iteratively include terms that lead to the largest increase in the evidence
- iterative BCS (iBCS) (Sargsyan 2012):
  - adaptive iterative order growth
  - BCS on order-p Legendre-Uniform PC
  - repeat with order-$p+1$ terms added to surviving p-th order terms

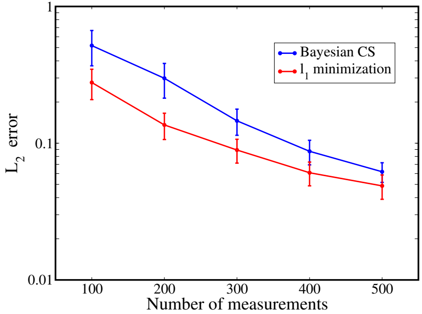
CS and BCS

Corner-peak Genz function

- $f(x) = (1 + \sum_{i=1}^{n} a_i x_i)^{-(n+1)}; \quad a_i \propto 1/i^2$
- Legendre-Uniform PC, 10^{th}-order/5d; 5^{th}-order/10d



5d

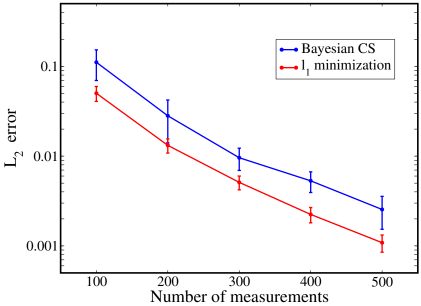


10d

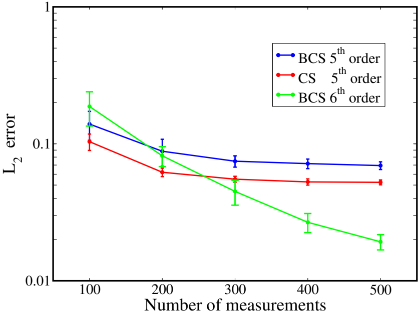
CS and BCS

Oscillatory Genz function

- $f(x) = \cos(2\pi r + \sum_{i=1}^{n} a_i x_i); \quad a_i \propto 1/i^2; \quad r = 0$
- Legendre-Uniform PC, 10^{th}-order/5d; $(5,6)^{th}$-order/10d

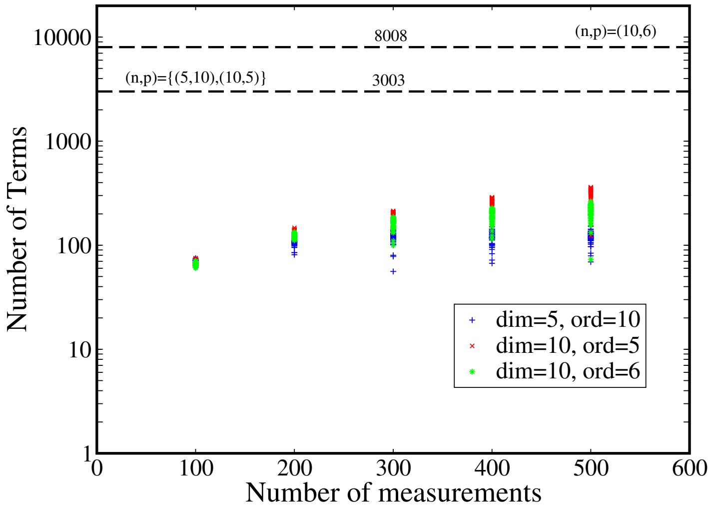


5d

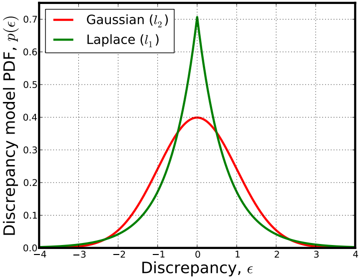


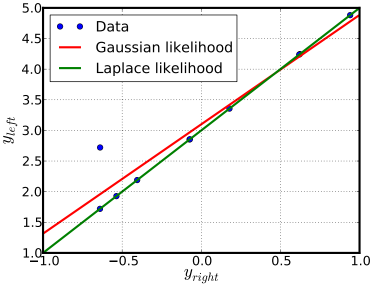
10d

Oscillatory function – BCS number of terms



ℓ_1 norm fitting – Robustness to outliers





- Using ℓ_1-norm fitting, or Laplace likelihood, provides significant robustness to outliers
- The ℓ_1-norm effectively minimizes the number of significant error terms
  - Neglects occasional outlier with large error

