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 $\mathcal{M} = \{M_1, M_2, \ldots\}$ 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

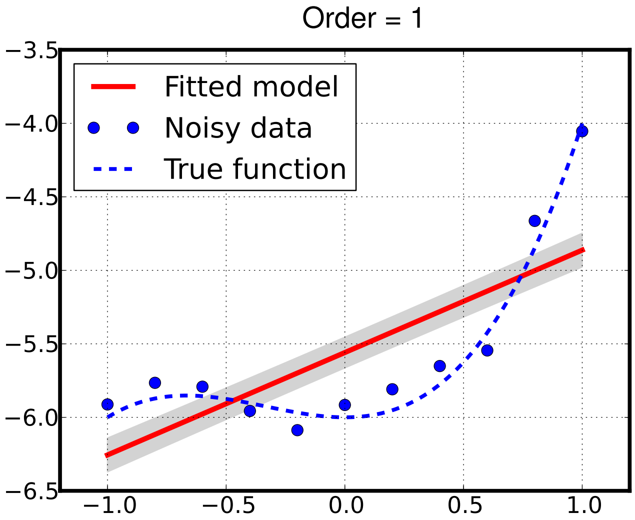
$$y_t = x^3 + x^2 - 6$$

- 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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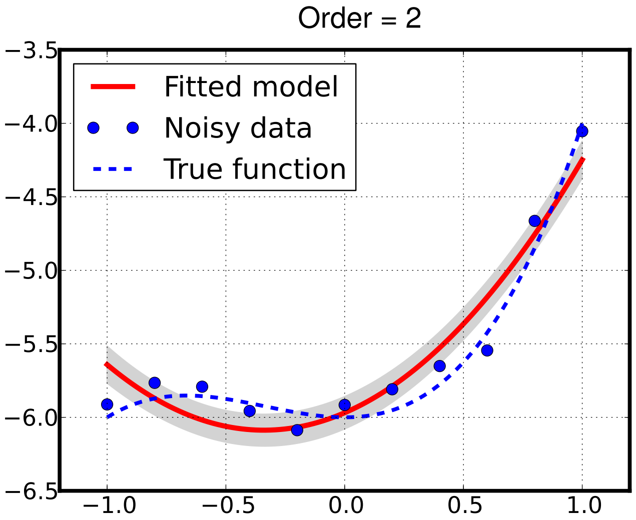

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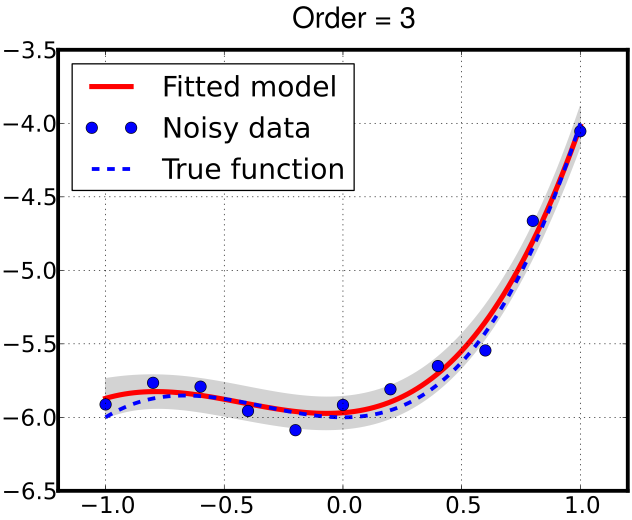

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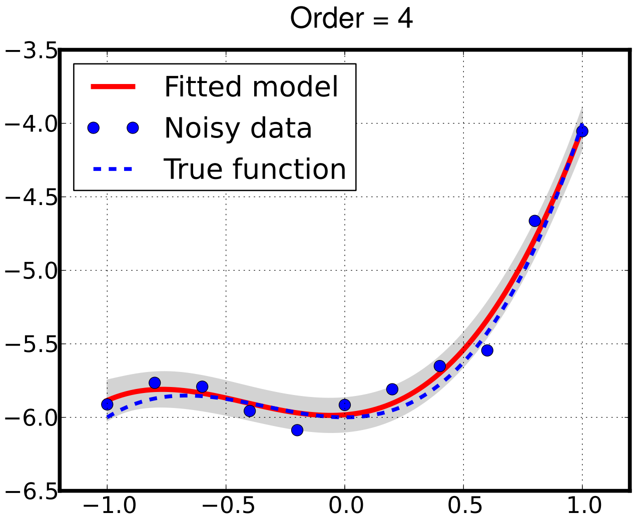

