Pattern Recognition 2018
Linear Models for Regression

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Linear Regression Model

The central assumption of linear regression is

$$\mathbb{E}[t|x] = y(x) = w_0 + w_1 x$$

Or, alternatively

$$t = w_0 + w_1 x + \varepsilon$$

with $\mathbb{E}[\varepsilon|x] = 0$.

Usually, we also assume that $\mathrm{var}[t|x] = \sigma^2$, i.e. t has the same variance for each value of x.
For ML estimation, we typically assume $\varepsilon \sim \mathcal{N}(0, \sigma^2)$.

Minimizing empirical loss

Given training data

$$D = \{(x_1, t_1), (x_2, t_2), \ldots, (x_N, t_N)\},$$

find the values of w_0 and w_1 such that the sum of squared errors

$$\begin{aligned} E_D(w_0, w_1) &= \sum_{n=1}^{N} (t_n - \overbrace{(w_0 + w_1 x_n)}^{\text{prediction for } t_n})^2 \\ &= \sum_{n=1}^{N} (t_n - w_0 - w_1 x_n)^2 \end{aligned}$$

is minimized.

General Solution: Calculus

Partial derivative with respect to intercept:

$$\begin{aligned}\frac{\partial E_D}{\partial w_0} &= \sum_{n=1}^{N} 2(t_n - w_0 - w_1 x_n)(-1) \\ &= -2\sum_{n=1}^{N}(t_n - w_0 - w_1 x_n)\end{aligned}$$

Equate to zero

$$\sum_{n=1}^{N}(t_n - w_0 - w_1 x_n) = \sum_{n=1}^{N} e_n = 0$$

General Solution: Calculus

Partial derivative with respect to slope:

$$\begin{aligned}\frac{\partial E_D}{\partial w_1} &= \sum_{n=1}^{N} 2(t_n - w_0 - w_1 x_n)(-x_n) \\ &= -2\sum_{n=1}^{N} x_n(t_n - w_0 - w_1 x_n)\end{aligned}$$

Equate to zero

$$\sum_{n=1}^{N} x_n(t_n - w_0 - w_1 x_n) = \sum_{n=1}^{N} x_n e_n = 0$$

General Solution: Calculus

Expand and collect terms:

$$\begin{aligned}\sum_{n=1}^{N} t_n &= N w_0 + w_1 \sum_{n=1}^{N} x_n && (1)\\ \sum_{n=1}^{N} x_n t_n &= w_0 \sum_{n=1}^{N} x_n + w_1 \sum_{n=1}^{N} x_n^2 && (2)\end{aligned}$$

To solve for w_0 divide (1) by N:

$$w_0 = \bar{t} - w_1 \bar{x}$$

Hence, the least squares fitted line goes through the point of means $(\bar{x}, \bar{t})$.

General Solution: Calculus

To solve for w_1, multiply (1) by $\sum x_n$ and (2) by N

$$\begin{aligned} \sum x_n \sum t_n &= N w_0 \sum x_n + w_1 \left(\sum x_n\right)^2 && (3) \\ N \sum x_n t_n &= N w_0 \sum x_n + N w_1 \sum x_n^2 && (4) \end{aligned}$$

Subtract (3) from (4) and solve for w_1:

$$w_1 = \frac{N \sum x_n t_n - \sum x_n \sum t_n}{N \sum x_n^2 - (\sum x_n)^2}$$

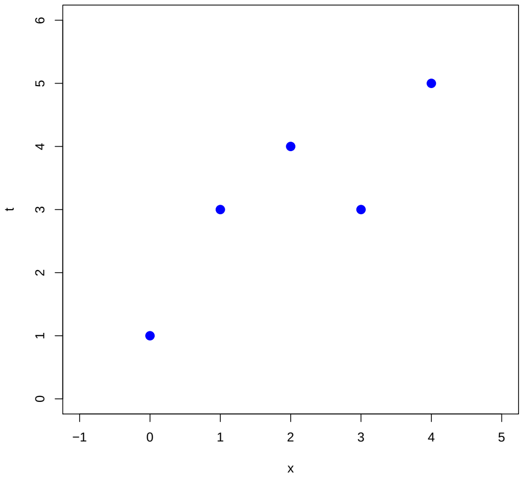
Example

n	x_n	t_n	$x_n t_n$	x_n^2
1	0	1	0	0
2	1	3	3	1
3	2	4	8	4
4	3	3	9	9
5	4	5	20	16
$\sum$	10	16	40	30