Exploring the Posterior – MCMC

- Given any sample λ, the un-normalized posterior probability can be easily computed

$$p(\lambda|y) \propto p(y|\lambda)p(\lambda)$$

- Explore posterior w/ Markov Chain Monte Carlo (MCMC)
  - Metropolis-Hastings algorithm:
    - Random walk with proposal PDF & rejection rules
  - Computationally intensive, $\mathcal{O}(10^5)$ samples
  - Each sample: evaluation of the forward model
    - Surrogate models
- Evaluate moments/marginals from the MCMC statistics

Metropolis-Hastings MCMC sampling of density $\pi(x)$

Algorithm:

- Given a starting point x_0 and proposal density $p(y|x_n)$
- Draw a proposed sample y from proposal density
- Calculate acceptance ratio

$$\alpha(x_n, y) = \min\left\{1, \frac{\pi(y)q(x_n|y)}{\pi(x_n)q(y|x_n)}\right\}$$

- Put

$$x_{n+1} = \begin{cases} y, & \text{with probability } \alpha(x_n, y) \\ x_n, & \text{with probability } 1 - \alpha(x_n, y) \end{cases}$$

Note:

- If $q(y|x_n) \propto \pi(y)$ then $\alpha = 1$
- q does not have to be symmetric.
- π need be evaluated only up to a multiplicative constant

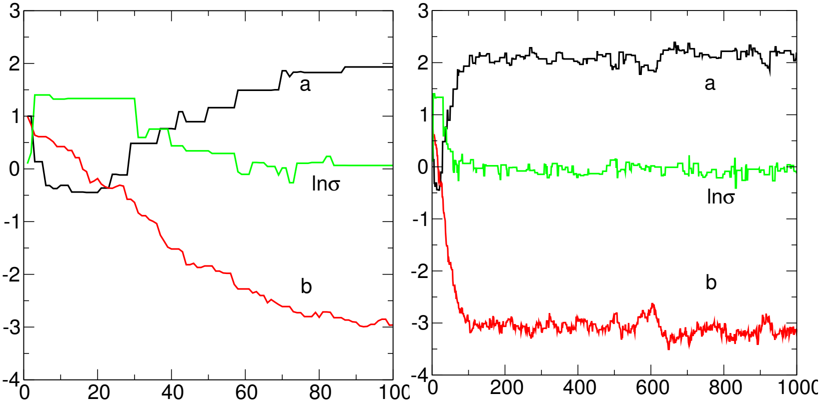
Adaptive Metropolis

- Idea: learn a better proposal $q(y|x)$ from past samples.
  - Learn an appropriate proposal **scale**.
  - Learn an appropriate proposal **orientation** and anisotropy; this is *essential* in problems with strong correlation in π
- Adaptive Metropolis scheme of [Haario *et al.* 2001]:
  - Covariance matrix at step n

    $$C_n^* = s_d \mathbf{Cov}\left(x_0, \ldots, x_n\right) + s_d \epsilon I_d$$

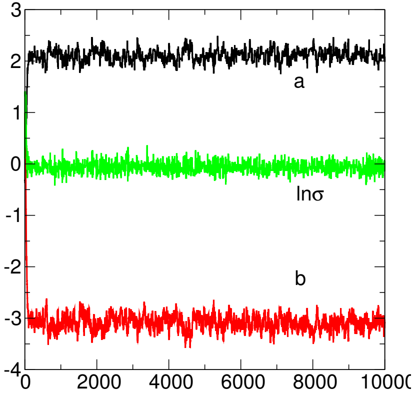
    where $\epsilon > 0$, d is the dimension of the state, and $s_d = 2.4^2/d$ (scaling rule-of-thumb).
  - Proposals are Gaussians centered at x_n.
  - Use fixed covariance C_0 for the first n_0 steps, then use C_n^*.
  - Chain is not Markov.
  - Nonetheless, one can prove that the chain converges to π
- Other adaptive MCMC ideas have been developed

Line fitting example – MCMC – $(a, b, \ln\sigma)$ samples



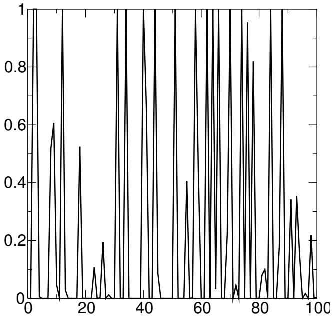
- Initial transient "Burn-in" period, ≈ 100 steps
- Problem and initial condition dependent