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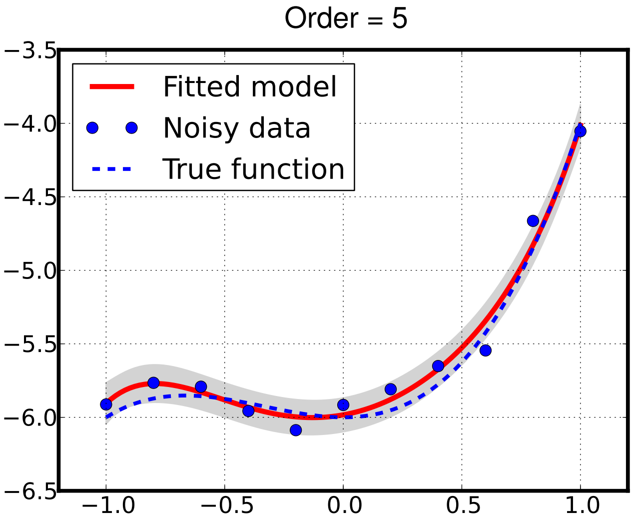

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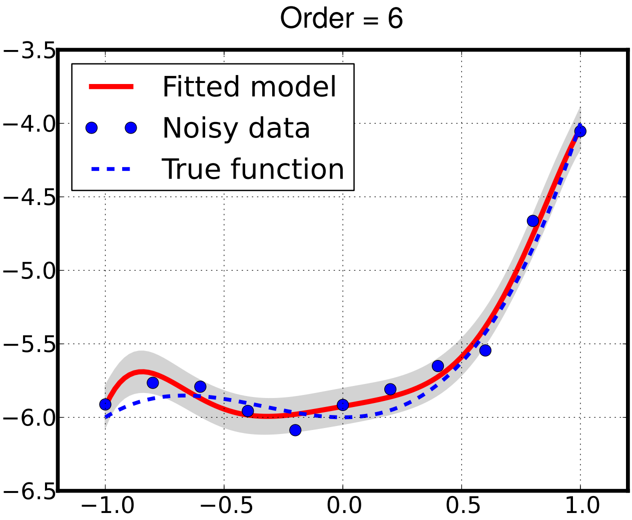

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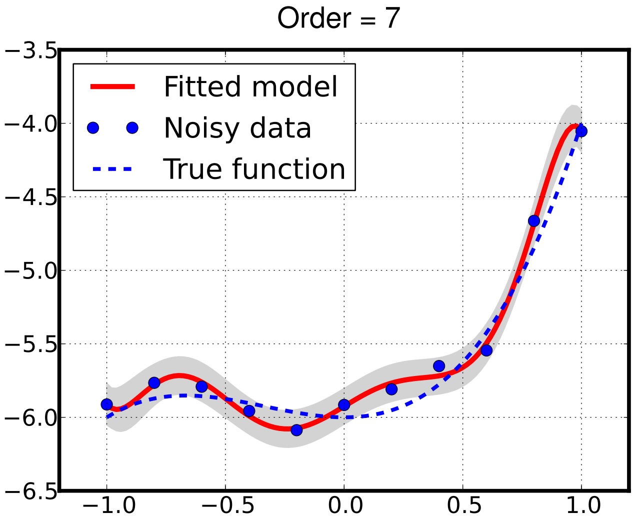

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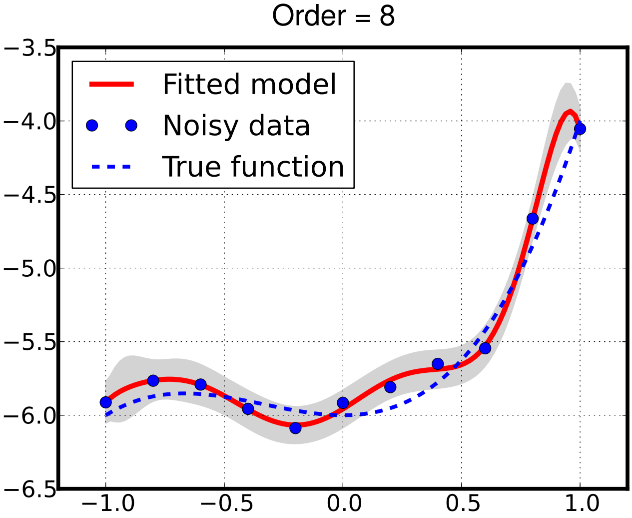

