

# Model Selection Tutorial #1: Akaike's Information Criterion

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- 2 Estimation
- 3 AIC
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# Problem

- We have observed  $n$  data points  $\mathbf{y}^n = (y_1, \dots, y_n)$  from some *unknown*, probabilistic source  $p^*$ , i.e.

$$\mathbf{y}^n \sim p^*$$

where  $\mathbf{y}^n \in \mathcal{Y}^n$ .

- We wish to *learn* about  $p^*$  from  $\mathbf{y}^n$ .
- More precisely, we would like to discover the generating source  $p^*$ , or at least a *good* approximation of it, from nothing but  $\mathbf{y}^n$

# Statistical Models

- To approximate  $p^*$  we will restrict ourself to a set of potential statistical models
- Informally, a statistical model can be viewed as a conditional probability distribution over the potential dataspace  $\mathcal{Y}^n$

$$p(\mathbf{y}^n|\theta), \theta \in \Theta$$

where  $\theta = (\theta_1, \dots, \theta_p)$  is a *parameter* vector that indexes the particular model

- Such models satisfy

$$\int_{\mathbf{y}^n \in \mathcal{Y}^n} p(\mathbf{y}^n|\theta) d\mathbf{y}^n = 1$$

for a *fixed*  $\theta$

# Statistical Models ...

- An example would be the univariate normal distribution.

$$p(\mathbf{y}^n|\boldsymbol{\theta}) = \left(\frac{1}{2\pi\tau}\right)^{\frac{n}{2}} \exp\left(-\frac{1}{2\tau} \sum_{i=1}^n (y_i - \mu)^2\right)$$

where

- $p = 2$
- $\boldsymbol{\theta} = (\mu, \tau)$  are the parameters
- $\mathcal{Y}^n = \mathbb{R}^n$
- $\boldsymbol{\Theta} = \mathbb{R} \times \mathbb{R}_+$

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# Parameter Estimation

- Given a statistical model and data  $\mathbf{y}^n$ , we would like to take a guess at a plausible value of  $\theta$
- The guess should be ‘good’ in some sense
- Many ways to approach this problem; we shall discuss one particularly relevant and important method : Maximum Likelihood

# Method of Maximum Likelihood (ML), Part 1

- A heuristic procedure introduced by R. A. Fisher
- Possesses good properties in many cases
- Is very general and easy to understand
- To estimate parameters  $\theta$  for a statistical model from  $\mathbf{y}^n$ , solve

$$\hat{\theta}(\mathbf{y}^n) = \arg \max_{\theta \in \Theta} \{p(\mathbf{y}^n|\theta)\}$$

or, more conveniently

$$\hat{\theta}(\mathbf{y}^n) = \arg \min_{\theta \in \Theta} \{-\log p(\mathbf{y}^n|\theta)\}$$



# Method of Maximum Likelihood (ML), Part 2

- Example : Estimating the mean parameter  $\mu$  of a univariate normal distribution
- Negative log-likelihood function :

$$L(\mu, \tau) = \frac{n}{2} \log(2\pi\tau) + \frac{1}{2\tau} \sum_{i=1}^n (y_i - \mu)^2$$

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- Differentiating  $L(\cdot)$  with respect to  $\mu$  yields

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- Setting this to zero, and solving for  $\mu$  yields

$$\hat{\mu}(\mathbf{y}^n) = \frac{1}{n} \sum_{i=1}^n y_i$$

# Univariate Polynomial Regression

- A more complex model :  $k$ -order polynomial regression

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- Let each  $y(x)$  be distributed as per a univariate normal with variance  $\tau$  and a special mean

$$\mu(\mathbf{x}) = \beta_0 + \beta_1 \mathbf{x} + \beta_2 \mathbf{x}^2 \dots \beta_k \mathbf{x}^k$$

The parameters of this model are  $\theta^{(k)} = (\tau, \beta_0, \dots, \beta_k)$ .

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- In this model the data  $\mathbf{y}^n$  is associated with a  $\mathbf{x}^n$  which are *known*
- *Given* an order  $k$ , maximum likelihood can be used to estimate  $\theta^{(k)}$
- But it cannot be used to provide a suitable estimate of order  $k$  !



# Univariate Polynomial Regression

- If we let

$$\hat{\mu}^{(k)}(\mathbf{x}) = \hat{\beta}_0 + \hat{\beta}_1 \mathbf{x} + \hat{\beta}_2 \mathbf{x}^2 \dots \hat{\beta}_k \mathbf{x}^k$$

Maximum Likelihood chooses  $\hat{\beta}^{(k)}(\mathbf{y}^n)$  to minimise

$$\hat{\tau}^{(k)}(\mathbf{y}^n) = \frac{1}{n} \sum_{i=1}^n \left( y_i - \hat{\mu}^{(k)}(\mathbf{x}_i) \right)^2$$

This is called the *residual variance*.