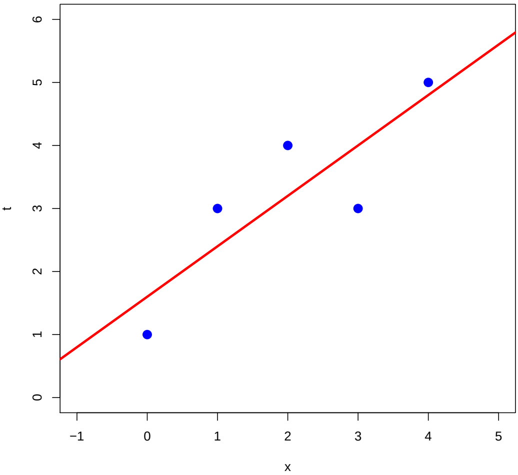
$$\begin{aligned} w_1 &= \frac{N \sum x_n t_n - \sum x_n \sum t_n}{N \sum x_n^2 - (\sum x_n)^2} \\ &= \frac{5 \times 40 - 10 \times 16}{5 \times 30 - 10^2} = \frac{4}{5} \end{aligned}$$

$$w_0 = \bar{t} - w_1 \bar{x} = \frac{16}{5} - \left(\frac{4}{5}\right)\left(\frac{10}{5}\right) = \frac{8}{5}$$

Scatter plot of Training Data



Fitted Line: $y(x) = 1.6 + 0.8\ x$



Decomposition of total sample variation in t

1. $\sum(t_n - \bar{t})^2$ = total sum of squares = SST
2. $\sum(y_n - \bar{t})^2$ = explained sum of squares = SSR
3. $\sum(t_n - y_n)^2 = \sum e_n^2$ = error sum of squares = SSE

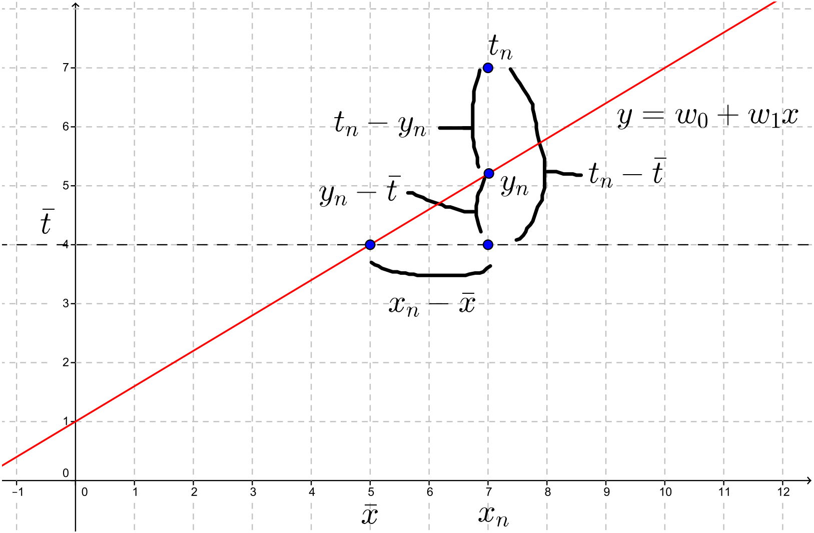
We have

$$\mathrm{SST} = \mathrm{SSR} + \mathrm{SSE}$$

Proportion of variation in t explained by x:

$$\boxed{R^2 = \frac{\mathrm{SSR}}{\mathrm{SST}} = 1 - \frac{\mathrm{SSE}}{\mathrm{SST}}}$$

Decomposition of variation in t



Example: Computation of R^2

Fitted model

$$y(x) = 1.6 + 0.8x$$

n	x_n	t_n	y_n	e_n	e_n^2	$(t_n - \bar{t})^2$	$(y_n - \bar{t})^2$
1	0	1	$8/5$	$-3/5$	$9/25$	$121/25$	$64/25$
2	1	3	$12/5$	$3/5$	$9/25$	$1/25$	$16/25$
3	2	4	$16/5$	$4/5$	$16/25$	$16/25$	0
4	3	3	$20/5$	-1	$25/25$	$1/25$	$16/25$
5	4	5	$24/5$	$1/5$	$1/25$	$81/25$	$64/25$
$\sum$	10	16	16	0	$60/25$	$220/25$	$160/25$

$$\begin{array}{ccccc} 220/25 & = & 60/25 & + & 160/25 \\ (SST) & & (SSE) & & (SSR) \end{array}$$

$$R^2 = \frac{SSR}{SST} = \frac{160}{220} \approx 0.73$$

Linear regression through the origin

Suppose we know that the population regression line goes through the origin, i.e.

$$\mathbb{E}[t|x] = wx$$

Find the value of w such that the sum of squared errors

$$E_D(w) = \sum_{n=1}^{N} (t_n - wx_n)^2$$

is minimized.

