Least Squares

EES 4891/5891

Probability & Statistics for Geosciences

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Learning Goals

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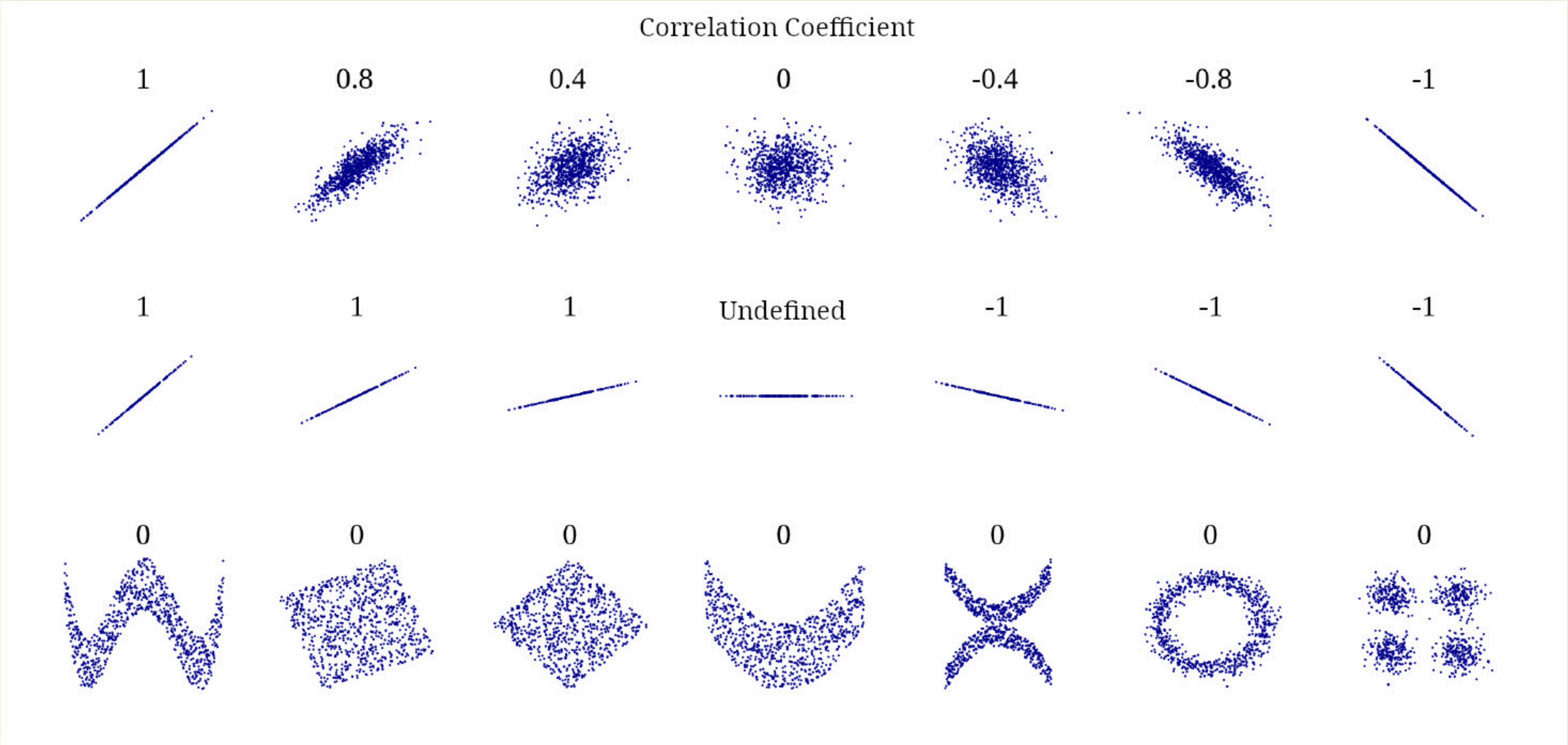
Introducing Least Squares

The Basic Problem

- We've learned about estimating parameters for probability distributions from data:
  - Univariate data:
    - Method of Moments
    - Maximum Likelihood Estimation
    - Bayesian Methods
  - Multivariate Normal
    - Estimating mean and covariance matrix
- Covariance and correlation tell you that there's a relationship between variables,
  - Don't tell you what the relationship is.
  - Different relationships can have the same correlation or covariance



- Least-Squares Analysis:
  - Estimate parameters Θ for a functional relationship between variables in multivariate data

$$x_p = f(x_1, x_2, \ldots, x_{p-1} | \Theta)$$
$$\Theta = (\theta_1, \theta_2, \ldots, \theta_k)$$

    - Bivariate: $x_2 = f(x_1 | \Theta)$

Ordinary Least Squares

- Consider N observations of bivariate data (x_i, y_i):

$$\begin{bmatrix} x_1 & y_1 \\ x_2 & y_2 \\ \vdots & \vdots \\ x_N & y_N \end{bmatrix}$$

- Assume a linear relationship:

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i,$$

where β are parameters and ε represents a random residual.

