ST451 - Lent term
Bayesian Machine Learning

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Bayesian Inference Concepts - Linear Regression

Outline

Outline

Summary of last lecture

- Define model (likelihood) $f(y|\theta)$ and prior $\pi(\theta)$.
- Obtain posterior via Bayes theorem

$$\pi(\theta|y) = \frac{f(y|\theta)\pi(\theta)}{\int f(y|\theta)\pi(\theta)d\theta} \propto f(y|\theta)\pi(\theta)$$

- Bayes Estimators: posterior mean, median or mode.
- Bayesian 95% credible intervals: 2.5-th and 97.5-th percentiles. θ is in them with probability 95%
- Bayesian forecasting for future data y_n via the (posterior-)predictive distribution

$$f(y_n|y) = \int f(y_n|\theta)\pi(\theta|y)d\theta.$$

Example: Normal-Normal

Likelihood: Let $y = (y_1, \ldots, y_n)$ be a random sample from a N(θ, σ^2) - σ^2 known. The likelihood is given by the joint density of the sample

$$f(y|\theta) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y_i - \theta)^2}{2\sigma^2}\right) \propto \exp\left(-\frac{\sum_{i=1}^{n}(y_i - \theta)^2}{2\sigma^2}\right)$$

Prior: We assume the Normal prior N$(\mu, \tau^2\sigma^2)$ for θ, which gives

$$\pi(\theta) \propto \exp\left(-\frac{(\theta - \mu)^2}{2\tau^2\sigma^2}\right)$$

Example Normal-Normal - completing the square

Posterior: The posterior can then be obtained as

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

$$\propto \cdots \propto \exp\left(-\frac{\theta^2 - 2\theta\frac{\bar{y}\tau^2+\mu\frac{1}{n}}{\frac{1}{n}+\tau^2}}{2\frac{\sigma^2}{\frac{1}{\tau^2}+n}}\right) \stackrel{\mathcal{D}}{=} \mathrm{N}\left(\frac{\frac{1}{n}\mu+\tau^2\bar{y}}{\frac{1}{n}+\tau^2}, \frac{\sigma^2}{\frac{1}{\tau^2}+n}\right)$$

Bayes Estimators: Posterior mean, median and mode are all equal to

$$\frac{\frac{1}{n}\mu+\tau^2\bar{y}}{\frac{1}{n}+\tau^2} = \frac{\tau^2}{\frac{1}{n}+\tau^2}\bar{y} + \left(1-\frac{\tau^2}{\frac{1}{n}+\tau^2}\right)\mu,$$

a weighted average between the prior mean μ and the MLE $\bar{y}$

Example Normal-Normal (cont'd)

Bayesian 95% credible intervals: With $\mathcal{Z}_{2.5}$ being the 2.5-th percentile of the $N(0,1)$, we get

$$\frac{\frac{1}{n}\mu + \tau^2 \bar{y}}{\tau^2 + \frac{1}{n}} \pm \mathcal{Z}_{2.5} \sqrt{\frac{\sigma^2}{\frac{1}{\tau^2} + n}}$$

Predictive distribution: Given θ a future observation y_n will be $N(\theta, \sigma^2)$, so using standard properties of Normal distributions we get that the predictive is also a Normal with mean

$$\frac{\frac{1}{n}\mu + \tau^2 \bar{y}}{\tau^2 + \frac{1}{n}}$$

and variance

$$\frac{\sigma^2}{\frac{1}{\tau^2} + n} + \sigma^2$$

Example Normal-Normal: Jeffreys prior

To find Jeffreys prior we perform the following steps:

$$\log f(y|\theta) = -\frac{\sum_{i=1}^{n}(y_i-\theta)^2}{2\sigma^2}, \quad \frac{\partial}{\partial\theta}\log f(y|\theta) = \frac{\sum_{i=1}^{n}(y_i-\theta)}{\sigma^2}$$

$$\mathcal{I}(\theta|y) = -E_Y\left(\frac{\partial^2}{\partial\theta^2}\log f(y|\theta)\right) = -E_Y\left(-\frac{n}{\sigma^2}\right) = \frac{n}{\sigma^2}$$

Hence the Jeffreys prior: $\pi(\theta) \propto 1$.

Example Normal-Normal: Inference with Jeffreys prior

Posterior: The posterior from Jeffreys prior is

$$\begin{aligned}\pi(\theta|y) &\propto \exp\left(-\frac{\sum_{i=1}^{n}(y_i-\theta)^2}{2\sigma^2}\right) \propto \exp\left(-\frac{n\theta^2-2\theta\sum_{i=1}^{n}y_i}{2\sigma^2}\right)\\ &\propto \exp\left(-\frac{\theta^2-2\theta\bar{y}}{2\frac{\sigma^2}{n}}\right) \overset{\mathcal{D}}{=} \mathrm{N}\left(\bar{y},\frac{\sigma^2}{n}\right)\end{aligned}$$

Bayes Estimators: All are the same as the MLE, i.e. $\bar{y}$.