Regression through the origin: calculus

Take the derivative

$$\frac{dE_D}{dw} = -2 \sum (t_n - w x_n) x_n$$

and equate to zero

$$\sum x_n t_n - w \sum x_n^2 = 0$$

so we get

$$w = \frac{\sum x_n t_n}{\sum x_n^2}$$

Regression through the origin: geometry

Regression through the origin: $y_n = wx_n$

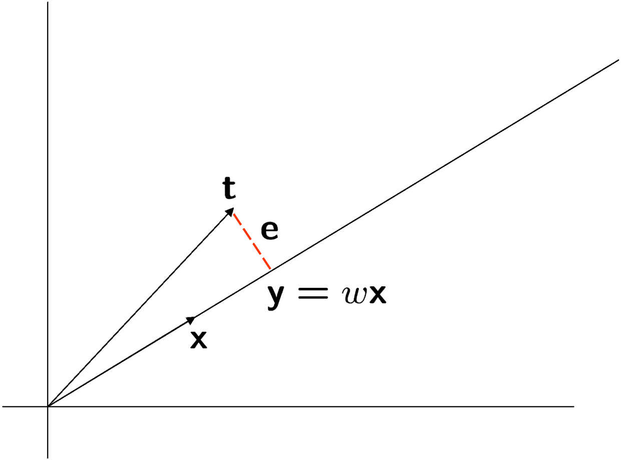
$D = \{(2,5),(1,3)\}$ contains only two observations.

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 2 \\ 1 \end{bmatrix} \text{ and } \mathbf{t} = \begin{bmatrix} t_1 \\ t_2 \end{bmatrix} = \begin{bmatrix} 5 \\ 3 \end{bmatrix}$$

$$\mathbf{e} = \begin{bmatrix} e_1 \\ e_2 \end{bmatrix} \text{ and } \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

$$\mathbf{y} = w\mathbf{x} \text{ and } \mathbf{e} = \mathbf{t} - w\mathbf{x}$$

Least Squares Solution (*N* dimensional space!)



Length of $\mathbf{e} = \sqrt{\mathbf{e} \cdot \mathbf{e}} = \sqrt{e_1^2 + e_2^2}$.

Least Squares Solution

To minimize the length of $\mathbf{e}$, it must be perpendicular to $\mathbf{x}$ so $\mathbf{x} \cdot \mathbf{e} = 0$.

$$\mathbf{x} \cdot \mathbf{e} = \mathbf{x} \cdot (\mathbf{t} - w\mathbf{x}) = \mathbf{x} \cdot \mathbf{t} - w\mathbf{x} \cdot \mathbf{x} = 0$$

Therefore

$$w = \frac{\mathbf{x} \cdot \mathbf{t}}{\mathbf{x} \cdot \mathbf{x}}$$

Matrix notation

$$w = \frac{\mathbf{x}^\top \mathbf{t}}{\mathbf{x}^\top \mathbf{x}} \qquad \text{or} \qquad w = (\mathbf{x}^\top \mathbf{x})^{-1} \mathbf{x}^\top \mathbf{t}$$

Solution of Numerical Example

Solution of the numerical example

$$\mathbf{x}^\top \mathbf{t} = [2 \;\; 1] \begin{bmatrix} 5 \\ 3 \end{bmatrix} = 13$$

and

$$\mathbf{x}^\top \mathbf{x} = [2 \;\; 1] \begin{bmatrix} 2 \\ 1 \end{bmatrix} = 5$$

which yields

$$w = \frac{\mathbf{x}^\top \mathbf{t}}{\mathbf{x}^\top \mathbf{x}} = \frac{13}{5} = 2.6$$

Simple linear regression in matrix terms

We can write the observed t values as

$$t_n = w_0 + w_1 x_n + e_n \qquad\qquad n = 1, \ldots, N$$

which is short for

$$\begin{aligned} t_1 &= w_0 + w_1 x_1 + e_1 \\ t_2 &= w_0 + w_1 x_2 + e_2 \\ &\vdots \\ t_N &= w_0 + w_1 x_N + e_N \end{aligned}$$

Matrix Notation

$$\mathbf{X} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \\ 1 & x_N \end{bmatrix} \mathbf{t} = \begin{bmatrix} t_1 \\ t_2 \\ \vdots \\ t_N \end{bmatrix} \mathbf{e} = \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_N \end{bmatrix} \mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \end{bmatrix}$$

Then we can simply write

$$\mathbf{t} = \mathbf{X}\mathbf{w} + \mathbf{e}$$

Check

$$\mathbf{t} = \mathbf{X}\mathbf{w} + \mathbf{e}$$

$$\begin{aligned}
\begin{bmatrix} t_1 \\ t_2 \\ \vdots \\ t_N \end{bmatrix} &= \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \\ 1 & x_N \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \end{bmatrix} + \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_N \end{bmatrix} \\
&= \begin{bmatrix} w_0 + w_1 x_1 \\ w_0 + w_1 x_2 \\ \vdots \\ w_0 + w_1 x_N \end{bmatrix} + \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_N \end{bmatrix} \\
&= \begin{bmatrix} w_0 + w_1 x_1 + e_1 \\ w_0 + w_1 x_2 + e_2 \\ \vdots \\ w_0 + w_1 x_N + e_N \end{bmatrix}
\end{aligned}$$