  - ε represents the residual variance not explained by $\beta_0 + \beta_1 x$

- The problem: Estimate the best values for β, given data (x_i, y_i) for $i \in 1, 2, \ldots N$
  - Criterion for best values: make ε as small as possible ("least squares").
    - Specifically: minimize

$$\sum_{i=1}^{N} \epsilon_i^2 = \sum_{i=1}^{N} (y_i - (\beta_0 + \beta_1 x_i))^2$$

    - If ε is normally distributed ($\varepsilon \sim \mathcal{N}(0, \sigma)$), then the maximum-likelihood values for β will minimize $\sum_i \epsilon_i^2$
      - Ordinary Least Squares is equivalent to Maximum Likelihood.

Multivariate Case

- More generally, if we have p-dimensional multivariate data,

$$\begin{bmatrix} x_{1,1} & x_{1,2}, & \cdots & x_{1,p} \\ x_{2,1} & x_{2,2}, & \cdots & x_{2,p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{N,1} & x_{N,2}, & \cdots & x_{N,p} \end{bmatrix}$$

we use a linear relationship

$$x_{i,p} = \beta_0 + \sum_{j=1}^{p-1} \beta_j x_{i,j} + \epsilon_i$$

and find values for $\beta = (\beta_0, \beta_1, \ldots, \beta_{p-1})$ that minimize the sum of the squares of ϵ_i

Least-Squares in R

Least-Squares in R

- Start by creating fake data with known parameters:

$$\begin{aligned}\beta_0 &= 3.5\\ \beta_1 &= 7.2\end{aligned}$$

  - Generate 100 samples with $y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$, where $\varepsilon \sim \mathcal{N}(\mu = 0, \sigma = 10)$

```
set.seed(12345)
b0 <- 3.5
b1 <- 7.2
sigma = 10
df <- tibble(x = seq(0, 10, length.out = 100),
             y = b0 + b1 * x +
               rnorm(length(x), 0, sigma))
```

- Use the `lm()` function to fit parameters to data:

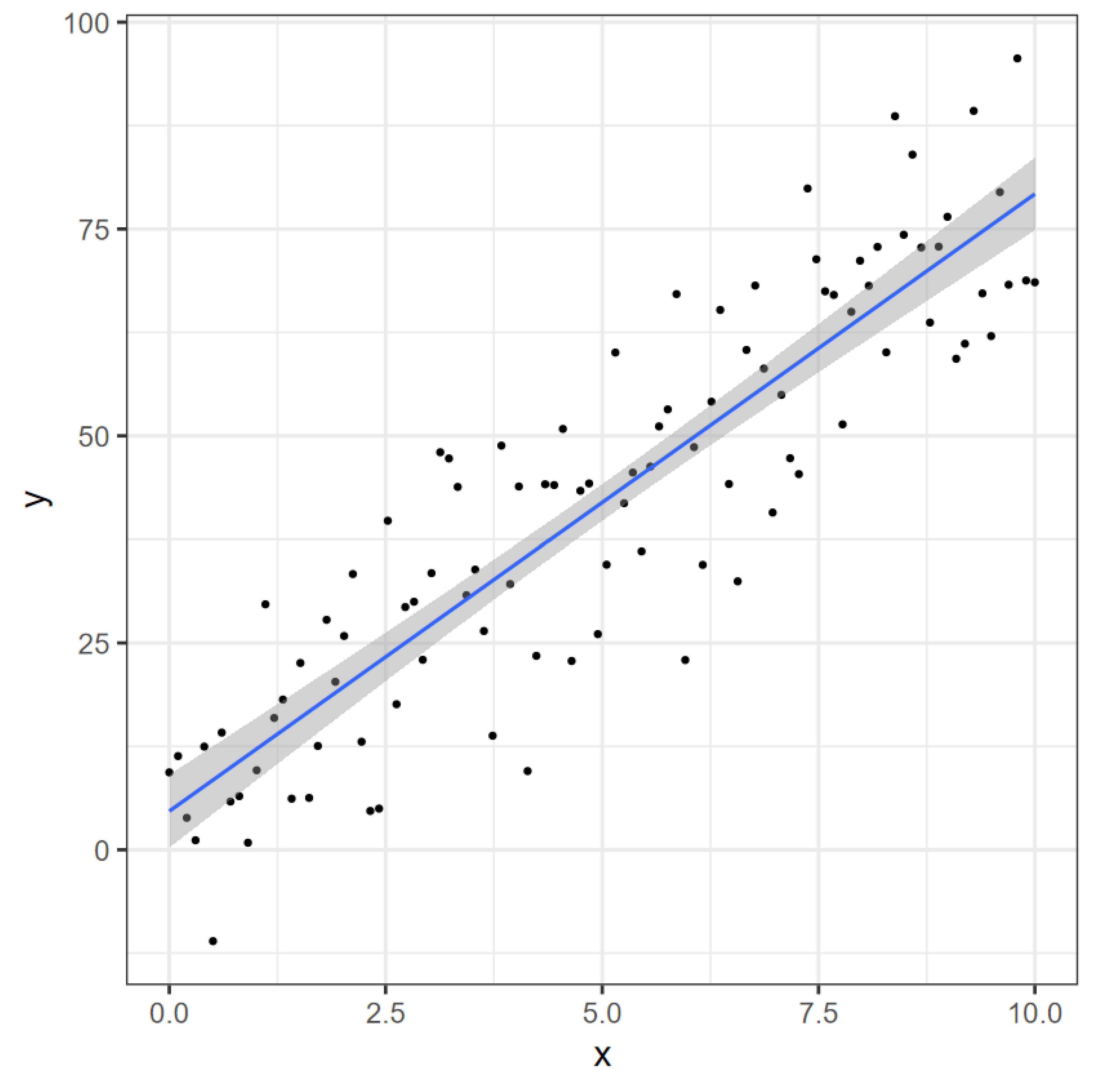
```
fit <- lm(y ~ x, df)
summary(fit)
```

```
##
## Call:
## lm(formula = y ~ x, data = df)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -26.168   -8.699    2.071    6.326   21.451
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)   4.6689     2.2190   2.104   0.0379 *
## x             7.4566     0.3834  19.450   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.'
0.1 ' ' 1
##
## Residual standard error: 11.18 on 98 degrees of
freedom
## Multiple R-squared:  0.7942, Adjusted R-squared:
0.7921
## F-statistic: 378.3 on 1 and 98 DF,  p-value: < 2.2e-
16
```