Bayesian 95% credible intervals: $\bar{y} \pm \mathcal{Z}_{2.5}\sqrt{\frac{\sigma^2}{n}}$.
Same as in the frequentist case but with different interpretation.

Predictive distribution: We get $N(\bar{y}, \frac{\sigma^2}{n}+\sigma^2)$.

Outline

Motivating Example: Prostate Cancer

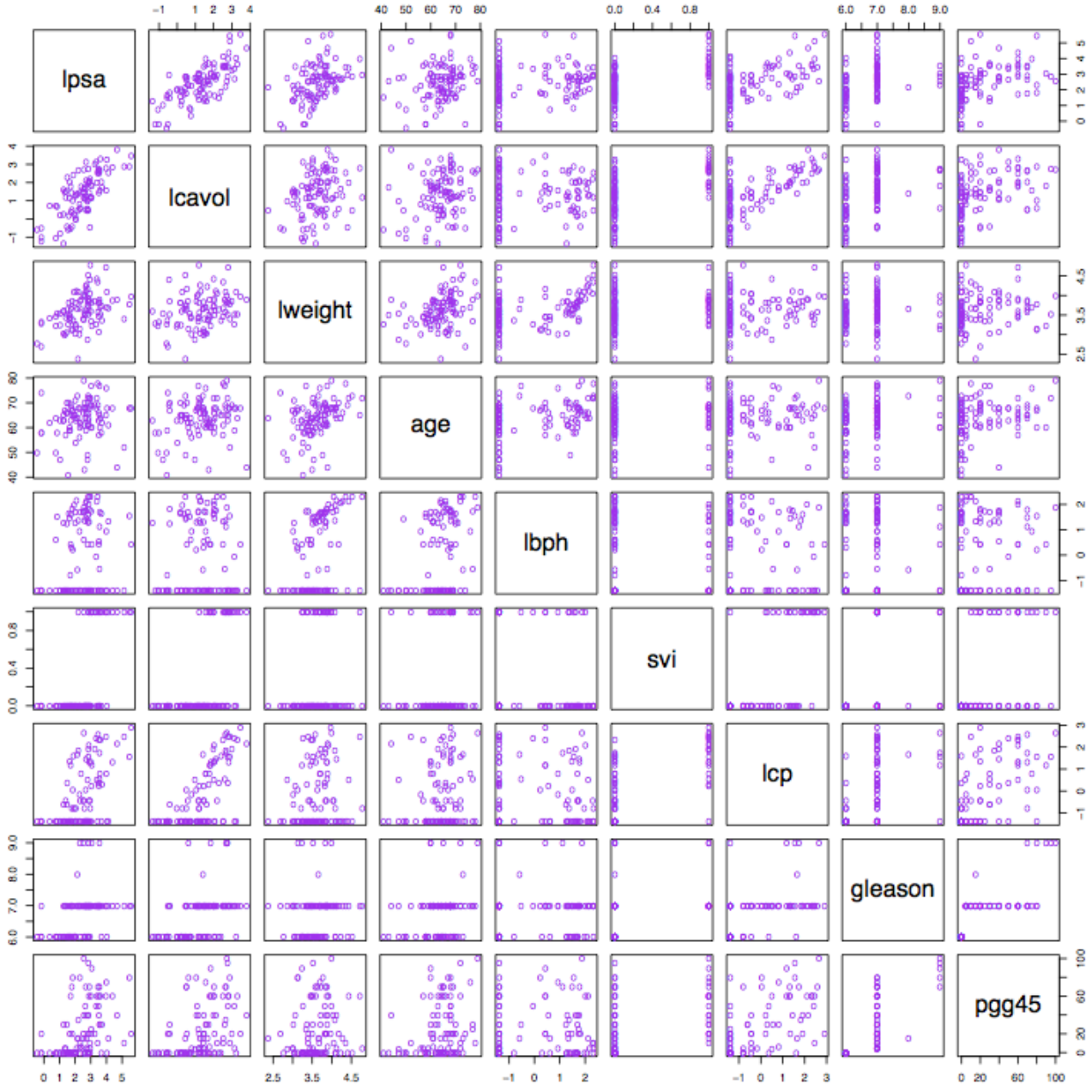
Data from the following study on prostate cancer

Stamey, T., et al. (1989). Prostate specific antigen in the diagnosis and treatment of adenocarcinoma of the prostate II radical prostatectomy treated patients, Journal of Urology 16: 1076-1083.