Least Squares Solution

$\mathbf{y}$ is a linear combination of the columns of $\mathbf{X}$:

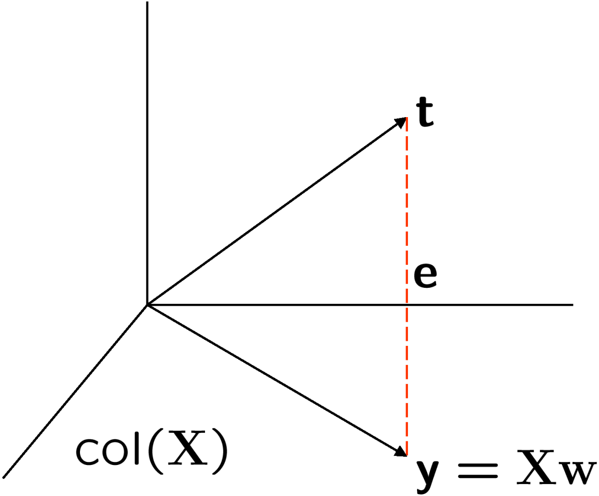
$$\mathbf{y} = \mathbf{X}\mathbf{w}$$

Typically, $\mathbf{t}$ is not in the column space of $\mathbf{X}$. Find the value of $\mathbf{y}$ that is closest to $\mathbf{t}$. For this to be the case, the error vector

$$\mathbf{e} = \mathbf{t} - \mathbf{X}\mathbf{w}$$

must be orthogonal to *all columns* of $\mathbf{X}$.

Least Squares Solution (N dimensional space)



Least Squares Solution

In other words, we should have

$$\mathbf{X}^\top \mathbf{e} = \mathbf{0}.$$

Since

$$\mathbf{e} = (\mathbf{t} - \mathbf{X}\mathbf{w})$$

we should have

$$\mathbf{X}^\top(\mathbf{t} - \mathbf{X}\mathbf{w}) = \mathbf{X}^\top\mathbf{t} - \mathbf{X}^\top\mathbf{X}\mathbf{w} = \mathbf{0}.$$

It follows that

$$\mathbf{X}^\top\mathbf{X}\mathbf{w} = \mathbf{X}^\top\mathbf{t}$$

Least Squares Solution

So we have

$$\mathbf{X}^\top \mathbf{X}\mathbf{w} = \mathbf{X}^\top \mathbf{t}$$

Premultiply both sides by the inverse of $\mathbf{X}^\top \mathbf{X}$:

$$(\mathbf{X}^\top \mathbf{X})^{-1}\mathbf{X}^\top \mathbf{X}\mathbf{w} = (\mathbf{X}^\top \mathbf{X})^{-1}\mathbf{X}^\top \mathbf{t}$$

We then find, since $(\mathbf{X}^\top \mathbf{X})^{-1}\mathbf{X}^\top \mathbf{X} = \mathbf{I}$ and $\mathbf{I}\mathbf{w} = \mathbf{w}$:

$$\boxed{\mathbf{w} = (\mathbf{X}^\top \mathbf{X})^{-1}\mathbf{X}^\top \mathbf{t}} \qquad (3.15)$$

Numeric example

$$D = \{(0,1),(1,1),(2,2),(3,2)\}$$

$$\mathbf{X} = \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix} \quad \mathbf{t} = \begin{bmatrix} 1 \\ 1 \\ 2 \\ 2 \end{bmatrix}$$

$$\mathbf{X}^\top \mathbf{X} = \begin{bmatrix} 4 & 6 \\ 6 & 14 \end{bmatrix} \quad \mathbf{X}^\top \mathbf{t} = \begin{bmatrix} 6 \\ 11 \end{bmatrix}$$

Numeric Example

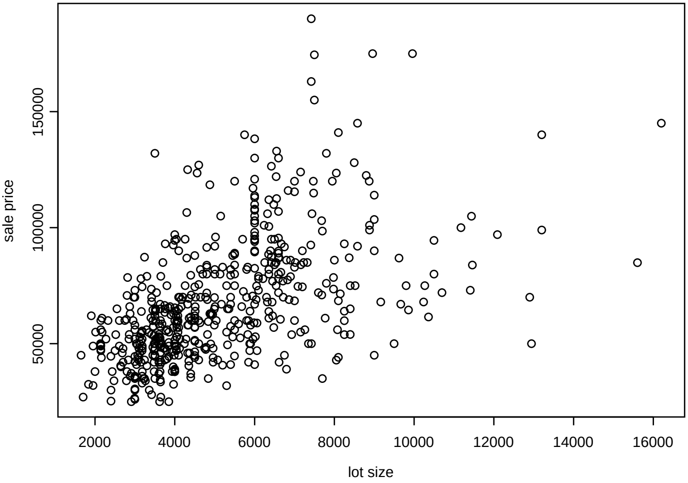
Now, since

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1} = \frac{1}{ad-bc}\begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$$