Plotting Least-Squares

- Always plot your data
  - Your eyes are better at seeing patterns in plots than interpreting numbers like *p*-values
- The `geom_smooth()` function can plot the result of a least-squares analysis.
  - The gray area indicates the 95% confidence interval of the fitted line.

```
ggplot(df, aes(x = x, y = y)) +
  geom_point() +
  geom_smooth(method = "lm")
```



Least-Squares with Real Data

- Paleoclimate data: tree-ring growth index vs. minimum summer air temperature from the MacKenzie Delta, NW Canada,
  - Data from T.J. Porter *et al.*, *Quaternary Res.* **80**, 167 (2013), DOI: 10.1016/j.yqres.2013.05.004.
- Load the data:

```
paleo <- read_rds("tree-rings.rds")
glimpse(paleo)
```

```
## Rows: 106
## Columns: 3
## $ year_ad      <dbl> 1893, 1894, 1895,…
## $ t_min        <dbl> 4.64, 4.52, 5.42,…
## $ growth_index <dbl> 0.90, 0.98, 1.08,…
```

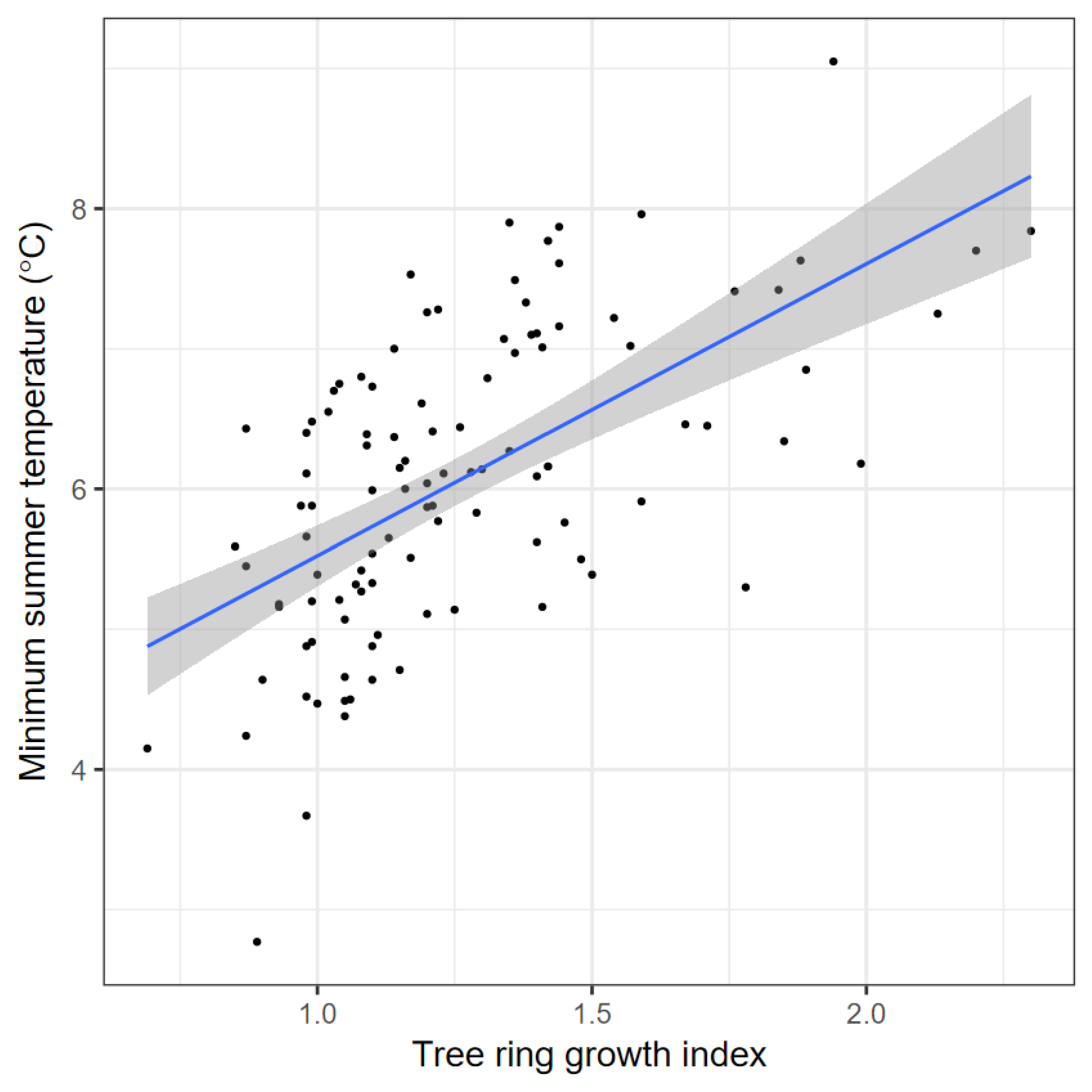
- Fit parameters to the data:

```
fit_paleo <- lm(t_min ~ growth_index, paleo)
summary(fit_paleo)
```

```
##
## Call:
## lm(formula = t_min ~ growth_index, data = paleo)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -2.52464 -0.62025 -0.03916  0.66740  1.65240
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)    3.4417     0.3516   9.789  < 2e-16
***
## growth_index   2.0820     0.2706   7.694 8.52e-12
***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.'
0.1 ' ' 1
##
## Residual standard error: 0.8676 on 104 degrees of
freedom
## Multiple R-squared:  0.3627, Adjusted R-squared:
0.3566
## F-statistic:  59.2 on 1 and 104 DF,  p-value:
8.517e-12
```