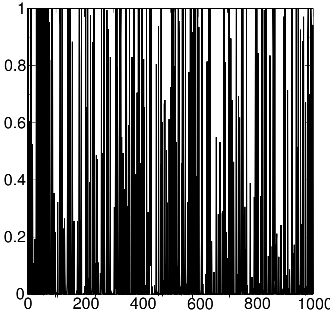
Line fitting example – MCMC – $(a, b, \ln\sigma)$ samples



- Visual inspection reveals “good mixing”
- No significant long-term correlation or periodicity

Line fitting example – MCMC – acceptance probability

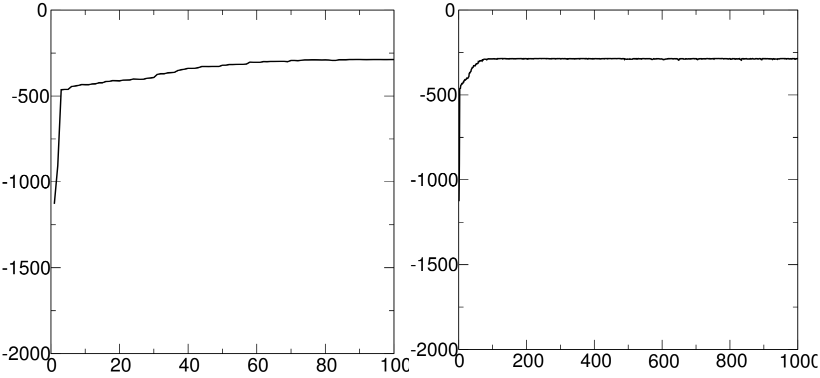




- An average acceptance probability of ~ 0.2 is "good"
- A typical compromise between accepting most samples
    - not moving much, strong correlation

  and rejecting most samples
    - moving too far off, wasted CPU time in rejections

Line fitting example – MCMC – posterior density



- Chain finds high posterior density (HPD) region
- stays there generating many random samples

MCMC practicalities

Effective use of MCMC still requires some (problem-specific) experience. Some useful rules of thumb:

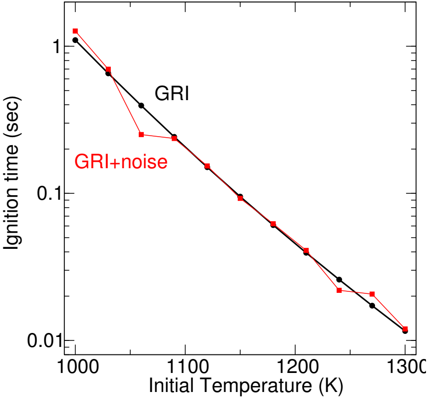
- Adaptive schemes are not a panacea.
- Whenever possible, parameterize the problem in order to minimize posterior correlations.
- What to do, if anything, about "burn-in?"
- Visual inspection of chain components is often the first and best convergence diagnostic.
- Also look at:
  - autocorrelation plots
  - multivariate potential scale reduction factor (MPSRF, Gelman & Brooks)
  - and other diagnostics.
- Optimal acceptance rates? Maybe ... $\sim$0.2
  - But in practice it's best to explore chain diagnostics

Chemical Rate Parameter Estimation example

Synthetic ignition data generated using a detailed model+noise

- Ignition using GRImech3.0 methane-air chemistry
- Ignition time versus Initial Temperature
- Multiplicative noise error model
- 11 data points:

$$\tau_i^d = \tau^{\mathrm{GRI}}(T_i^o)\,(1 + \sigma\epsilon_i)$$
$$\epsilon \sim N(0,1)$$

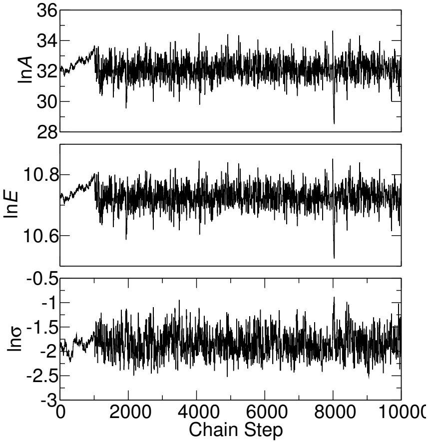


Fitting with a simple chemical model

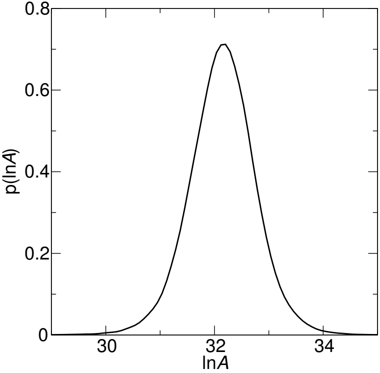
- Fit a global single-step irreversible chemical model