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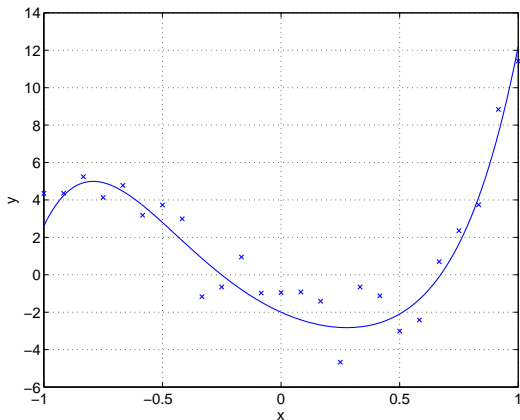
This is called the *residual variance*.

- The likelihood function  $L(\mathbf{y}^n | \hat{\theta}^{(k)}(\mathbf{y}^n))$  made by plugging in the Maximum Likelihood estimates is

$$L(\mathbf{y}^n | \hat{\theta}^{(k)}(\mathbf{y}^n)) = \frac{n}{2} \log \left( 2\pi \hat{\tau}^{(k)}(\mathbf{y}^n) \right) + \frac{n}{2}$$

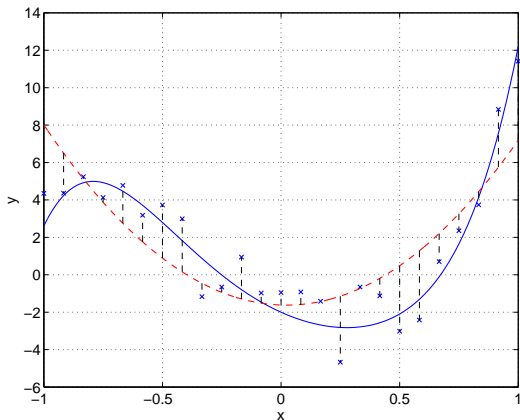
# Method of Maximum Likelihood (ML), Part 4

'Truth' :  $\mu(x) = 9.7x^5 + 0.8x^3 + 9.4x^2 - 5.7x - 2, \tau = 1$



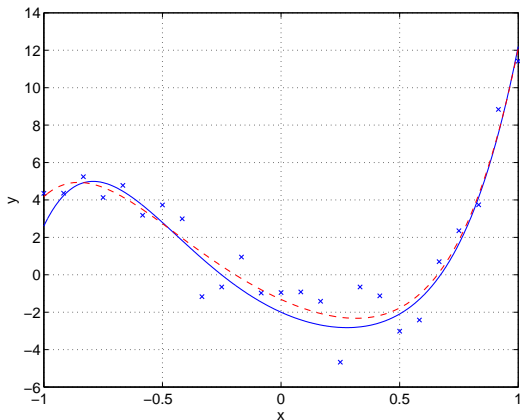
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Polynomial fit,  $k = 2$ ,  $\hat{\tau}^{(2)}(\mathbf{y}) = 4.6919$



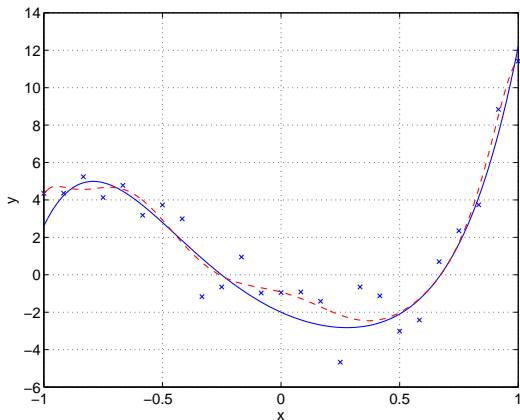
# Method of Maximum Likelihood (ML), Part 4

Polynomial fit,  $k = 5$ ,  $\hat{\tau}^{(5)}(\mathbf{y}) = 1.1388$



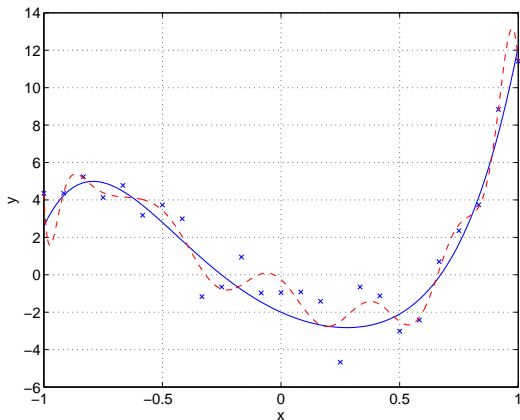
# Method of Maximum Likelihood (ML), Part 4