Plot Data

```
ggplot(paleo, aes(x = growth_index, y = t_min)) +
  geom_point() +
  geom_smooth(method="lm") +
  labs(x = "Tree ring growth index",
       y = expression(paste("Minimum summer temperature
        (",
                           degree * C, ")")))
```



General Least Squares

General Least Squares

- Ordinary least squares models linear relationships between x and y.
  - We can also use least-squares methods for nonlinear relationships betwen x and y, as long as there is a linear relationship between the parameters β and the dependent variable.
    - Polynomial fits

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^2 + \varepsilon$$

    - Transformed data

$$\log(y) = \beta_0 + \beta_1 \log(x) + \varepsilon$$

  - But we can't fit non-linear relationships between the parameters and the dependent variable.
    - The following won't work:

$$\begin{aligned} y =& \beta_0 + x^{\beta_1} + \varepsilon \\ y =& \sin(\beta_1 x) + \varepsilon \end{aligned}$$

Example of General Least Squares

- Diffusion coefficients for ^{40}Ar in biotite at different temperatures
  - Data from T.M. Harrison *et al.*, *Geomchim. Geocosm. Act.* **49**, 2461 (1985). DOI: 10.1016/0016-7037(85)90246-7
- Load the data

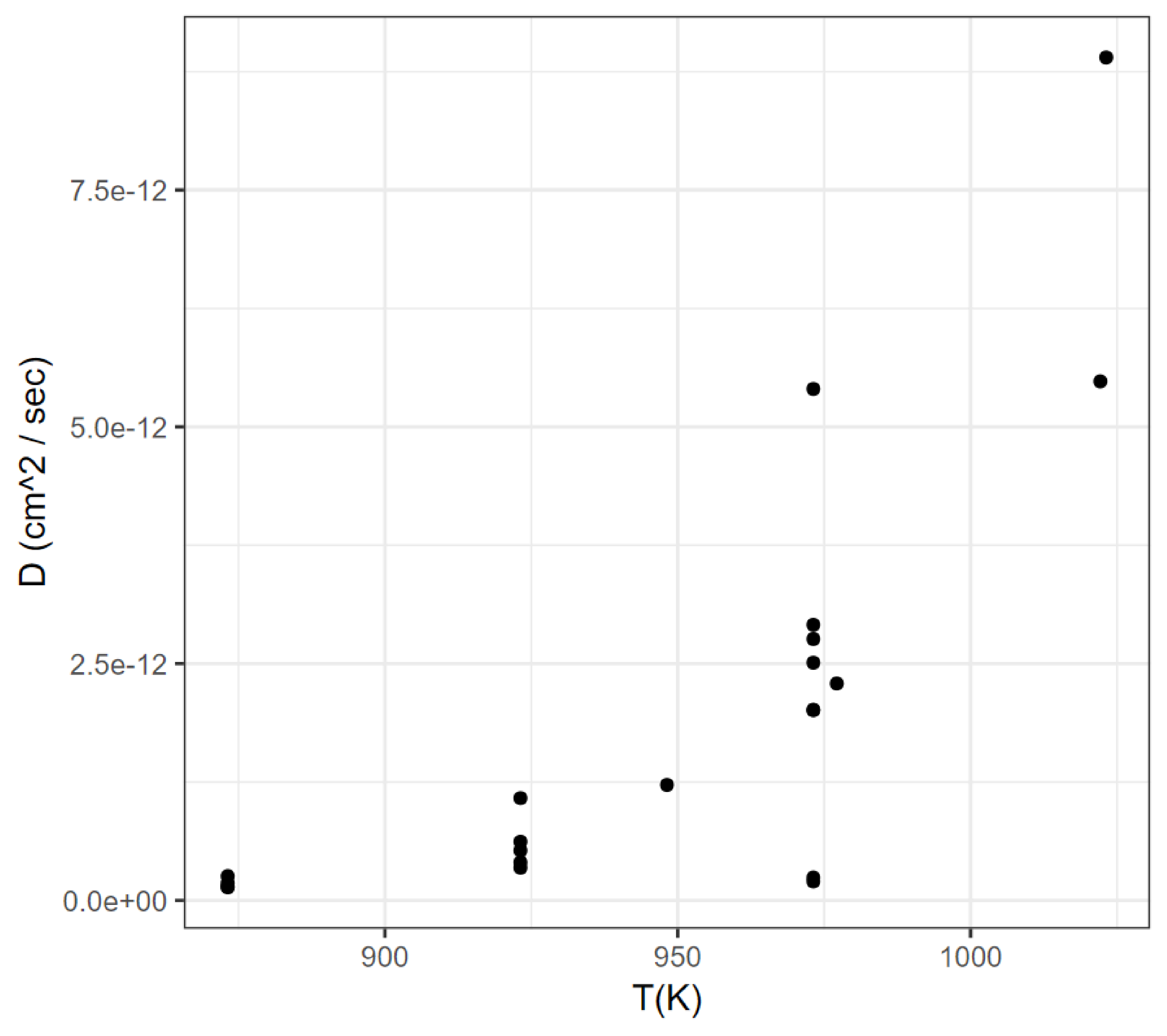
```
diffus <- read_rds("argon-diffusion.rds")
glimpse(diffus)
```

```
## Rows: 21
## Columns: 5
## $ run <chr> "CB-100", "m-101", "CB-103…
## $ t   <dbl> 973.15, 973.15, 873.15, 92…
## $ a   <dbl> 97, 97, 97, 97, 202, 97, 9…
## $ d   <dbl> 2.01e-12, 2.51e-12, 1.38e-…
## $ P   <dbl> 1, 1, 1, 1, 1, 1, 1, 1, 1,…
```