Examines association between the level of prostate-specific antigen (PSA) and a number of clinical measures in men who were about to receive a radical prostatectomy.

The variables are cancer volume (lcavol), prostate weight (lweight), age, amount of benign prostatic hyperplasia (lbph), seminal vesicle invasion (svi), capsular penetration (lcp), Gleason score (gleason), and percent of Gleason scores 4 or 5 (pgg45).

Motivating Example: Data



Motivating Example: Aims of the analysis

- Determine the level of PSA on a future patient based on the clinical measurements. Otherwise detailed histological and morphometric analysis is required.
- How is each of these variables associated with PSA? Is the association linear?
- Are any of these variables redundant in the presence of the others? Which are the most important?
- Are there any synergies between these variables?

Data setup

Data consist of measurements on all these variables on several individuals.

We typically denote value of the response variable, in this case log-PSA, on the individual i with Y_i. The vector $Y = (Y_1, \ldots, Y_n)$ is assumed to be a $n-$dimensional random variable.

The remaining variables $X_1, \ldots, X_p$ contain the clinical measurements. X_{ji} refers to the value of the clinical measurement j of the individual i.

The $X's$ are not assumed to be random they are treated as fixed inputs, with Y being regarded as the output.

Linear Regression

The linear regression model is written as

$$Y_i = \beta_0 + \beta_1 X_{1i} + \cdots + \beta_p X_{pi} + \epsilon_i, \quad i = 1, \ldots, n.$$

It is more convenient to use matrix algebra. Define $y = (Y_1, \ldots, Y_n)$, $\epsilon = (\epsilon_1, \ldots, \epsilon_n)^T$ the error terms, $\beta = (\beta_0, \ldots, \beta_p)^T$ denoting the regression coefficients and the design matrix

$$X = \begin{pmatrix} 1 & X_{11} & \ldots & X_{p1} \\ 1 & X_{12} & \ldots & X_{p2} \\ \vdots & \vdots & & \vdots \\ 1 & X_{1n} & \ldots & X_{pn} \end{pmatrix}.$$

Then we can rewrite the model in matrix notation as

$$y = X\beta + \epsilon,$$

Example: Prostate Cancer Regression Coefficients

Test your understanding on interpreting coefficients in the table below:

Term	Coefficient	Std. Error	Z Score
`Intercept`	2.46	0.09	27.60
`lcavol`	0.68	0.13	5.37
`lweight`	0.26	0.10	2.75
`age`	−0.14	0.10	−1.40
`lbph`	0.21	0.10	2.06
`svi`	0.31	0.12	2.47
`lcp`	−0.29	0.15	−1.87
`gleason`	−0.02	0.15	−0.15
`pgg45`	0.27	0.15	1.74

MLE of Linear Regression

The MLE and the least squares estimators can be shown to be:

$$\widehat{\beta} = (X^T X)^{-1} X^T Y.$$

The variance of the MLE is given by

$$\text{Var}(\widehat{\beta}) = \widehat{\sigma}^2 (X^T X)^{-1},$$

where $\widehat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^{n} (Y_i - X_i \widehat{\beta})^2$ or $\widehat{\sigma}^2 = \frac{1}{n-p-1} \sum_{i=1}^{n} (Y_i - X_i \widehat{\beta})^2$.

The distribution of the MLE is the t-distribution with $n - p$ degrees of freedom.

Linear Basis Functions

The model is linear its parameters β not X so we can replace each X_i with $\phi(X_i)$. We can then write the model as

$$y = \phi(X)\beta + \epsilon$$

Examples include dummy variables, polynomial terms, Gaussian kernels, sigmoid functions etc.