we get

$$\begin{aligned} \mathbf{w} = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{t} &= \frac{1}{20}\begin{bmatrix} 14 & -6 \\ -6 & 4 \end{bmatrix}\begin{bmatrix} 6 \\ 11 \end{bmatrix} \\ &= \frac{1}{20}\begin{bmatrix} 18 \\ 8 \end{bmatrix} = \begin{bmatrix} 9/10 \\ 4/10 \end{bmatrix} = \begin{bmatrix} w_0 \\ w_1 \end{bmatrix} \end{aligned}$$

Scatter plot of lot size and sale price



Least Squares fitted line

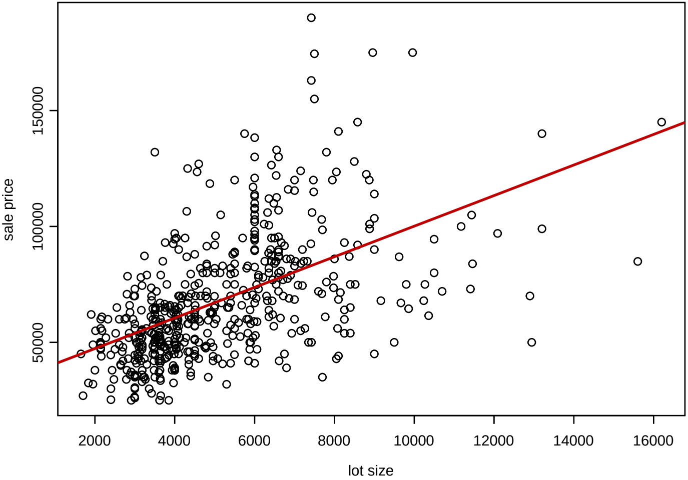
Using `R` we find:

$$\text{sale price} = 34136.1916 + 6.5988 \times \text{lot size}$$

$R^2 = 0.2871$

Model explains only about 30% of variation in sale price.

Least Squares fitted line



Multiple Linear Regression

Usually, you want to use more than one input variable to predict t.

The basic assumption is

$$\mathbb{E}[t|\mathbf{x}] = w_0 + w_1 x_1 + w_2 x_2 + \ldots + w_{M-1} x_{M-1}$$

Multiple Linear Regression

We can write the observed t values as

$$t_n = w_0 + w_1 x_{n,1} + w_2 x_{n,2} + \ldots + w_{M-1} x_{n,M-1} + e_n$$

which is short for

$$\begin{aligned}
t_1 &= w_0 + w_1 x_{1,1} + w_2 x_{1,2} + \ldots + w_{M-1} x_{1,M-1} + e_1 \\
t_2 &= w_0 + w_1 x_{2,1} + w_2 x_{2,2} + \ldots + w_{M-1} x_{2,M-1} + e_2 \\
&\vdots \\
t_N &= w_0 + w_1 x_{N,1} + w_2 x_{N,2} + \ldots + w_{M-1} x_{N,M-1} + e_N
\end{aligned}$$

Notation and Least Squares Solution

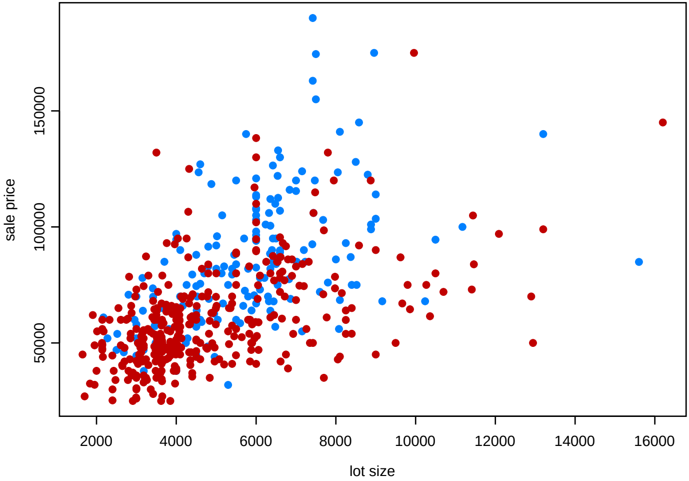
$$\mathbf{X} = \begin{bmatrix} 1 & x_{1,1} & x_{1,2} & \dots & x_{1,M-1} \\ 1 & x_{2,1} & x_{2,2} & \dots & x_{2,M-1} \\ \vdots & & & & \\ 1 & x_{N,1} & x_{N,2} & \dots & x_{N,M-1} \end{bmatrix}$$

$$\mathbf{t} = \begin{bmatrix} t_1 \\ t_2 \\ \vdots \\ t_N \end{bmatrix} \mathbf{e} = \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_N \end{bmatrix} \mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_{M-1} \end{bmatrix}$$