  - `t`: temperature (K),
  - `a`: grain radius (μm),
  - `d`: diffusion coefficient (cm^2/sec),
  - `P`: pressure (kbar)

- Plot the data:

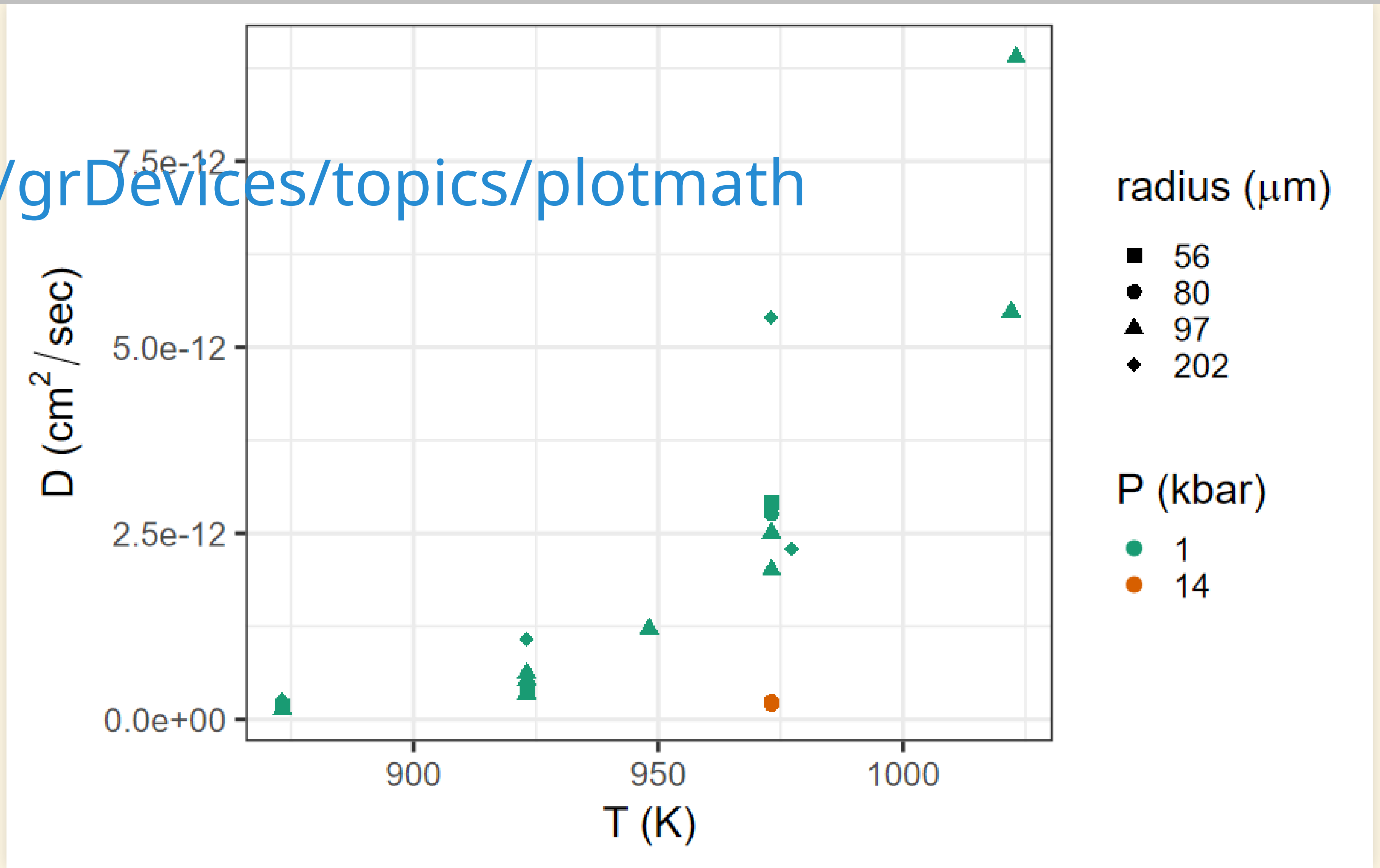
```
ggplot(diffus, aes(x = t, y = d)) +
  geom_point(size = 3) +
  labs(x = "T(K)", y = "D (cm^2 / sec)")
```