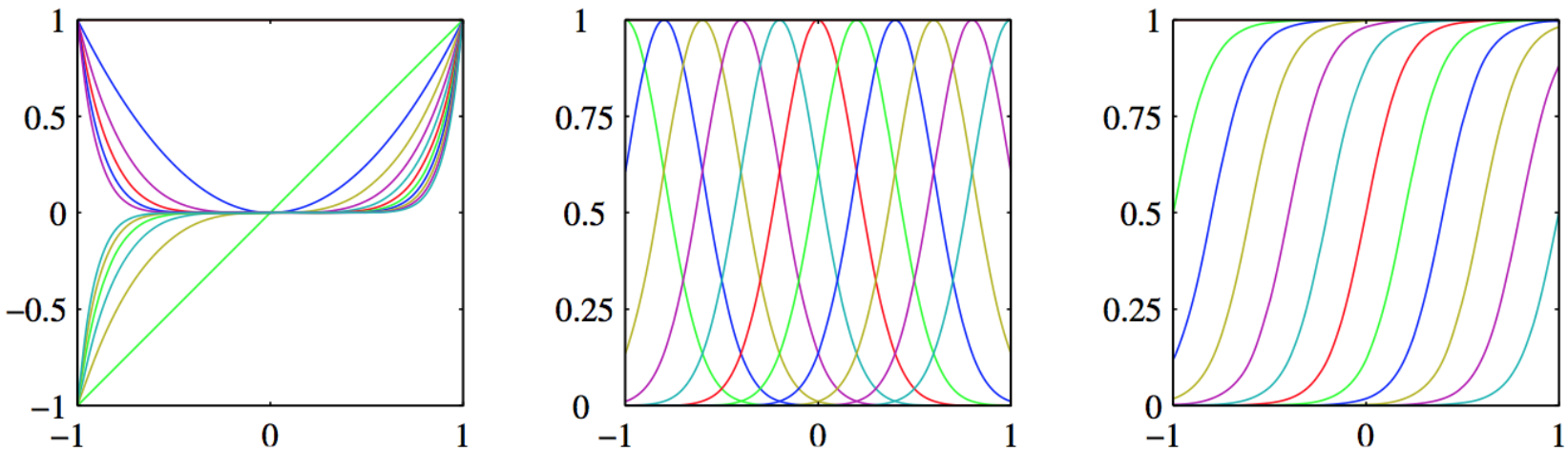
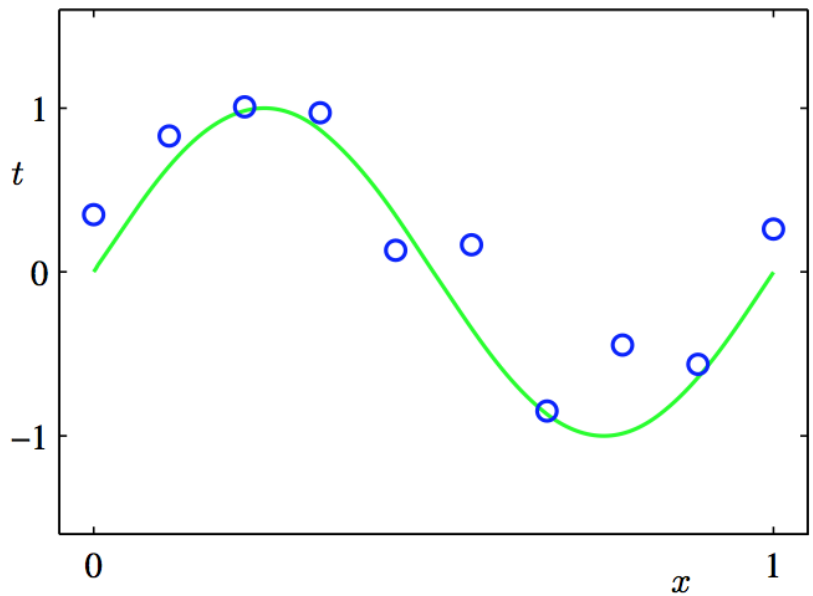


Figure 3.1 Examples of basis functions, showing polynomials on the left, Gaussians of the form (3.4) in the centre, and sigmoidal of the form (3.5) on the right.

Example: Polynomial Curve Fitting

Let's consider the following example on simulated data. The generating process is $\sin(2\pi x)$ and we observe this function on 10 different points in $[0, 1]$ with independent Gaussian error.