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$
$$\mathfrak{R} = [CH_4][O_2]k_f$$
$$k_f = A\exp(-E/R^oT)$$

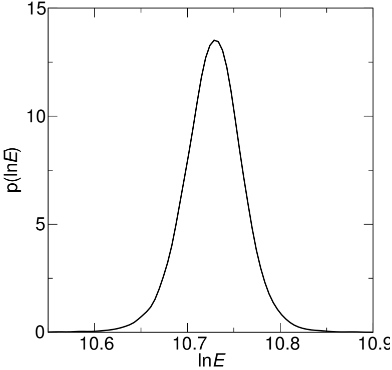
- Infer 3-D parameter vector $(\ln A, \ln E, \ln\sigma)$
- Good mixing with adaptive MCMC when start at MLE



Marginal Posteriors on $\ln A$ and $\ln E$

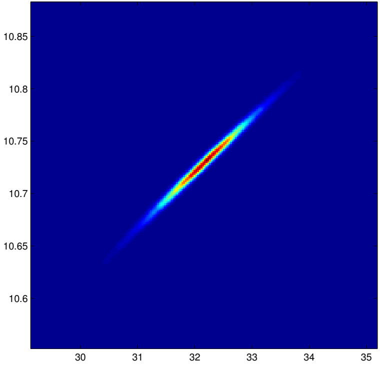


$$\ln A = 32.15 \pm 3 \times 0.61$$

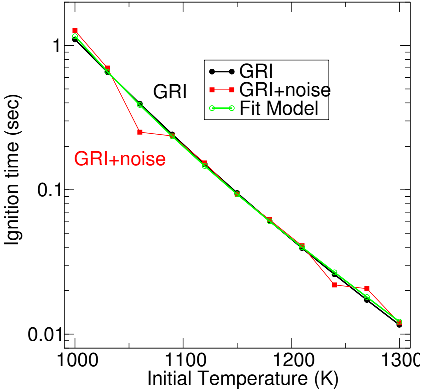


$$\ln E = 10.73 \pm 3 \times 0.032$$

Bayesian Inference Posterior and Nominal Prediction



Marginal joint posterior on $(\ln A, \ln E)$ exhibits strong correlation



Nominal fit model is consistent with the true model

Approximate Bayesian Computation (ABC)

- Data model: $y = f(x, \lambda) + \epsilon_{\mathrm{d}}, \qquad \epsilon_{\mathrm{d}} \sim N(0, \sigma^2)$ and $\alpha \equiv (\lambda, \sigma)$
- Full Likelihood: $L(\alpha) = p(D|\alpha) = p(y_{\mathrm{d}}|\alpha)$
- Often, the likelihood cannot be formulated or is too costly to compute, e.g.

$$
\begin{aligned}
L(\alpha) &:= L^*(\alpha)Z(\alpha) \quad \text{where } Z(\alpha) \text{ is unknown} \\
L(\alpha) &:= \int L^*(\alpha, u)\mathrm{d}u \quad \text{where } u \text{ is high dimensional}
\end{aligned}
$$

Resolution:

- Bypass computation of Likelihood
- Generate replicate data samples z from the data model
- Employ a pseudo-likelihood based on a kernel density that enforces select constraints on the predictions z
    - Constraint employs some distance measure between y_d and z

ABC Likelihood

With $\rho(\mathcal{S})$ being a metric of the statistic $\mathcal{S}$, use the kernel function as an ABC likelihood:

$$L_{\mathrm{ABC}}(\alpha) = \frac{1}{\epsilon} K\left(\frac{\rho(\mathcal{S})}{\epsilon}\right)$$

where ϵ controls the severity of the consistency control

Example, enforce the mean data prediction

$$\mathcal{S}(y) = \mathrm{E}(y) = \mu_y$$

with $z = z(\alpha)$, and

$$\rho(\mathcal{S}) := \mu_z(\alpha) - \mu_{y_d}$$

Propose the Gaussian kernel density:

$$L_\epsilon(\alpha) = \frac{1}{\epsilon\sqrt{2\pi}} \exp\left(-\frac{(\mu_z(\alpha) - \mu_{y_d})^2}{2\epsilon^2}\right)$$