Digression: Fancy Plotting

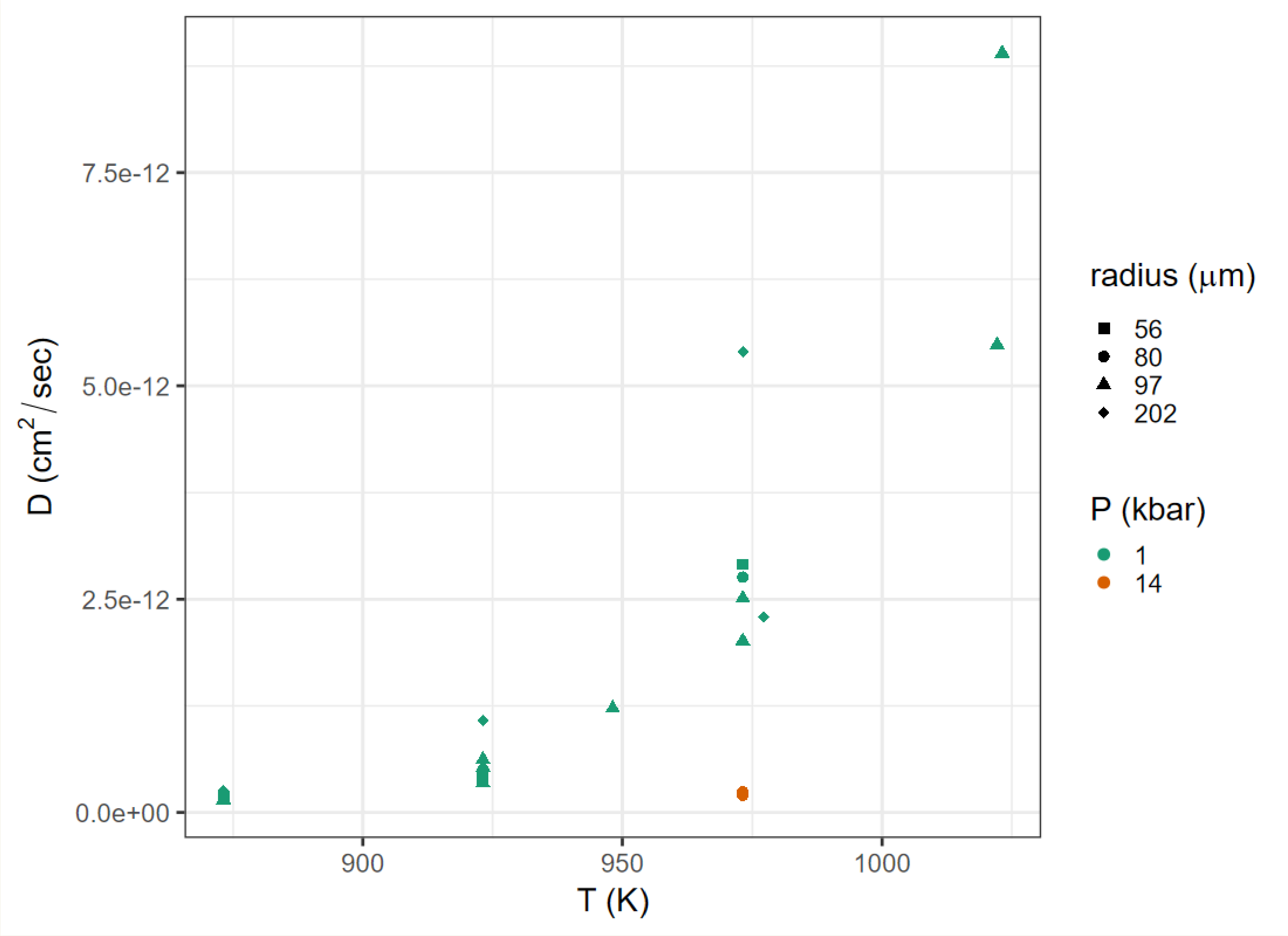
- Getting fancy with `ggplot()`:
  - To plot discrete colors and shapes, we have t
    into factors.
  - If we don't like the default shapes or colors R
    `scale_shape_manual()`, `scale_color_manual`
    shapes or colors to associate with each level
  - We can put mathematical expressions into la
    and `expression(paste())`.
    - Details at
      https://www.rdocumentation.org/packages/grDevices/topics/plotmath

```
diffus <- diffus |> mutate(P = factor(P), a = factor(a))
ggplot(diffus, aes(x = t, y = d)) +
  geom_point(aes(color = P, shape = a), size = 3) +
  scale_color_brewer(palette = "Dark2", name = "P (kbar)")
        +
  scale_shape_manual(values = c("56" = 15, "80" = 16,
                                "97" = 17, "202" = 18),
                     name = expression(paste("radius (",
                                             mu * m,
        ")"))) +
  labs(x = "T (K)",
       y = expression(paste("D (", cm^2 / sec, ")")))
```



Analyzing the Plot

- The data really don't look like they fall on a straight line the line.
- Transforming the data may produce a better linear relationship.
  - The physics of diffusion suggests that there should be a linear relationship between $\log(D)$ and $1/T$, where T is the Kelvin temperature.



