

6- numerical estimation and regression

regression

input variables = regressors, independent/ predictor/ explanatory/ exposure variables

output variables = regressands, dependent/ response/ explained/ outcome variables

if the model is non-linear, utilize the expectation maximization algorithm

linear regression = $y = mx + b$ for noise \rightarrow random variable $\leftarrow Y_j = \alpha + \beta x_j + E_j$ (error variable with mean 0, unbiased estimator)
 unknown parameters to be estimated

the least-squares estimator = $\sum_{j=1}^N (E_j)^2 = \sum_{j=1}^N (y_j - (\alpha + \beta x_j))^2$ minimize

$$\rightarrow \hat{\beta} \rightarrow \frac{\partial \sum (E_j)^2}{\partial \beta} = \sum -2x_j(y_j - \alpha - \beta x_j) = 0 \quad \hat{\alpha} = \bar{y} - \hat{\beta} \bar{x}$$

$$\rightarrow \hat{\alpha} \rightarrow \frac{\partial \sum (E_j)^2}{\partial \alpha} = \sum -2(y_j - \alpha - \beta x_j) = 0 \quad \hat{\beta} = \frac{\sum (y_j - \bar{y})(x_j - \bar{x})}{\sum (x_j - \bar{x})^2}$$

weighted least squares = normally error of each point has different var $\rightarrow \min(\sum w_j (y_j - \alpha - \beta x_j)^2)$

multiple regression = $Y_j = \alpha + \beta_1 x_{j1} + \beta_2 x_{j2} + \dots + \beta_k x_{jk} + E_j$

$$\rightarrow \text{matrix form: } Y = C\beta + E \quad \begin{aligned} Y &= (Y_1, Y_2, \dots, Y_n)^T \\ \beta &= (\alpha, \beta_1, \beta_2, \dots, \beta_k)^T \\ E &= (E_1, E_2, \dots, E_n)^T \end{aligned} \quad C = \begin{pmatrix} 1 & x_{11} & x_{12} & \dots & x_{1k} \\ 1 & x_{21} & x_{22} & \dots & x_{2k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \dots & x_{nk} \end{pmatrix} \rightarrow \hat{\beta} = (C^T C)^{-1} C^T Y$$

polynomial regression = $Y_j = \alpha + \beta_1 x_j + \beta_2 x_j^2 + \dots + \beta_k x_j^k + E_j$

change it like $(x = x_j, y = x_j^2, z = x_j^3) \rightarrow$ predict $z = y$, like it is linear

multivariate normal (multinormal) = generalization of the one-dimensional normal/gaussian distribution to higher dimensions

every combinations of dimensions is distributed normally

$$\rightarrow \Sigma_{ij} = \text{cov}(x_i, x_j) = E[(x_i - \mu_i)(x_j - \mu_j)] \quad \Sigma_{ij} = \begin{bmatrix} E[(x_1 - \mu_1)(x_1 - \mu_1)] & E[(x_1 - \mu_1)(x_2 - \mu_2)] & \dots & E[(x_1 - \mu_1)(x_n - \mu_n)] \\ E[(x_2 - \mu_2)(x_1 - \mu_1)] & E[(x_2 - \mu_2)(x_2 - \mu_2)] & \dots & E[(x_2 - \mu_2)(x_n - \mu_n)] \\ \vdots & \vdots & \ddots & \vdots \\ E[(x_n - \mu_n)(x_1 - \mu_1)] & E[(x_n - \mu_n)(x_2 - \mu_2)] & \dots & E[(x_n - \mu_n)(x_n - \mu_n)] \end{bmatrix}$$

$$\rightarrow \Sigma = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \rightarrow \text{no correlation} \quad \rightarrow \Sigma = \begin{pmatrix} 1 & 0.75 \\ 0.75 & 1 \end{pmatrix} \rightarrow \text{positive correlation between } x \text{ and } y$$

mixtures of multinormals = when only a mixture of gaussians can represent data

$$\left\{ \begin{array}{l} \text{0.7 } N((2,2), \Sigma_1) + 0.15 N((1,1), \Sigma_2) + 0.15 N((2,3), \Sigma_3) \end{array} \right\}$$

$$\rightarrow \text{density function} = \sum_{i=1}^k w_i N(\mu_i, \Sigma_i) \quad (\sum_{i=1}^k w_i = 1)$$

* if we know how many gaussians in the mixture:

① if which point belonged to which gaussian is given, the parameters can be found using maximum likelihood estimation

② if the parameters is given, we can find the assignments using expectation maximization algorithm

expectation maximization algorithm = guess the assignments \rightarrow use them to estimate parameters

\rightarrow use them to generate better assignments \rightarrow repeat until no improvement (like k-means)

\rightarrow expectation step = given parameters θ , find expected value on the latent variables z

$$z = E[z | x, \theta] \quad z_{ij} = \begin{cases} 1, & \text{if point } i \text{ in } j\text{th gaussian (assigning members to clusters)} \\ 0, & \text{otherwise} \end{cases}$$

\rightarrow (n x k) matrix

soft assignments = $0 \leq z_{ij} \leq 1$ (used here)

hard assignment = $z_{ij} = 1$, rest $z_{ik} = 0$

\rightarrow maximization step = estimate new parameters based on max likelihood

$$\theta' = \hat{\theta}_{MLE} = \arg \max_{\theta} \log L(\theta | x, z) \quad \theta = \{(\mu_1, \Sigma_1), \dots, (\mu_k, \Sigma_k)\} \quad (\text{calculating new means and covariance matrices})$$

③ if number of gaussians is unknown:

$\rightarrow k = n$, each point gets its own gaussian, max possible likelihood \rightarrow overfitting

$\rightarrow k = 1$, simple low likelihood \rightarrow underfitting

$$\text{bayesian information criterion (BIC)} = \underbrace{-2 \log L(\theta | x, z)}_{\text{accuracy}} + \underbrace{k \log(n)}_{\text{penalize for more parameters}} \quad \begin{aligned} k &= \# \text{ of regressors} \\ n &= \# \text{ of points} \end{aligned}$$

must be lowest

linear model in R:

- lm(<response var> ~ <input var>, <data frame>)

simple regression:

```
my_linear_model <- lm(y ~ x, my_data_frame)
```

```
predict(my_linear_model, data.frame(x=1:5))
```

multivariable regression:

$$y = \beta_1 x + \beta_2 + \alpha$$

```
my_multi_regression_model <- lm(y ~ x + z, my_data_frame)
```

polynomial regression:

$h(t) = k + v_0t + gt^2$

```
lm(h~t+t2,data.frame(h=ball$h, t=ball$t, t2= ball$t^2))
```

- <<- global assignment in R