Model UQ

- No model of a physical system is strictly true
- The probability of a model being strictly true is zero
- Given limited information, some models may be relied upon for describing the system

Let $\mathcal{M} = \{M_1, M_2, ...\}$ be the set of all models

- $p(M_k|I)$ is the probability that M_k is the model behind the available information
    - Model Plausibility
- Parameter estimation from data is conditioned on the model

$$p(\theta|D, M_k) = \frac{p(D|\theta, M_k)\pi(\theta|M_k)}{p(D|M_k)}$$

Bayesian Model Comparison

Evidence (marginal likelihood) for M_k:

$$p(D|M_k) = \int p(D|\theta, M_k)\pi(\theta|M_k)\mathrm{d}\theta$$

Bayes Factor B_{ij}:

$$B_{ij} = \frac{p(D|M_i)}{p(D|M_j)}$$

Plausibility of M_k:

$$p(M_k|D, \mathcal{M}) = \frac{p(D|M_k)\ \pi(M_k|\mathcal{M})}{\sum_s p(D|M_s)\pi(M_s|\mathcal{M})} \qquad k = 1, \ldots$$

Posterior odds:

$$\frac{p(M_i|D, \mathcal{M})}{p(M_j|D, \mathcal{M})} = B_{ij}\ \frac{\pi(M_i|\mathcal{M})}{\pi(M_j|\mathcal{M})}$$

Marginal Likelihood example

- Consider Fitting with data from a truth model

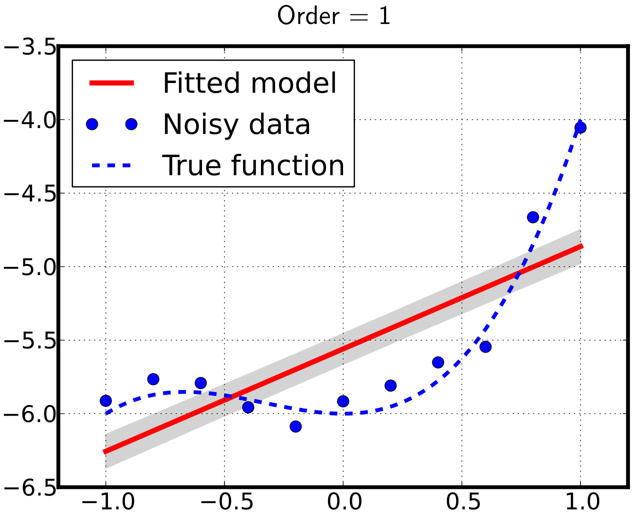
$$y_t = x^3 + x^2 - 6$$

- Gaussian *iid* additive noise model with fixed variance s
- Bayesian regression with a Gaussian Likelihood, *iid* and given s
- Consider a set of Legendre Polynomial expansion models, order 1-10

$$y_m = \sum_{k=0}^{P} c_k \psi_k(x)$$

- Uniform priors $[-D, D]$ on all coefficients

Too much model complexity leads to overfitting



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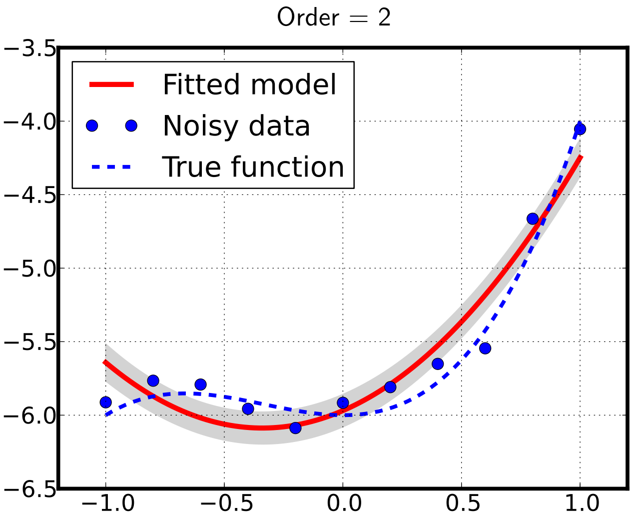