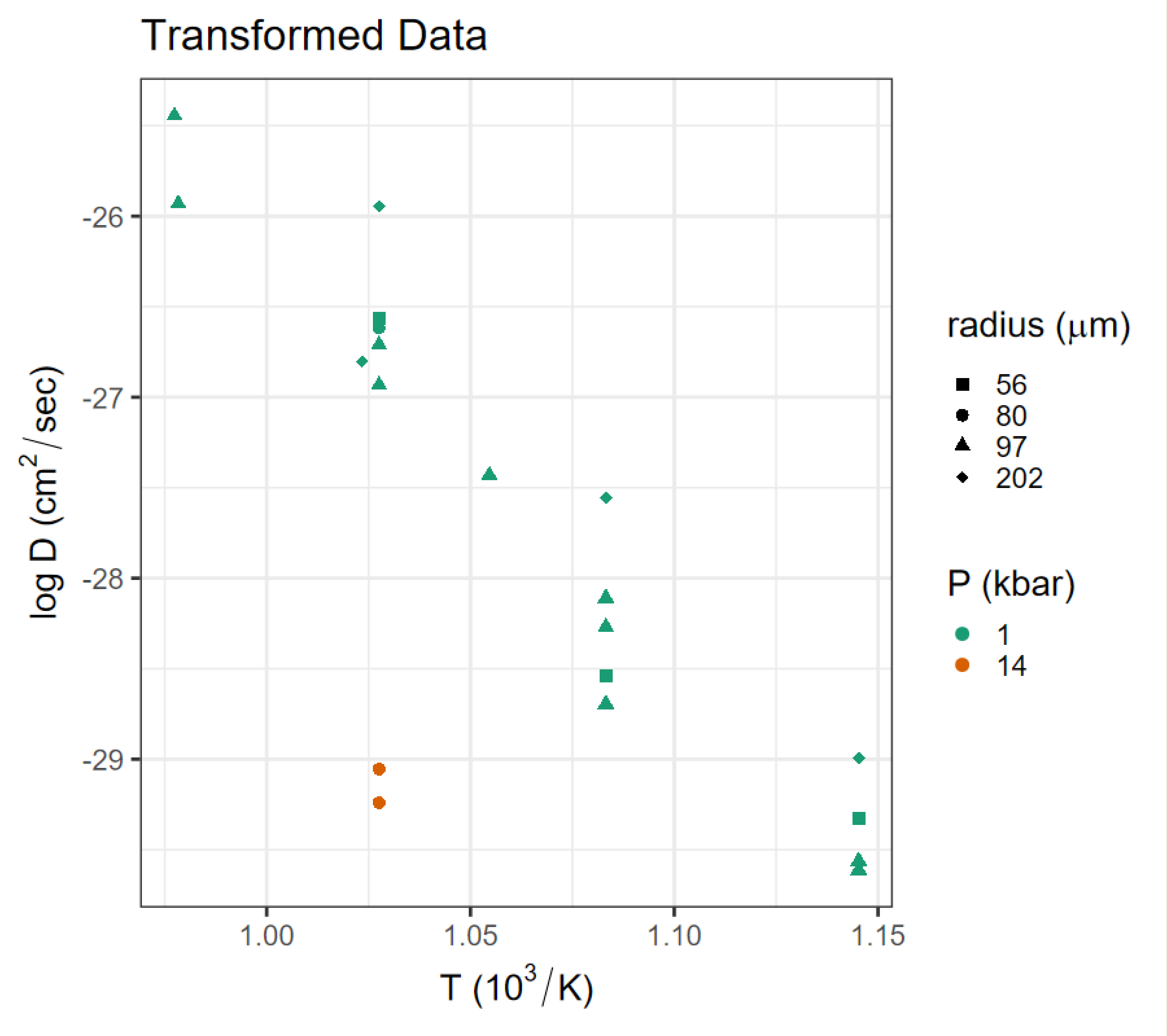
Transforming Data

- The physics of diffusion suggests that there should be a linear relationship between $\log(D)$ and $1/T$.
  - T is close to 1000 K, so transforming $1000/T$ gives numbers close to 1.

```
diffus <- diffus |> mutate(t_inv = 1000 / t,
                           log_d = log(d))
```

- Plot transformed data:

```
p_xform <- ggplot(diffus, aes(x = t_inv, y = log_d)) +
  geom_point(aes(color = P, shape = a), size = 3) +
  scale_color_brewer(palette = "Dark2",
                     name = "P (kbar)") +
  scale_shape_manual(values = c("56" = 15, "80" = 16,
                                "97" = 17, "202" = 18),
                     name = expression(paste("radius (",
                                             mu * m, ")"))
                     ) +
  labs(x = expression(paste("T (", 10^3 / K, ")")),
       y = expression(paste(log~D, " (", cm^2 / sec, ")")),
       title = "Transformed Data")
p_xform
```