Then we can write

$$\mathbf{t} = \mathbf{X}\mathbf{w} + \mathbf{e}, \quad \mathbf{w} = (\mathbf{X}^\top \mathbf{X})^{-1}\mathbf{X}^\top \mathbf{t}$$

Scatter plot of lot size, airco and sale price



Fitted Equation

$$\text{sale.price} = 32692.9 + 5.6 \times \text{lot.size} + 20174.5 \times \text{air.cond}$$

Or, since air.cond is binary:

$$\text{sale.price} = 32692.9 + 5.6 \times \text{lot.size}$$

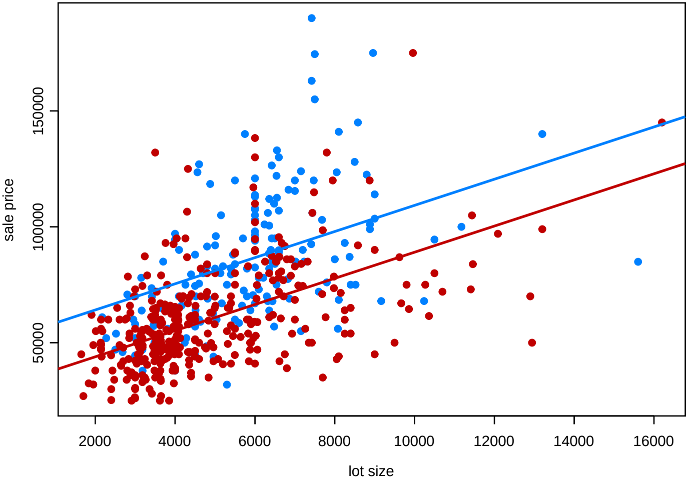
when air.cond=0.

$$\text{sale.price} = (32692.9 + 20174.5) + 5.6 \times \text{lot.size}$$

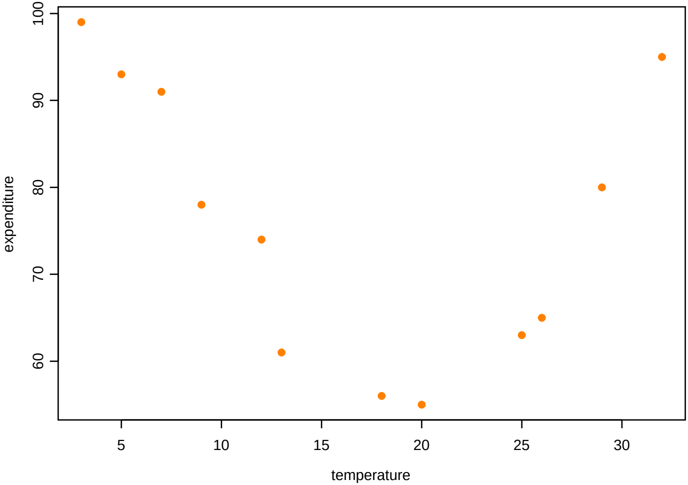
when air.cond=1.