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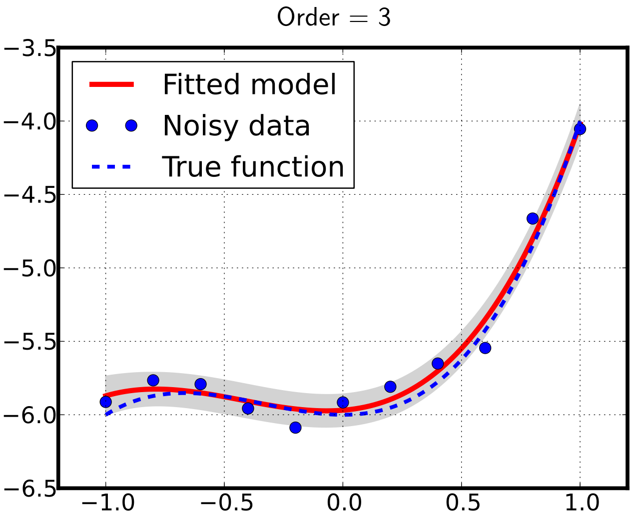

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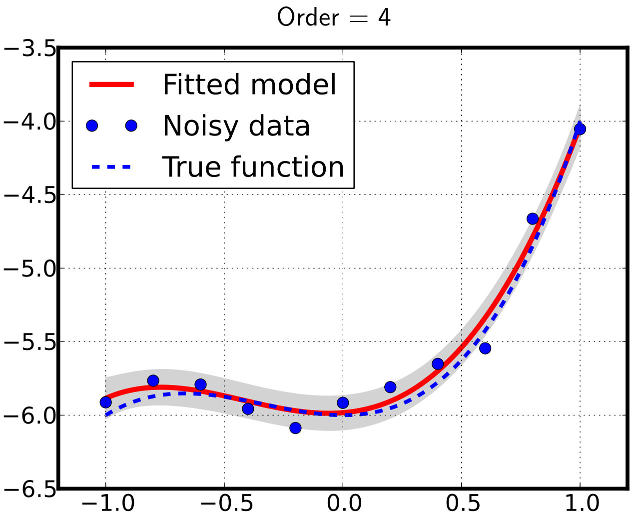

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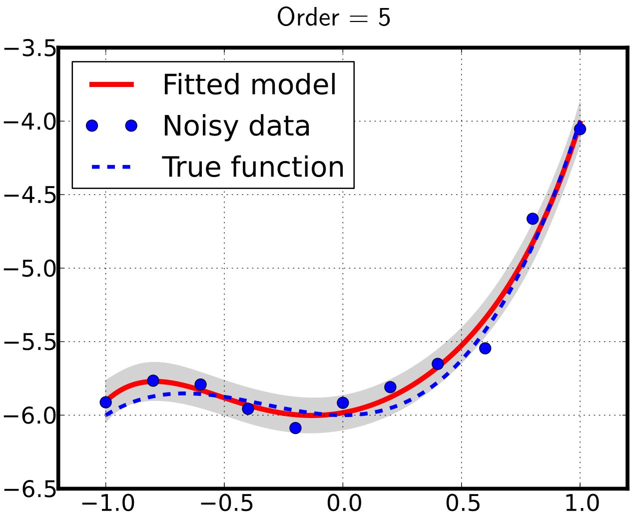

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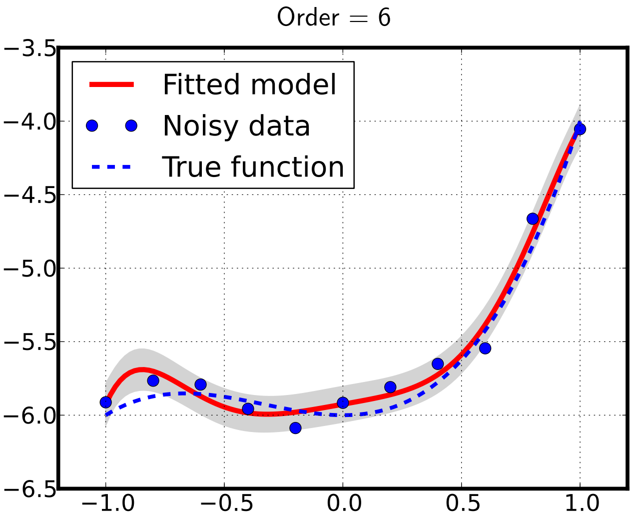

