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Data Literacy
Lecture 06: Linear Regression

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Plan for today

Linear regression: why it matters

Linear regression: The ‘Machine Learning’ view

Linear regression revisited: Estimation in linear Gaussian models

Linear regression: The Bayesian view

Summary

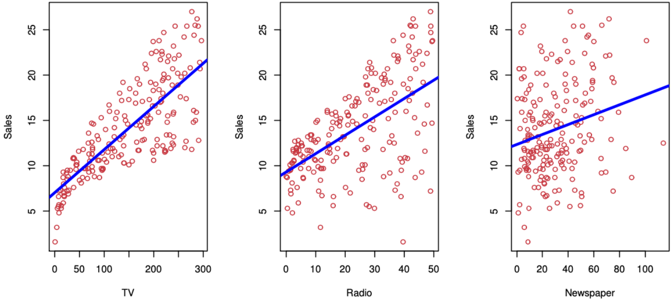
Regression

- *Regression analysis* aims to estimate the relationship between an *independent variable* x and a *dependent variable* t
- Often, we say we want to predict t from x.
- We want to find a function f with parameters ω such that

$$t \approx f(x, \omega), \tag{1}$$

  where x is (typically) an M-dimensional vector and t a scalar.
- Jargon:
  x is the *predictor*, *covariate*, *explanatory variable*, or *feature*.
  t is the *target*, *outcome*, or *response*.
- Often, we dont want to just *predict* t, but also *interpret* the relationship between x and t.

Example: Predicting sales from advertising



Source: James, Witten, Hastie, Tibshirani 2017

- Is there a relationship between advertising budget and sales?
- How strong is this relationship?
- Advertising in which media are most strongly associated with sales?
- Is the relationship linear?
- Are there synergies (or redundancies) among the different media?

Many other examples...

- How will Covid-Case Counts develop in the near future?
  (predict future counts from past counts)
- What vote-share will parties get at the next election?
  (predict votes from surveys, economic data)
- How will neural activity in the brain change when a particular image is shown (and which parts of the image are most important)?
- How well will students do in an exam?
- ...

Linear regression: The parent of all regression models

- Given data data $D = \{(\mathbf{x}_1, t_1), \ldots, (\mathbf{x}_N, t_N)\}$, we seek a linear model

$$\begin{aligned} t_n &= \omega_1 x_n^{(1)} + \ldots + \omega_N x_n^{(N)} + \varepsilon_n && (2) \\ &= \omega^\top x_n + \varepsilon_n, && (3) \end{aligned}$$

  where the ε_n are error terms (or 'residuals').
- This is sometimes written in matrix form,

$$\mathbf{t} = X\omega + \varepsilon, \qquad (4)$$

  where $\mathbf{t}$ is an $N \times 1$ vector, X is the $N \times M$ matrix of covariates (the *design matrix*), and ε is a vector of residuals.

Why is linear regression so important?

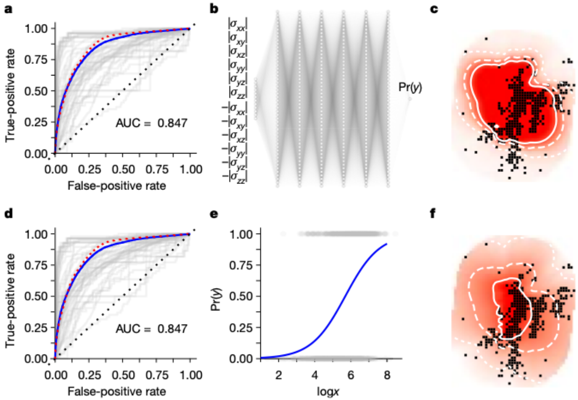
- The simplest regression model: (Almost) always try it first!
- Statistical properties of linear regression models (e.g. hypothesis tests) extremely well studied.
- Linear models are are easier to interpret (but even that is not always trivial, e.g. if covariates are correlated).
- It provides a building block for more complex, nonlinear models.