Polynomial fit,  $k = 10$ ,  $\hat{\tau}^{(10)}(\mathbf{y}) = 1.0038$



# Method of Maximum Likelihood (ML), Part 4

Polynomial fit,  $k = 20$ ,  $\hat{\tau}^{(20)}(\mathbf{y}) = 0.1612$



# A problem with Maximum Likelihood

- It is not difficult to show that

$$\hat{\tau}^{(0)} > \hat{\tau}^{(1)} > \hat{\tau}^{(2)} > \dots > \hat{\tau}^{(n-1)}$$

and furthermore that  $\hat{\tau}^{(n-1)} = 0$ .



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- From this it is obvious that attempting to estimate  $k$  using Maximum Likelihood will fail, i.e. the solution of

$$\hat{k} = \arg \min_{k \in \{0, \dots, n-1\}} \left\{ \frac{n}{2} \log 2\pi \hat{\tau}^{(k)}(\mathbf{y}^n) + \frac{n}{2} \right\}$$

is simply  $\hat{k} = (n - 1)$ , irrespective of  $\mathbf{y}^n$ .

# Some solutions ...

- The minimum encoding approach, pioneered by C.S. Wallace, D. Boulton and J.J. Rissanen
- The minimum discrepancy estimation approach, pioneered by H. Akaike

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# Kullback-Leibler Divergence

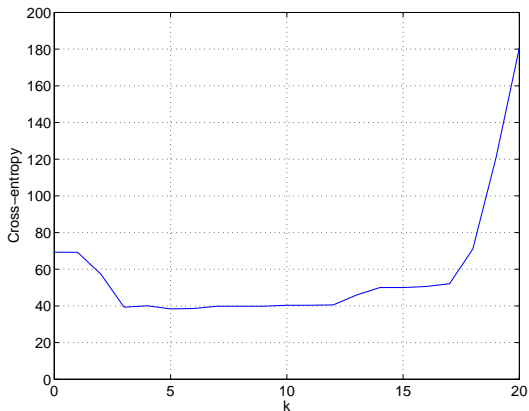
- AIC is based on estimating the Kullback-Leibler (KL) divergence
- The Kullback-Leibler divergence

$$KL(f||g) = \underbrace{- \int_{\mathcal{Y}^n} f(\mathbf{y}^n) \log g(\mathbf{y}^n) d\mathbf{y}^n}_{\text{Cross-entropy}} + \underbrace{\int_{\mathcal{Y}^n} f(\mathbf{y}^n) \log f(\mathbf{y}^n) d\mathbf{y}^n}_{\text{Entropy}}$$

- Cross-entropy,  $\Delta(f||g)$ , is the ‘expected negative log-likelihood’ of data coming from  $f$  under  $g$

# Kullback-Leibler Divergence

- Cross-entropy for polynomial fits of order  $k = \{0, \dots, 20\}$



# Akaike's Information Criterion

- Problem : KL divergence depends on knowing the truth (our  $p^*$ )
- Akaike's solution : Estimate it !

# Akaike's Information Criterion

- The AIC score for a model is

$$\text{AIC}(\hat{\theta}(\mathbf{y}^n)) = -\log p(\mathbf{y}^n | \hat{\theta}(\mathbf{y}^n)) + p$$

where  $p$  is the number of free model parameters.

- Using AIC one chooses the model that solves

$$\hat{k} = \arg \min_{k \in \{0, 1, \dots\}} \left\{ \text{AIC}(\hat{\theta}^{(k)}(\mathbf{y}^n)) \right\}$$

# Properties of AIC

- Under certain conditions the AIC score satisfies

$$\mathbb{E}_{\theta^*} \left[ \text{AIC}(\hat{\theta}(\mathbf{y}^n)) \right] = \mathbb{E}_{\theta^*} \left[ \Delta(\theta^* || \hat{\theta}(\mathbf{y}^n)) \right] + o_n(1)$$

where  $o_n(1) \rightarrow 0$  as  $n \rightarrow \infty$

- In words, the AIC score is an *asymptotically unbiased* estimate of the cross-entropy risk
- This means it is only valid if  $n$  is ‘large’