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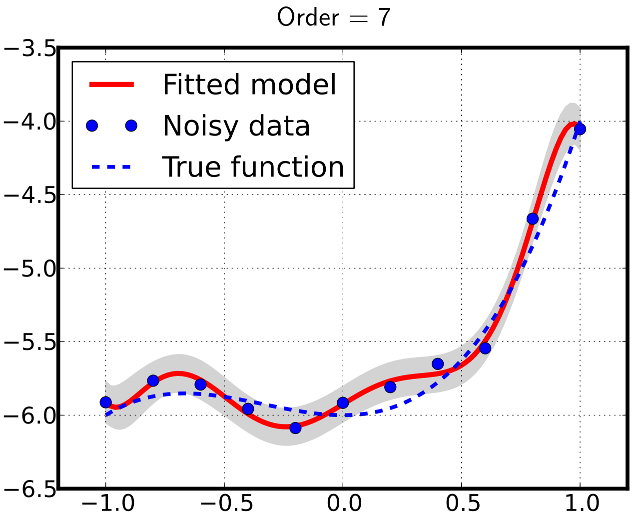

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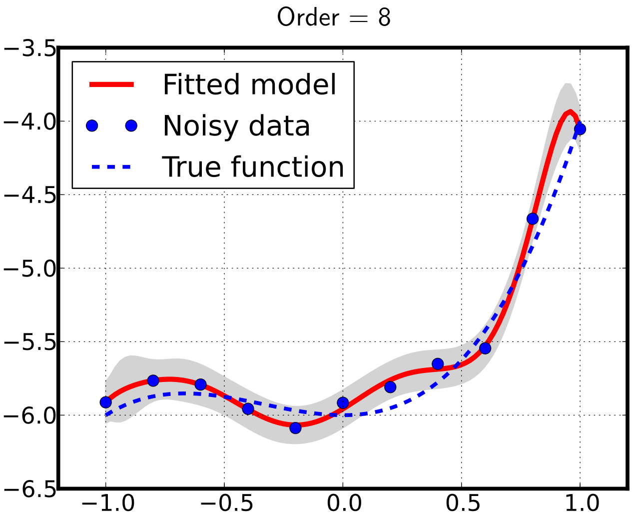

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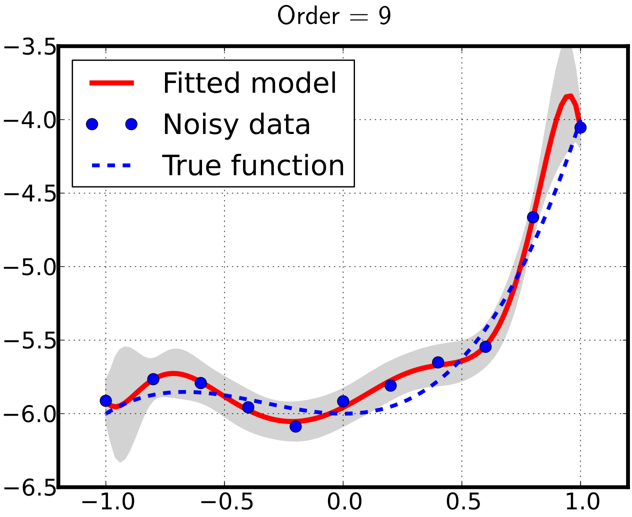

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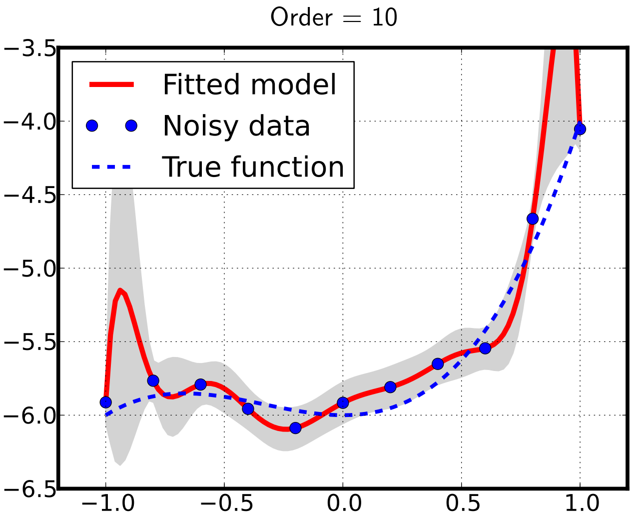
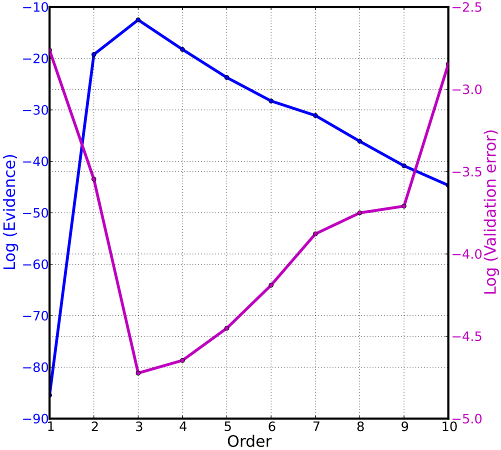