MATTERS ARISING

https://doi.org/10.1038/s41586-019-1582-8

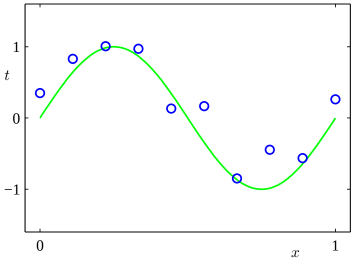
One neuron versus deep learning in aftershock prediction

Arnaud Mignan[1,2,3]* & Marco Broccardo[2,4]*



Linear regression: The ‘Machine Learning’ view

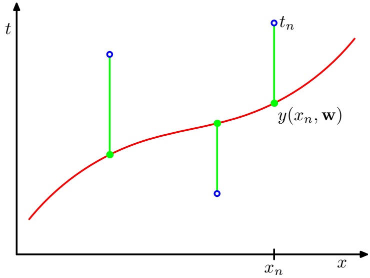
Using linear regression for nonlinear prediction problems



Source: Bishop PRML, Fig. 1.2.

$$
\begin{aligned}
y(x, \omega) &= \omega_0 + \omega_1 x + \omega_2 x^2 + \cdots + \omega_M x^M && (5)\\
&= \sum_{i=0}^{M} \omega_i x^i && (6)\\
&:= \omega^\top \phi(x) \qquad\qquad := \omega^\top z && (7)
\end{aligned}
$$

How to find ω? One idea: Minimize sum of squared errors



Source: Bishop PRML, Fig. 1.3.

$$E(\omega) = \frac{1}{2} \sum_{n=1}^{N} (y(x_n, \omega) - t_n)^2 \tag{8}$$

Minimum squared error solution for linear regression

$$
\begin{aligned}
E(\omega) &= \frac{1}{2}\sum_{n=1}^{N}(\omega^\top z_n - t_n)^2 && (9)\\
&= \frac{1}{2}\sum_{n=1}^{N}(\omega^\top z_n - t_n)(\omega^\top z_n - t_n)^\top && (10)\\
&= \frac{1}{2}\sum_{n=1}^{N}(\omega^\top z_n - t_n)(z_n^\top \omega - t_n) && (11)\\
&= \frac{1}{2}\sum_{n=1}^{N}\omega^\top z_n z_n^\top w - 2t_n\omega^\top z_n + t_n^2 && (12)\\
&= \omega^\top\left(\frac{1}{2}\sum_n z_n z_n^\top\right)\omega - \omega^\top\left(\sum_n t_n z_n\right) + \sum t_n^2 && (13)\\
&= \omega^\top \qquad A \qquad \omega + \omega^\top \qquad b \qquad + c && (14)
\end{aligned}
$$

Minimum squared error solution for linear regression

$$E(\omega) = \omega^\top A\omega + \omega^\top b + c \tag{15}$$

$$\Rightarrow \nabla_\omega E(\omega) = 2\omega^\top A + b^\top \tag{16}$$

$$= \omega^\top \left(\sum_n z_n z_n^\top\right) - \sum_n t_n z_n^\top \tag{17}$$

Setting the gradient to 0, we get the ω which minimizes the sum of squared errors,

$$\omega_{MSE} = \left(\sum_n z_n z_n^\top\right)^{-1} \sum_n t_n z_n \tag{18}$$

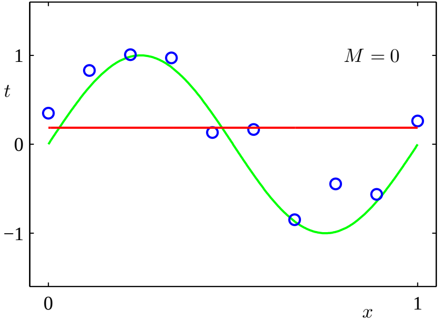
Note: If the z's have 0 mean, then

$$\mathrm{Cov}(z) = \frac{1}{N}\sum_n z_n z_n^\top \tag{19}$$

$$\mathrm{Cov}(z,t) = \frac{1}{N}\sum_n t_n z_n \tag{20}$$

Ok, but which *M* should we use?