# Properties of AIC

- AIC is good for prediction
- AIC is an *asymptotically efficient* model selection criterion
- In words, as  $n \rightarrow \infty$ , with probability approaching one, the model with the minimum AIC score will also possess the smallest Kullback-Leibler divergence
- It is not necessarily the best choice for *induction*

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- $L(\theta)$  must be twice differentiable with respect to  $\theta$  for all  $\theta \in \Theta$

# Some models to which AIC can be applied include ...

- Linear regression models, function approximation
- Generalised linear models
- Autoregressive Moving Average models, spectral estimation
- Constant bin-width histogram estimation
- Some forms of hypothesis testing



# When not to use AIC

- Multilayer Perceptron Neural Networks
  - Many different  $\theta$  map to the same distribution

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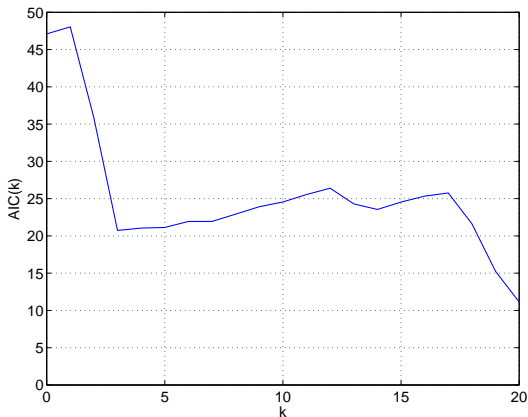
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- The AIC approach may still be applied to these problems, but the derivations need to be different

# Application to polynomials

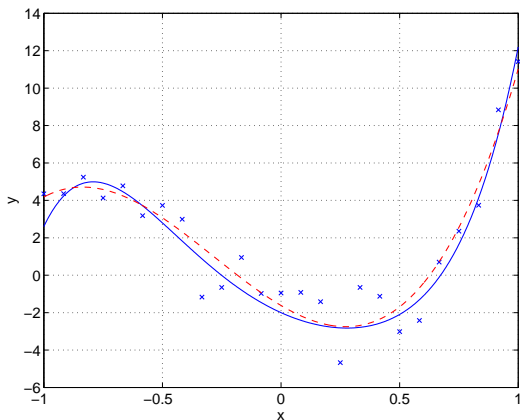
- AIC criterion for polynomials

$$\text{AIC}(k) = \frac{n}{2} \log 2\pi \hat{\sigma}^2(\mathbf{y}^n) + \frac{n}{2} + (k + 2)$$



# Application to polynomials

- AIC selects  $\hat{k} = 3$



# Improvements to AIC

- For some model types it is possible to derive improved estimates of the cross-entropy
- Under certain conditions, the ‘corrected’ AIC (AICc) criterion

$$\text{AIC}_c(\hat{\theta}(\mathbf{y}^n)) = -\log p(\mathbf{y}^n | \hat{\theta}(\mathbf{y}^n)) + \frac{n(p+1)}{n-p-2}$$

satisfies

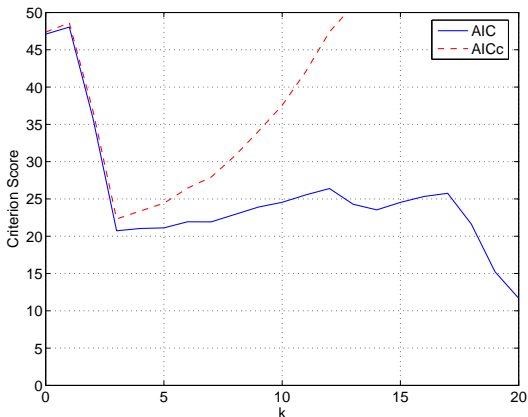
$$\mathbb{E}_{\theta^*} \left[ \text{AIC}_c(\hat{\theta}(\mathbf{y}^n)) \right] = \mathbb{E}_{\theta^*} \left[ \Delta(\theta^* || \hat{\theta}(\mathbf{y}^n)) \right]$$

- In words, it is an exactly unbiased estimator of the cross-entropy, even for finite  $n$

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# Using AICc

- Tends to perform better than AIC, especially when  $n/p$  is *small*
- Theoretically only valid for homoskedastic *linear models*; these include
  - Linear regression models, including linear function approximation
  - Autoregressive Moving Average (ARMA) models
  - Linear smoothers (kernel, local regression, etc)
- Practically, tends to perform well as long as the model class is suitably regular