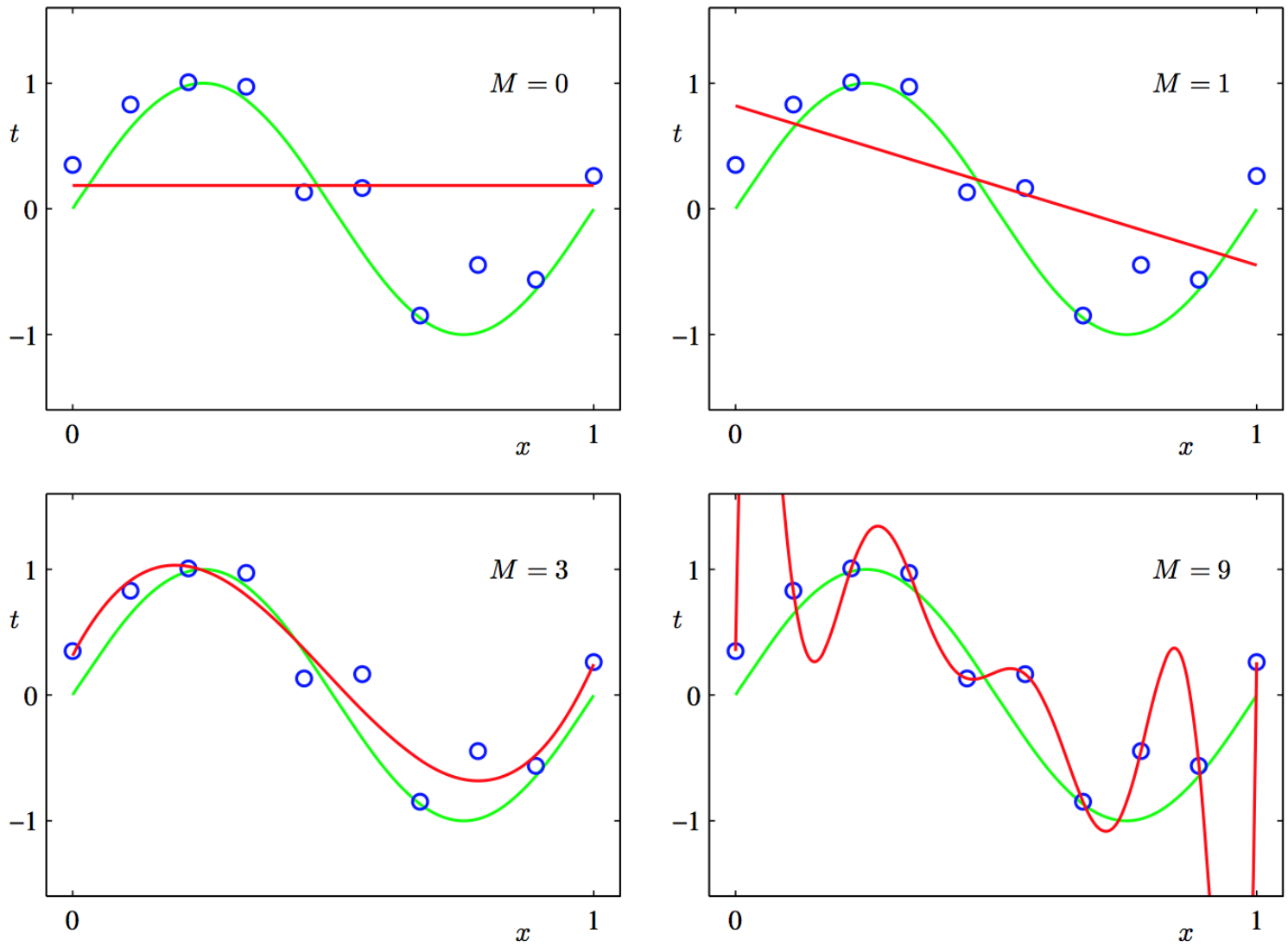


We fit a linear regression model with polynomial basis functions

$$y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \cdots + \beta_M x_i^M + \epsilon_i$$

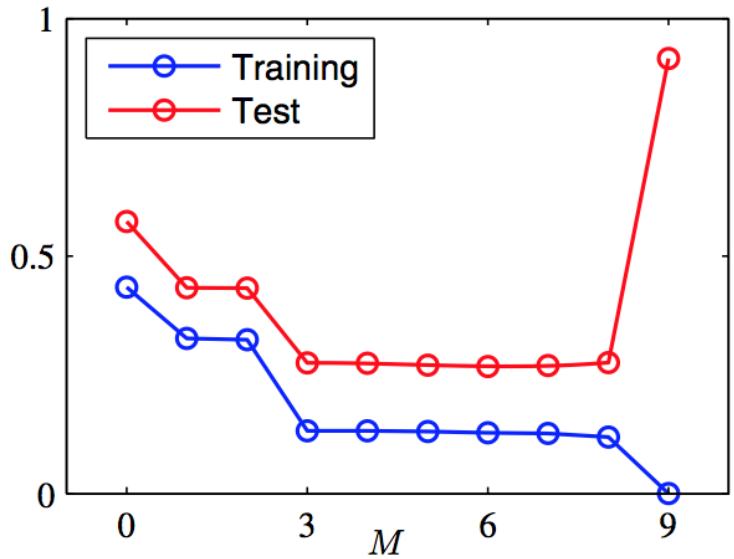
Example: Fit of different polynomials

For each order of polynomial we find the MLE and plot the corresponding function to assess its fit