M=0

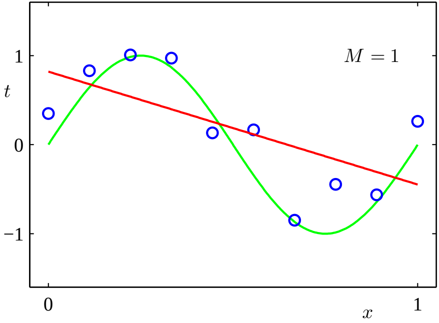


Source: Bishop PRML Fig. 1.4.

$$y = \omega_o \tag{21}$$

Ok, but which *M* should we use?

M=1

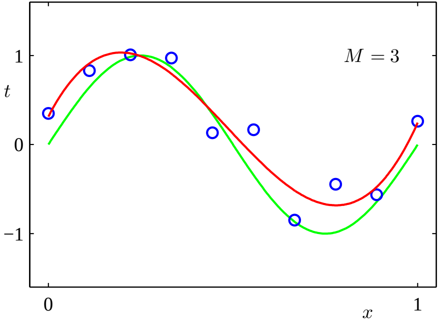


Source: Bishop PRML Fig. 1.4.

$$y = \omega_o + \omega_1 x \tag{22}$$

Ok, but which *M* should we use?

M=3

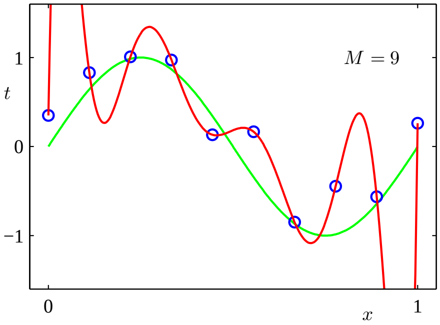


Source: Bishop PRML Fig. 1.4.

$$y = \omega_o + \omega_1 x + \omega_2 x^2 + \omega_3 x^3 \tag{23}$$

Ok, but which *M* should we use?

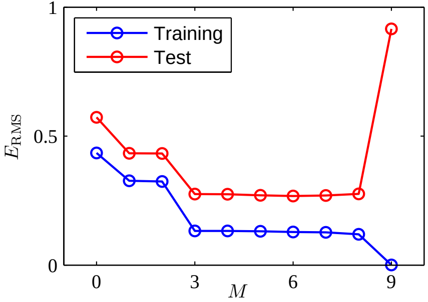
M=9



Source: Bishop PRML Fig. 1.4.

$$y = \omega_o + \omega_1 x + \omega_2 x^2 + \omega_3 x^3 \ldots + \omega_9 x^9 \tag{24}$$

Evaluating generalization performance: Use a separate test-set!



Source: Bishop PRML Fig. 1.5.

Note: The ‘optimal’ model will depend on *N*, i.e. the size of the data-set: With more data, we might favour more complex models.

Can we do better? Regularization

- Key idea: Penalize large parameters
- Add penalty on norm of ω to the loss function:

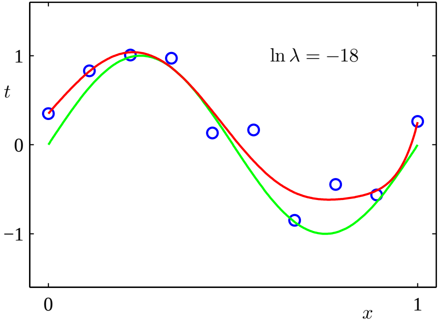
$$\tilde{E}(\omega|\lambda) = \frac{1}{2}\sum_{n=1}^{N}(y(x_n,\omega) - t_n)^2 + \frac{\lambda}{2}\|\omega\|^2 \tag{25}$$

- Solution:

$$\omega_{reg} = \left(\sum_{n=1}^{N} z_n z_n^\top + \lambda \mathbf{I}_M\right)^{-1} \sum_{n=1}^{N} z_n t_n \tag{26}$$

Can we do better? Regularization

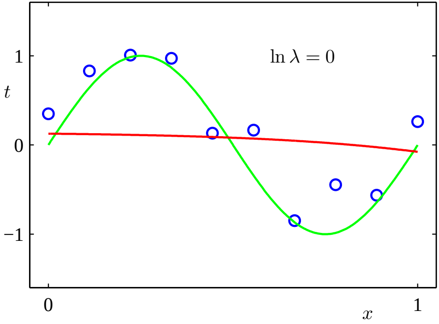
$\log \lambda = -18$



Source: Bishop PRML Fig. 1.7.