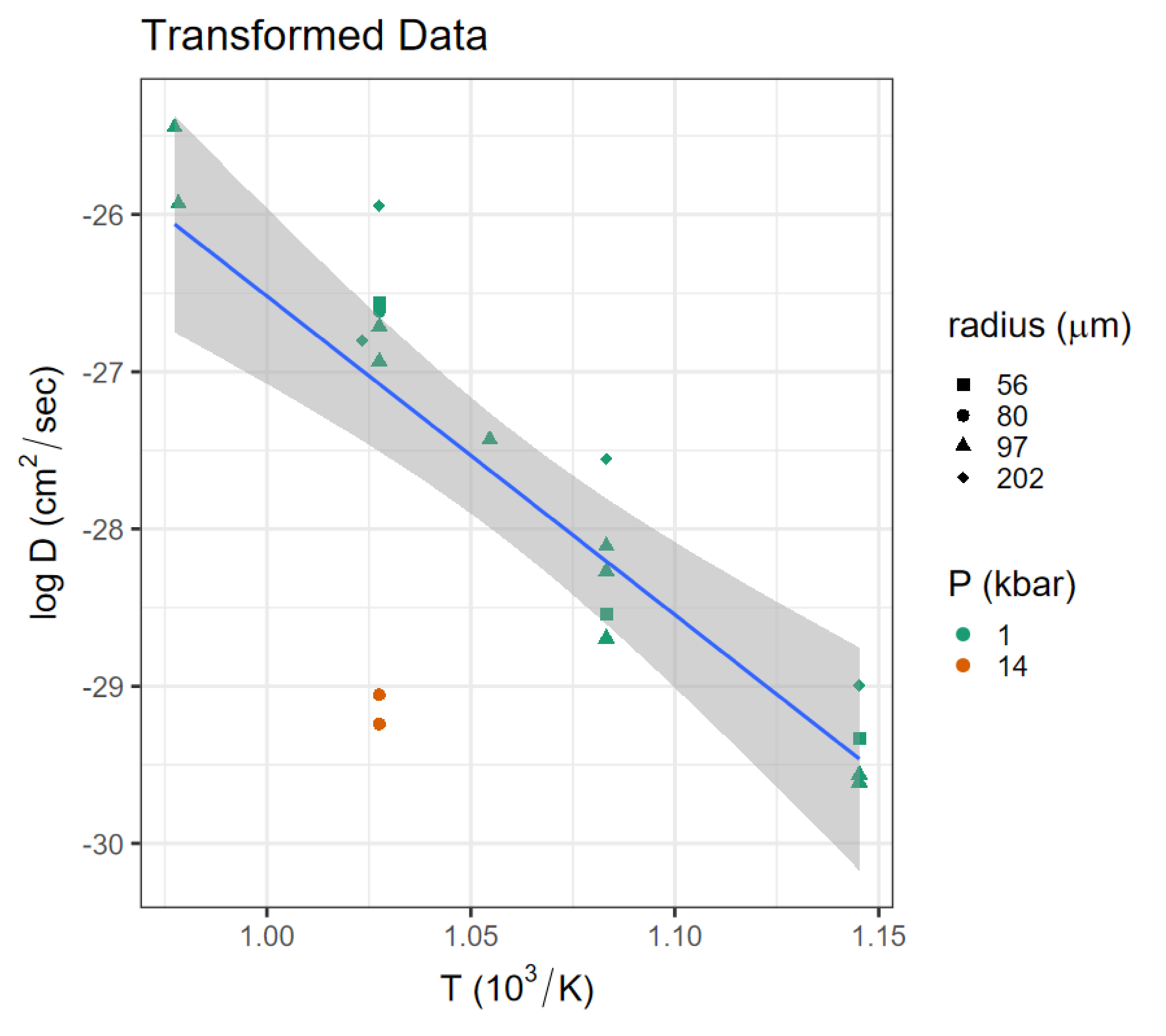
- 1-kbar data fall close to a straight line.
  - 14-kbar data don't.

General Least Squares in R

$$\log D = \beta_0 + \beta_1 \frac{1000}{T} + \varepsilon$$

```
fit_diffus <- lm(log_d ~ t_inv, diffus)
summary(fit_diffus)
```

```
##
## Call:
## lm(formula = log_d ~ t_inv, data = diffus)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -2.16200 -0.09938  0.14557  0.46267  1.13384
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)   -6.261      3.602  -1.738   0.0983 .
## t_inv        -20.259      3.395  -5.967 9.63e-06 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.'
0.1 ' ' 1
##
## Residual standard error: 0.7966 on 19 degrees of
freedom
## Multiple R-squared:  0.6521, Adjusted R-squared:
0.6337
## F-statistic: 35.61 on 1 and 19 DF,  p-value: 9.628e-06
```



- The fit is very good for 1-kbar data,
  - Poor for 14-kbar data.
  - 202 µm grains worse than smaller grains

Weighted Data

Weighted Data

- So far, we have assumed that each observation has the same measurement errors or uncertainty.
  - If some data have been measured more accurately than others, we can do *weighted least-squares* analysis, using a vector of weights w, the same length as the number of observations.
  - Ordinary least-squares minimizes

$$\sum_{i=1}^{N} \varepsilon_i^2 = \sum_{i=1}^{N} (y_i - (\beta_0 + \beta_1 x))$$

- Weighted least-squares minimizes

$$\sum_{i=1}^{N} w_i \varepsilon_i^2 = \sum_{i=1}^{N} w_i (y_i - (\beta_0 + \beta_1 x))$$

```
lm(y ~ x, data = df, weights = w)
```

  - Typially, if σ_i is the uncertainty in x_i, then $w_i = 1/\sigma_i^2$