Training and Test Error - Overfitting

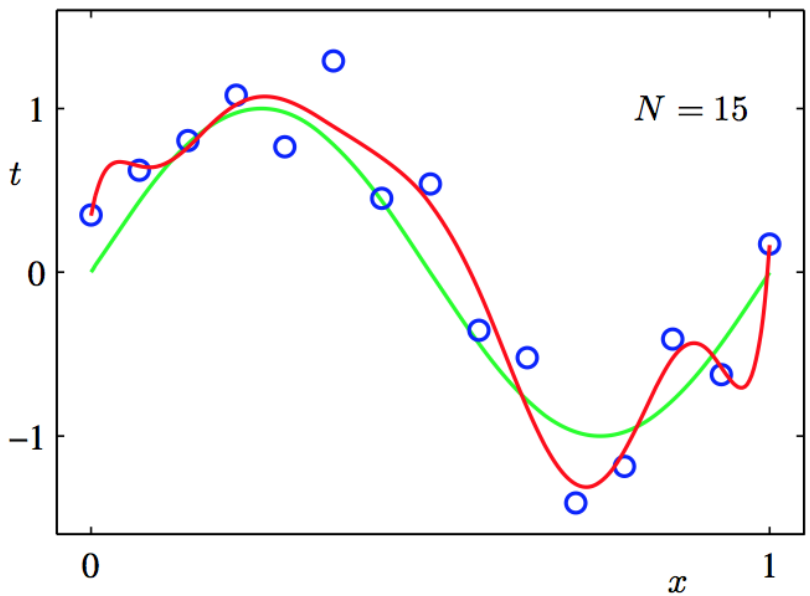
In addition to the training data set of 10 observations we simulate 100 more points in the same way and assess the training and test error.

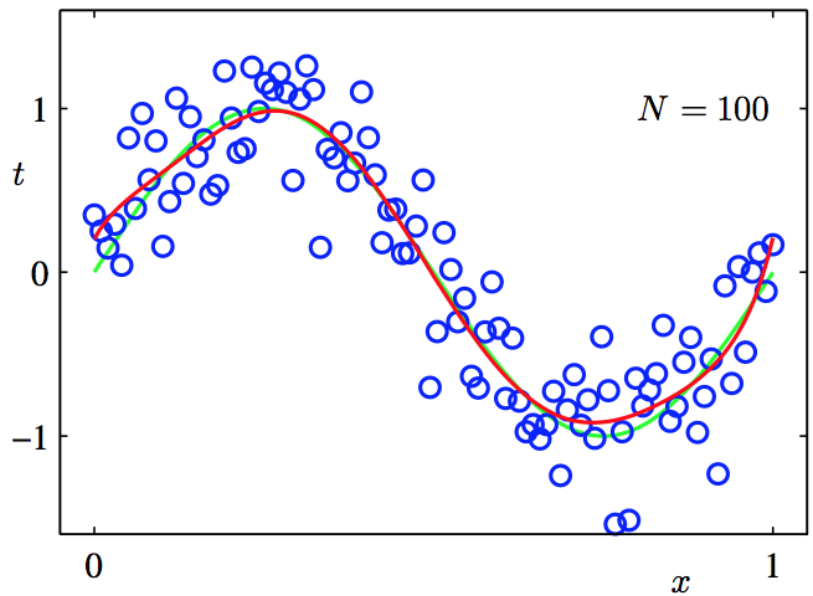


The test error decreases until $M = 6$ and increase afterwards. The training error keeps decreasing and drops to 0 for $M = 9$. MLE leads to overfit.

Model Complexity

In order to identify the data generating process our model should not be too complex compared to the data we are training it. Increasing the data improves learning for the model with $M = 9$.





Parameter Estimates

One way to reduce model complexity is to reduce the number of predictors. Not necessarily the best way.

More insight is obtained by looking at the parameter estimates for polynomials of different order.

$M = 0$	$M = 1$	$M = 6$	$M = 9$
0.19	0.82	0.31	0.35
	-1.27	7.99	232.37
		-25.43	-5321.83
		17.37	48568.31
			-231639.30
			640042.26
			-1061800.52
			1042400.18
			-557682.99
			125201.43

Regularisation

Instead of removing predictors we could instead restrict them closer to 0. In the least squares criterion

$$\sum_{i=1}^{n}(y_i - \beta_0 + \beta_1 x_i + \cdots + \beta_M x_i^M)^2,$$

we add a penalty term

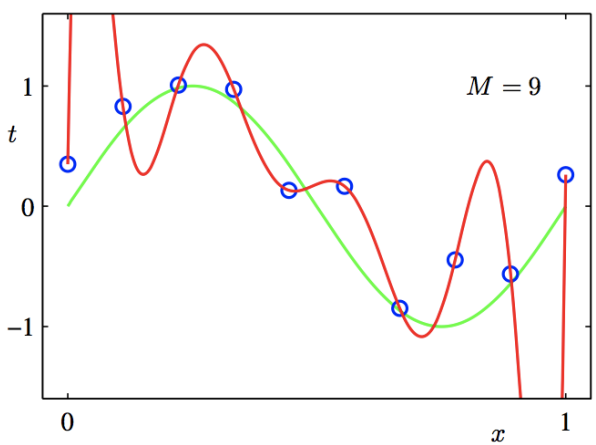
$$\sum_{i=1}^{n}(y_i - \beta_0 + \beta_1 x_i + \cdots + \beta_M x_i^M)^2 + \lambda \sum_{i=1}^{M} \beta_i^2.$$