Can we do better? Regularization

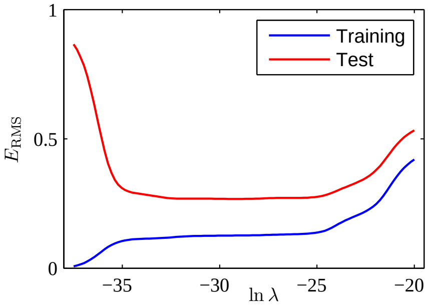
$\log \lambda = 0$



Origin: Bishop PRML Fig. 1.7.

Can we do better? Regularization

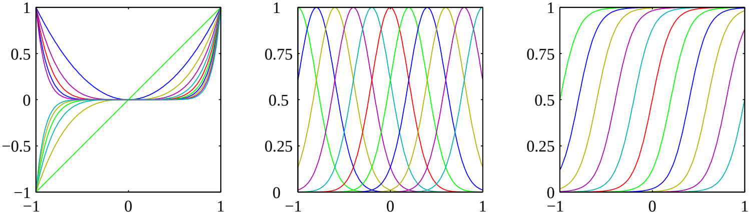
Cross-validation:



Source: Bishop PRML Fig. 1.8.

Linear regression with well-chosen basis functions ('features') can be a powerful modelling approach!.

- Basis functions $\phi(x)$ can model nonlinear relationships with $y(\omega, \mathbf{x}) = \omega^\top \phi(x)$.
- Polynomial regression: $\phi(x) = (1, x, x^2, x^3)$
- 'Gaussian bumps': $\phi_i(x) = \exp\left(-frac12(x - s_i)^2/\sigma_i^2\right)$
- Sigmoids $\phi_i(x) = 1/(1 + \exp(-x - s_i))$



Source: Bishop PRML Figures 3.1a-c

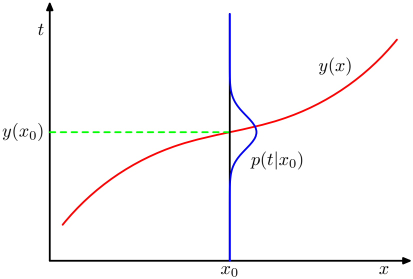
Linear regression revisited: Estimation in linear Gaussian models

Linear regression as MLE in a Gaussian model

- Suppose that we have data $D = \{(\mathbf{x}_1, t_1), \ldots, (\mathbf{x}_N, t_N)\}$
- We model the data by $t_n \approx y(x, \omega) + \varepsilon$, where ε is additive Gaussian noise.
- We assume that noise is independent, identically distributed and Gaussian:

$$\varepsilon \sim \mathcal{N}(0, \sigma^2) \tag{27}$$

$$t|\mathbf{x}, \omega, \sigma^2 \sim \mathcal{N}(y(\mathbf{x}, \omega), \sigma^2) \tag{28}$$



Source: Bishop PRML Figure 1.28

Linear regression as MLE in a Gaussian model

- We consider a linear model $y(\mathbf{x}, \omega) = \omega^\top \mathbf{x}$
- We want to infer ω by maximizing the log-likelihood, which is

$$\log P(D|\omega) = C - \frac{1}{2\sigma^2} \sum_{n=1}^{N} (y(\mathbf{x}_n, \omega) - t_n)^2 \tag{29}$$

- Thus, maximizing the likelihood for linear regression is the same as minimizing the sum of squared errors, and we get the MLE

$$\omega_{MLE} = \left(\sum_n \mathbf{x}_n \mathbf{x}_n^\top \right)^{-1} \sum_n \mathbf{x}_n t_n \tag{30}$$

Linear regression as MLE in a Gaussian model

$$y = \beta^\top x + \varepsilon_n \tag{31}$$

$$\varepsilon \sim \mathcal{N}(0, \sigma^2) \text{ i.i.d} \tag{32}$$

- The first entry of x is almost always a '1', and the corresponding parameter β_o is called the 'offset'.
- There is extensive, classical statistical theory for linear Gaussian models.
- Hypothesis tests: e.g. can one reject the null-hypothesis of all $\beta' s$ being 0?
- Confidence intervals: How well can we constrain each 'effect' β?
- Interpretation of β's: What does it 'mean' that a particular value of β is big?
- Are the assumptions of the model valid? Is the relationship linear? Are the errors independent, Gaussian, and all have the same variance?