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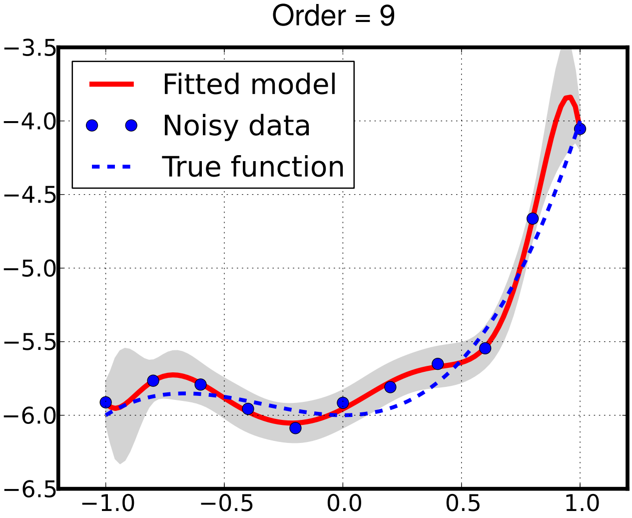

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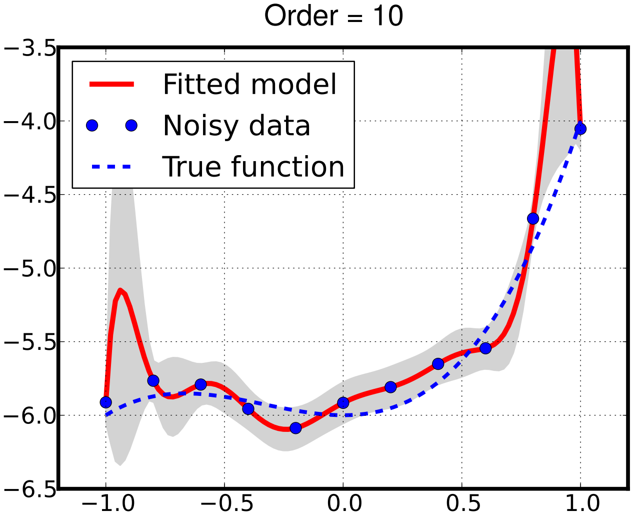
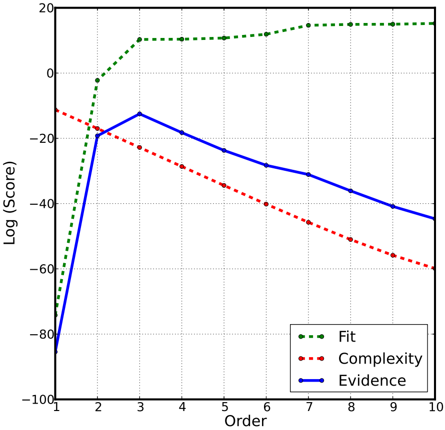
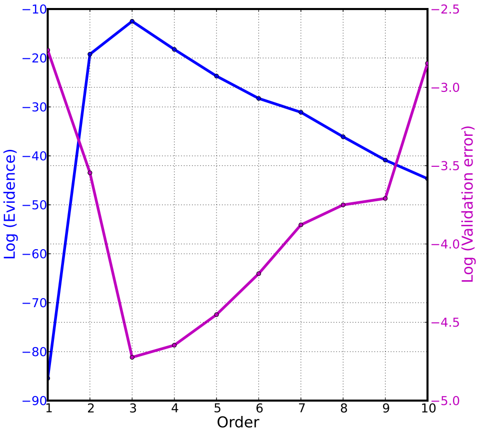


Evidence – Marginal Likelihood



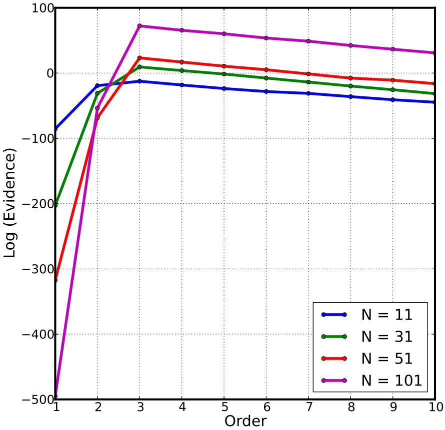
- Log evidence: sum of two scores, balances complexity & fit
- Peaks at 3rd order

Evidence and Validation Error



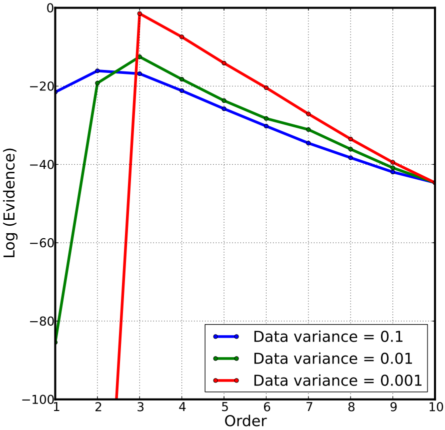
- Validation error – ℓ_2 error for a random set of 1000 points
- Validation error is minimal at the 3rd-order evidence peak

Evidence



- Discrimination among models is more clear-cut with higher amount of data

Evidence



- Discrimination among models is more clear-cut with 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

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 PFP data predictor

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:

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