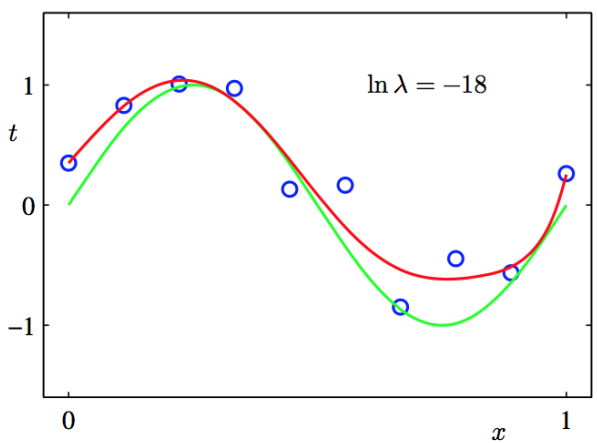
In the general case of a linear regression model $y = X\beta + \epsilon$ the above is minimised at the point

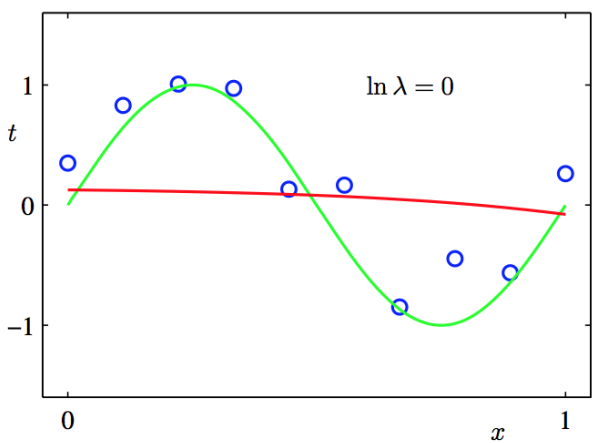
$$\hat{\beta}^{\lambda} = (X^T X + \lambda^2 I_p)^{-1} X^T y$$

Output From Regularised Approach

$\ln \lambda = -\infty$	$\ln \lambda = -18$	$\ln \lambda = 0$
0.35	0.35	0.13
232.37	4.74	-0.05
-5321.83	-0.77	-0.06
48568.31	-31.97	-0.05
-231639.30	-3.89	-0.03
640042.26	55.28	-0.02
-1061800.52	41.32	-0.01
1042400.18	-45.95	-0.00
-557682.99	-91.53	0.00
125201.43	72.68	0.01







Outline

Bayesian Linear Regression

Techniques like this come under the names shrinkage, ridge regression or weight decay in the context of neural networks.

But how can it be justified from a Statistical Inference point of view?

Adjusting for overfit is automatic under the Bayesian framework and comes in a natural way.

It turns out that this is a special case of Bayesian Linear Regression.

Case of known σ^2

We will first assume that σ^2 is known.

The likelihood $f(y|\beta)$ is the N$(X\beta, \sigma^2 I_n)$, where I_n is the identity matrix of dimension n.

The prior on β can be set to $N(\mu_0, \sigma^2\Omega_0)$

The posterior is then the N$(\mu_n, \sigma^2\Omega_n)$, where

$$\begin{aligned} \Omega_n &= (X^T X + \Omega_0^{-1})^{-1}, \\ \mu_n &= (X^T X + \Omega_0^{-1})^{-1}(\Omega_0^{-1}\mu_0 + X^T y), \end{aligned}$$

If we set $\mu_0 = 0$ and $\Omega_0 = g^2 I_p$ the Bayes Estimator coincides with the ridge regression estimator with $g = 1/\lambda$.

Notes on Bayesian Linear Regression

The Bayes estimate is a weighted average between the prior mean and the MLE.

The prior N(μ_0, $\sigma^2\Omega_0$) shrinks the parameters to μ_0. This can be interpreted as prior information.

The amount of force is determined by Ω_0. Prior can be viewed as a tuning parameter in the Machine Learning context.

The Bayes/ridge regression estimator is biased but has smaller variance due to the 'shrinking effect'.