Checking model assumptions in linear regresssion

- Are the residuals Gaussian? Plot histogram of residuals, check for Gaussianity (either by visual inspection or by running a statistical test). In particular, check for any 'outliers', i.e. values which seem overly small or big– these will likely have a very big influence on the estimated fit!
- Are the residuals uncorrelated? For data which is 'ordered', e.g. time-series data, calculate the correlation between adjacent residuals, to check whether they are uncorrelated.
- Do the residuals have a constant variance? (Jargon: constant variance = 'homeoscedastic', non-constant variance = 'heteroscedastic'. Plot the fitted values (y) against the residuals, and check whether there is a correlation.

Linear regression: The Bayesian view

Maximum-a-posteriori (MAP) solution for linear regression:

- We use a multivariate Gaussian as prior for ω:

$$\omega_i \sim \mathcal{N}(0, \alpha^{-1}) \tag{33}$$

$$p(\omega|\alpha) = \left(\frac{\alpha}{2\pi}\right)^{M/2} \exp\left(-\frac{\alpha}{2}\omega^\top \omega\right) \tag{34}$$

- Finding the maximum-a-posteriori of ω:

$$\omega_{MAP} = \left(\sum_{n=1}^{N} x_n x_n^\top + \frac{\alpha}{\gamma}\mathbf{I}_M\right)^{-1} \left(\sum_{n=1} x_n t_n\right), \tag{35}$$

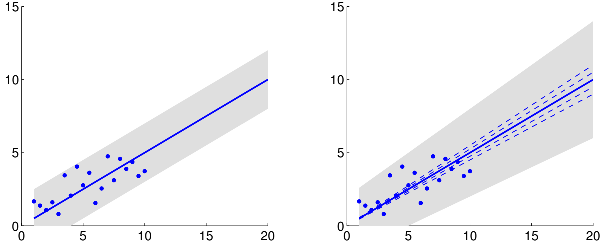
where $\gamma = 1/\sigma^2$.

In a linear Gaussian model, we can calculate the full posterior distribution in closed form (*)

$$p(\omega|D,\alpha,\gamma) = \mathcal{N}(\omega|\mu_{\text{post}},\Sigma_{\text{post}}), \text{ where} \tag{36}$$

$$\Sigma_{\text{post}}^{-1} = \alpha\mathbf{I} + \gamma\sum_n x_n x_n^\top \text{ and} \tag{37}$$

$$\mu_{post} = \gamma\Sigma_{post}\sum_n x_n t_n. \tag{38}$$



(*) Assuming that we fix α and γ– if we do not know them have to use MCMC or variational approximations.

Summary: Linear regression

- (Almost) always start with a linear regression!
- On nonlinear problems, use basis functions.
- ‘Machine learning view’: Minimize MSE, use regularization/cross-validation to control model complexity.
- ‘Statistical view’: Linear regression = Linear Gaussian model
- Can be used for hypothesis testing (e.g. ‘which, if any, parameters are significantly away from zero’).
- Care is needed when interpreting parameters!
- Bayesian linear regression: Model uncertainty over parameters. Closed form solutions (if we know prior and noise variances).
- Next week: Regression is just conditional density estimation.

Reading

- ‘Machine learning’ view of Linear Regression: Bishop PRML (“Pattern Recognition and Machine Learning” by Christopher Bishop, 2006) 3.1.1, 3.1.2, 3.1,4
- Statistical View of Linear Regression: “An introduction to statistical learning” by James, Witten, Hastie, Tibshirani, 2017, Chapter 3.
- Bayesian linear regression: Bishop PRML 3.3.1-3.3.2, 3.4-3.6 (advanced)