Evidence and Validation Error

Log Evidence:

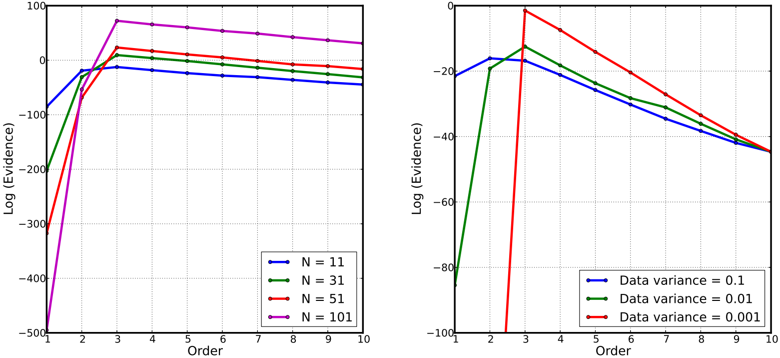
$$\ln p(D|M_k)$$



- Validation error – ℓ_2 error for a random set of 1000 points
  - Minimal at 3rd-order
- Log evidence: sum of two scores, balances complexity & fit
  - Peaks at 3rd order

Muto & Beck 2008

Evidence – Discrimination among Models



- Discrimination among models is more clear-cut with higher amount of data D and/or less data noise

Prediction

Consider that a model

$$y_m = f(x, \lambda)$$

was fitted according to

$$y = f(x, \lambda) + \epsilon, \quad \epsilon \sim N(0, \sigma^2),$$

providing:

- The posterior $p(\lambda, \sigma|D)$
- The marginal posterior $p(\lambda|D)$

Define:

- Pushed forward posterior (PFP) distribution : $p(y_m|x, D)$
- Posterior predictive (PP) distribution : $p(y|x, D)$

Pushed forward posterior (PFP)

- PFP distribution $p(y_m|x, D)$
- Push-forward of the marginal posterior measure on λ through $f(x, \lambda)$
- PFP random process

$$
\begin{aligned}
Y_m(x, \omega) &= f(x, \lambda(\omega)) \\
&\sim p(y_m|x, D)
\end{aligned}
$$

- The PFP provides the uncertain prediction by the calibrated model
  - Forward UQ
  - Mean prediction $E[Y_m]$
  - Predictive variance $V[Y_m]$

Posterior Predictive (PP)

Posterior Predictive distribution $p(y|x, D)$

- With $\alpha \equiv (\lambda, \sigma)$,

$$p(y|x, D) = \int p(y|x, \alpha, D)p(\alpha|D)\mathrm{d}\alpha$$

PP random process

$$\begin{aligned} Y^{PP}(x, \omega) &= \mathrm{E}_\alpha[Y(x, \omega)] \\ &\sim p(y|x, D) \end{aligned}$$

provides the marginal prediction of the data. Where

$$Y(x, \omega) = f(x, \lambda) + \epsilon(\omega, \sigma)$$

is the PP data predictor

- Posterior predictive check – evaluate distance between the PP and the actual/empirical distribution of the data

Validation

- Validity is a statement of model utility for predicting a given observable under given conditions
- Inspection of model utility requires accounting for uncertainty
- Statistical tool-chest for model validation
  - Cross-validation
  - Bayes Factor
  - Model Plausibility
  - Posterior Odds
  - Posterior predictive:

$$p(\tilde{D}|D, M_k) = \int p(\tilde{D}|\theta, M_k) p(\theta|D, M_k) d\theta$$

Model Averaging

- When multiple models are acceptable, and no model is a clear winner, model averaging can be used to provide a prediction of interest
- If prediction errors among models are uncorrelated, then averaging is expected to reduce prediction errors
  - Not likely if models are dependent, or if they have comparable large bias errors in a given observable of interest
- Bayesian Model Averaging

$$p(\phi|D,\mathcal{M}) = \sum_{k=1}^{N} p(\phi|D,M_k)p(M_k|D,\mathcal{M})$$

where

$$\mathcal{M} = \{M_1,\ldots,M_N\}$$

Closure

- Inverse problems are ubiquitous in science and engineering
- Where possible, employing the Bayesian framework provides for more robust, reliable and informed solutions
- Bayesian inversion facilitates subsequent prediction with uncertainty
- Bayesian model selection strategies are relevant to the identification of parsimonious models that explain empirical data