$R^2 = 0.4048$

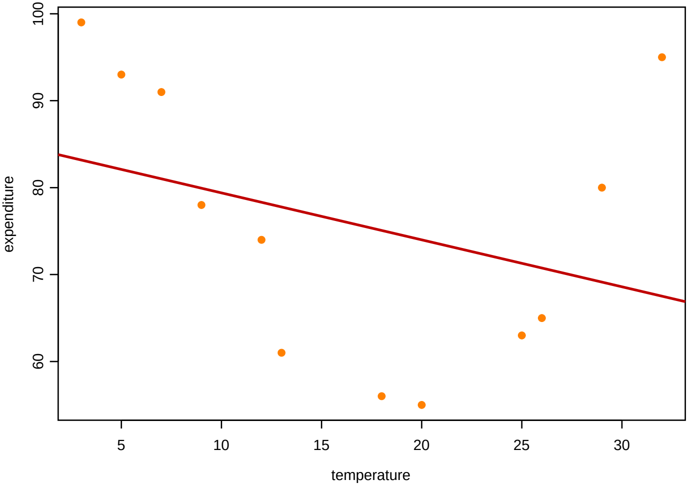
Fitted Equation



Scatter plot of Temperature and Energy Use



Fitting a Linear Function



Linear Equation

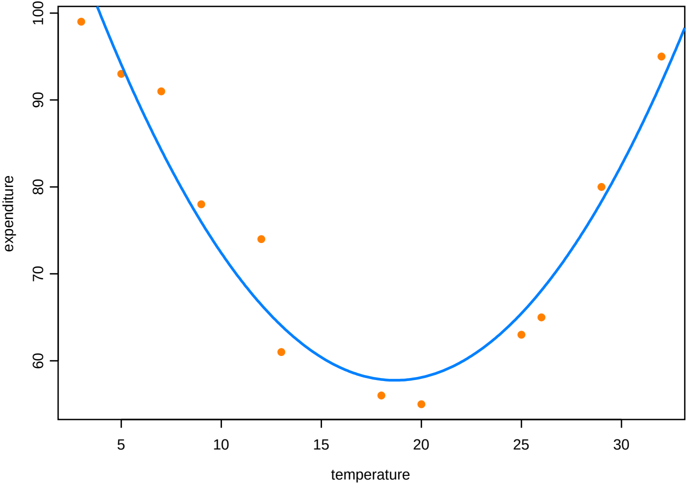
Fitted equation:

$$\text{expenditure} = 84.78 - 0.54 \times \text{temperature}$$

$R^2 \approx 0.11$

Bad fit!

Fitting a Quadratic Function



Quadratic Equation

Fitted equation:

$$\text{expenditure} = 125.44 - 7.24 \times \text{temp} + 0.19 \times \text{temp}^2$$

$R^2 \approx 0.93$

Spectacular improvement for only one extra parameter!

General Linear Model (OK, so I lied ...)

The term *linear* in linear regression means linear in the *parameters*, not linear in the *input variables*!

For example:

$$t = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_1^2 + w_4 x_1 x_2 + \varepsilon$$

is still a linear regression model.

General Linear Model

Linear in the features, but not necessarily linear in the input variables that generate them.

$$\phi(t_n) = w_0\phi_0(\mathbf{x}_n) + w_1\phi_1(\mathbf{x}_n) + \ldots + w_{M-1}\phi_{M-1}(\mathbf{x}_n) + \varepsilon_n$$

- $\mathbf{x}_n = (x_{n,1}, \ldots, x_{n,D})$
- $w_0, w_1, \ldots, w_{M-1}$: unknown parameters to be estimated;
- $\phi(\cdot), \phi_0(\cdot), \ldots, \phi_{M-1}(\cdot)$: functions that do not involve unknown parameters; "basis functions".

Modeling Pizza Expenditure

Linear Model

$$\mathbb{E}(\text{pizza}) = w_0 + w_1 \times \text{inc} + w_2 \times \text{age}$$

$$\frac{\partial \mathbb{E}(\text{pizza})}{\partial \text{inc}} = w_1 \qquad \frac{\partial \mathbb{E}(\text{pizza})}{\partial \text{age}} = w_2$$

Fitted equation:

$$\text{pizza} = 342.88 + 0.0024 \times \text{inc} - 7.58 \times \text{age}$$

$R^2 \approx 0.33$

Modeling Pizza Expenditure

Model with interaction between income and age:

$$\mathbb{E}(\text{pizza}) = w_0 + w_1 \times \text{inc} + w_2 \times \text{age} + w_3 \times (\text{age} \times \text{inc})$$

Effects of income and age:

$$\frac{\partial \mathbb{E}(\text{pizza})}{\partial \text{inc}} = w_1 + w_3 \times \text{age}$$

$$\frac{\partial \mathbb{E}(\text{pizza})}{\partial \text{age}} = w_2 + w_3 \times \text{inc}$$

Modeling Pizza Expenditure

Fitted equation:

$$\begin{aligned}\text{pizza} &= 161.47 + 0.01 \times \text{inc} - 2.98 \times \text{age} \\ &- 0.0002 \times (\text{age} \times \text{inc})\end{aligned}$$

$R^2 \approx 0.39$

Effect of income on pizza expenditure

$$
\begin{aligned}
\frac{\partial \mathbb{E}(\text{pizza})}{\partial \text{inc}} &= w_1 + w_3 \times \text{age} = 0.01 - 0.0002 \times \text{age} \\
&= \begin{cases} 0.006 & \text{for age} = 20 \\ 0 & \text{for age} = 50 \end{cases}
\end{aligned}
$$

So on average, a 20 year old will spend 60 cents on pizza of every 100 dollar of extra income.