Bayesian Lassso

If we use the Laplace prior La$(0, 1/\gamma)$ for β the Bayes estimator corresponding to the posterior mode is the Lasso Regression estimator.

The Laplace prior can also be written as a hierarchical Normal-Exponential prior:

$$\beta_i \sim N\left(0, \sigma^2\tau_i^2\right), \quad \tau_i^2 \sim \text{Exponential}\left(\frac{\gamma^2}{2}\right),$$

where $\lambda = \gamma/\sigma$.

Note however that the posterior mean and median provide different Bayes estimators.

Example: Results

Term	LS	Best Subset	Ridge	Lasso	PCR	PLS
Intercept	2.465	2.477	2.452	2.468	2.497	2.452
lcavol	0.680	0.740	0.420	0.533	0.543	0.419
lweight	0.263	0.316	0.238	0.169	0.289	0.344
age	−0.141		−0.046		−0.152	−0.026
lbph	0.210		0.162	0.002	0.214	0.220
svi	0.305		0.227	0.094	0.315	0.243
lcp	−0.288		0.000		−0.051	0.079
gleason	−0.021		0.040		0.232	0.011
pgg45	0.267		0.133		−0.056	0.084
Test Error	0.521	0.492	0.492	0.479	0.449	0.528
Std Error	0.179	0.143	0.165	0.164	0.105	0.152

Predictive distribution

For the predictive distribution of a new observation y_* given a new set of covariates X_*, we need to derive

$$f(y_*|y) = \int_0^\infty f(y_*|X_*, \beta, \sigma^2)\pi(\beta|y, X, \sigma^2)d\beta,$$

where the first term is $N(X_*\beta, \sigma^2)$ and the second term is N(μ_n, $\sigma^2\Omega_n$).

Using standard properties of the Normal distribution we get that the predictive distribution is

$$N\left(\mu_n X_*,\ \sigma^2 + X_*^T\sigma^2\Omega_n X_*\right)$$

Outline

Detour: Statistical Decision Theory

Given $f(y|\theta)$, a statistical decision problem consists of

1. The parameter space Θ.
2. A set $\mathcal{A}$ of all possible actions a, e.g. $\hat{\theta}$, choice of H_0 vs H_1.
3. A loss function $L(a, \theta) : \mathcal{A} \times \Theta \to \mathcal{R}$, reflecting the loss for action a and true parameter value θ.
4. One or more decision rules, i.e. functions $\delta(y) : \mathcal{R} \to \mathcal{A}$ that indicate the action a based on y.

Frequentist Risk

The aim is to minimise some king of risk, e.g. the frequentist risk.

$$R(\delta(y), \theta) = E_{Y|\theta}\left(L(\delta(y), \theta)\right) = \int L(\delta(y), \theta) f(y|\theta) dy.$$

Example: Let $\delta(y)$ be a point estimator $\hat{\theta}$ and $L(\hat{\theta}, \theta) = (\hat{\theta} - \theta)^2$. Then $R(\hat{\theta}, \theta) = E[(\hat{\theta} - \theta)^2]$, i.e. the Mean Squared Error. of $\hat{\theta}$.

In frequentist inference we aim to minimising the frequentist risk. Not always easy because it depends on unknown θ, hence we want the optimal $\delta(y)$ for all θ.

Often rely on conservative approaches such as the minimax or ad-hoc criteria such as minimum variance unbiased estimators or most powerful tests.

Bayes Risk

In Bayesian inference we minimise the Bayes Risk given a prior $\pi(\theta)$

$$r(\delta(y), \pi(\theta)) = E_\theta \left[R(\delta(y), \theta)\right] = \int R(\delta(y), \theta)\pi(\theta) d\theta.$$

Easier as it doesn't depend on θ, essentially we are 'averaging' the frequentist risk over θ according to $\pi(\theta)$.

So averaging over potential y still takes place in Bayesian inference but only under the Bayesian design where $\pi(\theta)$ is also involved.

The decision rule that minimises Bayes risk is called Bayes rule.

Bayes Estimators

- Bayes estimators minimise the Bayes risk: posterior mean, median and mode corresponds to quadratic, absolute and $0-1$ error loss functions respectively.
- They are typically biased (in case of proper priors) but they tend to have lower variance and are typically admissible estimators (no other estimator has smaller frequentist risk for all θ).
- Asymptotically they converge to the MLEs.

Today's lecture - Reading

Murphy: 1.7, 5.3.1, 5.3.3 ,5.7.1, 7.5, 7.6.1 and 7.6.2

Bishop: 1.1, 3.1.1, 3.1.4, 3.3.1 and 3.3.2