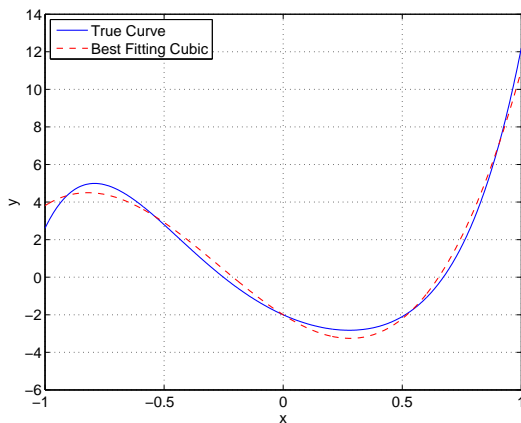
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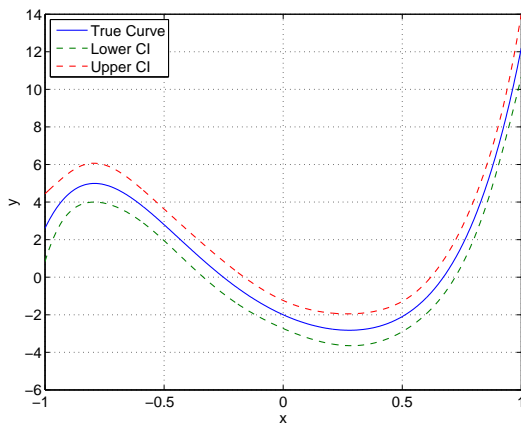
# Some theory

- Let  $k^*$  be the true number of parameters, and assume that the model space is nested
- Two sources of error/discrepancy in model selection
- Discrepancy due to approximation
  - Main source of error when *underfitting*, i.e. when  $\hat{k} < k^*$
- Discrepancy due to estimation
  - Source of error when exactly fitting or *overfitting*, i.e. when  $\hat{k} \geq k^*$

# Discrepancy due to Approximation



# Discrepancy due to Estimation



# Derivation

- The aim is to show that

$$\mathbb{E}_{\theta^*} \left[ L(\mathbf{y}^n | \hat{\theta}) + p \right] = \mathbb{E}_{\theta^*} \left[ \Delta(\theta^* || \hat{\theta}) \right] + o_n(1)$$

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- Note that (under certain conditions)

$$E_{\theta^*} \left[ \Delta(\theta^* || \hat{\theta}) \right] = \Delta(\theta^* || \theta_0) + \frac{1}{2}(\hat{\theta} - \theta_0)' \mathbf{J}(\theta_0)(\hat{\theta} - \theta_0) + o_n(1)$$

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- ... and

$$\Delta(\theta^* || \theta_0) = \mathbb{E}_{\theta^*} \left[ L(\mathbf{y}^n | \hat{\theta}) \right] + \frac{1}{2}(\hat{\theta} - \theta_0)' \mathbf{H}(\hat{\theta})(\hat{\theta} - \theta_0) + o_n(1)$$



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- Where

$$\mathbf{J}(\theta_0) = \left[ \frac{\partial^2 \Delta(\theta^* | \theta)}{\partial \theta \partial \theta'} \Big|_{\theta=\theta_0} \right], \quad \mathbf{H}(\hat{\theta}) = \left[ \frac{\partial^2 L(\mathbf{y}^n | \theta)}{\partial \theta \partial \theta'} \Big|_{\theta=\hat{\theta}} \right]$$

# Derivation

- Since

$$\begin{aligned}\frac{1}{2}E_{\theta^*} \left[ (\hat{\theta} - \theta_0)' \mathbf{J}(\theta_0) (\hat{\theta} - \theta_0) \right] &= \frac{p}{2} + o_n(1) \\ \frac{1}{2}E_{\theta^*} \left[ (\hat{\theta} - \theta_0)' \mathbf{H}(\hat{\theta}) (\hat{\theta} - \theta_0) \right] &= \frac{p}{2} + o_n(1)\end{aligned}$$

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- Then, substituting

$$\begin{aligned}\mathbb{E}_{\theta^*} \left[ \Delta(\theta^* || \hat{\theta}) \right] &= \left( \mathbb{E}_{\theta^*} \left[ L(\mathbf{y}^n | \hat{\theta}) \right] + \frac{p}{2} + o_n(1) \right) + \frac{p}{2} + o_n(1) \\ &= \underbrace{\mathbb{E}_{\theta^*} \left[ L(\mathbf{y}^n | \hat{\theta}) + p \right]}_{\text{AIC}(\hat{\theta})} + o_n(1)\end{aligned}$$

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