How to in R

```
# read data (put header=T if first row in data file contains
# names of variables)

> pizza.dat <- read.table("C:/PR/pizza.txt", header=T)

# show first 5 rows

> pizza.dat[1:5,]

  pizza sex edu1 edu2 edu3 income age
1   109   1    0    0    0  15000  25
2     0   1    0    0    0  30000  45
3     0   1    0    0    0  12000  20
4   108   1    0    0    0  20000  28
5   220   1    1    0    0  15000  25
```

How to in R

```
# fit model with interaction between age and income

> pizza.model1 <- lm(pizza ∼ age + income + age:income,
data=pizza.dat)

# show results (stuff deleted)

> summary(pizza.model1)

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)  1.615e+02  1.207e+02   1.338   0.1892
age         -2.977e+00  3.352e+00  -0.888   0.3803
income       9.074e-03  3.670e-03   2.473   0.0183 *
age:income  -1.602e-04  8.673e-05  -1.847   0.0730 .

Multiple R-Squared: 0.3873
```

Interaction with a binary variable: house prices

$$\mathbb{E}(\text{sale.price}) = w_0 + w_1 \times \text{lot.size} + w_2 \times (\text{air.cond} \times \text{lot.size})$$

Price per square foot depends on presence of airco:

$$\mathbb{E}(\text{sale.price}) = w_0 + w_1 \times \text{lot.size}$$

if no airco (air.cond=0), and

$$\mathbb{E}(\text{sale.price}) = w_0 + (w_1 + w_2) \times \text{lot.size}$$

if air.cond=1.

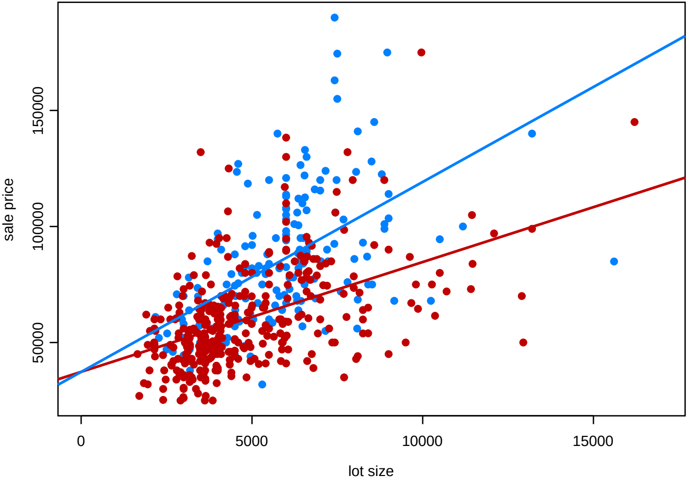
Fitted Equation

Fitted equation:

$$\begin{aligned}\text{sale.price} &= 37341.69 + 4.73 \times \text{lot.size} + \\ &\quad 3.45 \times (\text{air.cond} \times \text{lot.size})\end{aligned}$$

$R^2 \approx 0.41$.

Graph of fitted equation



Regularized Least Squares

Add regularization term to control overfitting

$$E(\mathbf{w}) = E_D(\mathbf{w}) + \lambda E_W(\mathbf{w}) \tag{3.24}$$

Ridge regression

$$E_W(\mathbf{w}) = \sum_i w_i^2 = \mathbf{w}^\top \mathbf{w} \tag{3.25}$$

The ridge regression error function is minimized by:

$$\mathbf{w} = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{t} \tag{3.28}$$

Regularization

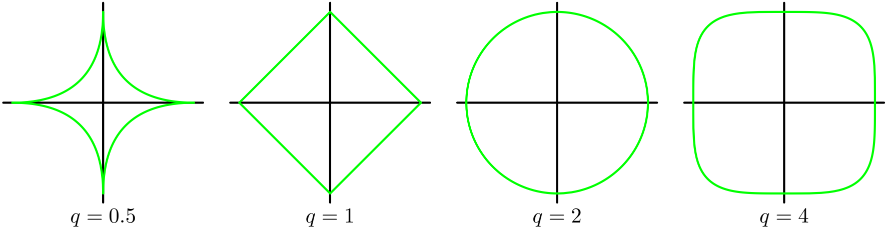
A more general regularizer

$$\sum_{n=1}^{N}\{t_n - \mathbf{w}^\top \mathbf{x}_n\}^2 + \lambda \sum_{j=0}^{M-1} |w_j|^q \qquad (3.29)$$

where $q = 2$ corresponds the ridge regression.

The case of $q = 1$ is known as the LASSO.

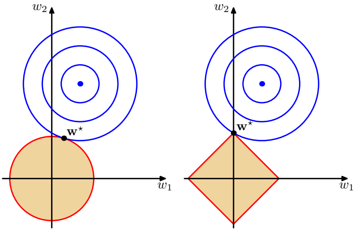
Contours of Regularization Term



LASSO

RIDGE

LASSO gives sparse solution



Minimize

$$E_D(\mathbf{w}) = \sum_{n=1}^{N} \{t_n - \mathbf{w}^\top \mathbf{x}_n\}^2 \tag{3.12}$$

subject to

$$\sum_{j=0}^{M-1} |w_j|^q \leq \eta \tag{3.30}$$

for an appropriate value of the parameter η.