Residual Analysis + Generalized Linear Models

Lecture 04

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`dukestm` package

This is a companion package for the course where I will be putting useful functions for some of our common tasks in the course.

This is not a official or polished package but I've tried to include documentation for most functions. If you notice a problem open and issue or send me an email.

To install,

```r
devtools::install_github("sta344-644-fa23/dukestm")
```

Updates will be made throughout the semester and I will attempt to remind you when something new is available, reruning the above will get you the latest version.

Example - `epred_draws_fix()`

```r
tidybayes::epred_draws(b, newdata=d)
```

```
# A tibble: 400,000 × 7
# Groups:   x, y, .row [100]
       x     y  .row .chain .iteration .draw
   <int> <dbl> <int>  <int>      <int> <int>
 1     1 -3.24     1     NA         NA     1
 2     1 -3.24     1     NA         NA     2
 3     1 -3.24     1     NA         NA     3
 4     1 -3.24     1     NA         NA     4
 5     1 -3.24     1     NA         NA     5
 6     1 -3.24     1     NA         NA     6
 7     1 -3.24     1     NA         NA     7
 8     1 -3.24     1     NA         NA     8
 9     1 -3.24     1     NA         NA     9
10     1 -3.24     1     NA         NA    10
# ℹ 399,990 more rows
# ℹ 1 more variable: .epred <dbl>
```

```r
dukestm::epred_draws_fix(b, newdata=d)
```

```
# A tibble: 400,000 × 7
       x     y  .row .chain .iteration .draw
   <int> <dbl> <int>  <int>      <int> <int>
 1     1 -3.24     1      1          1     1
 2     1 -3.24     1      1          2     2
 3     1 -3.24     1      1          3     3
 4     1 -3.24     1      1          4     4
 5     1 -3.24     1      1          5     5
 6     1 -3.24     1      1          6     6
 7     1 -3.24     1      1          7     7
 8     1 -3.24     1      1          8     8
 9     1 -3.24     1      1          9     9
10     1 -3.24     1      1         10    10
# ℹ 399,990 more rows
# ℹ 1 more variable: .epred <dbl>
```

`dukestm()` also has implementations of `predicted_draws_fix()` and `residual_draws_fix()`

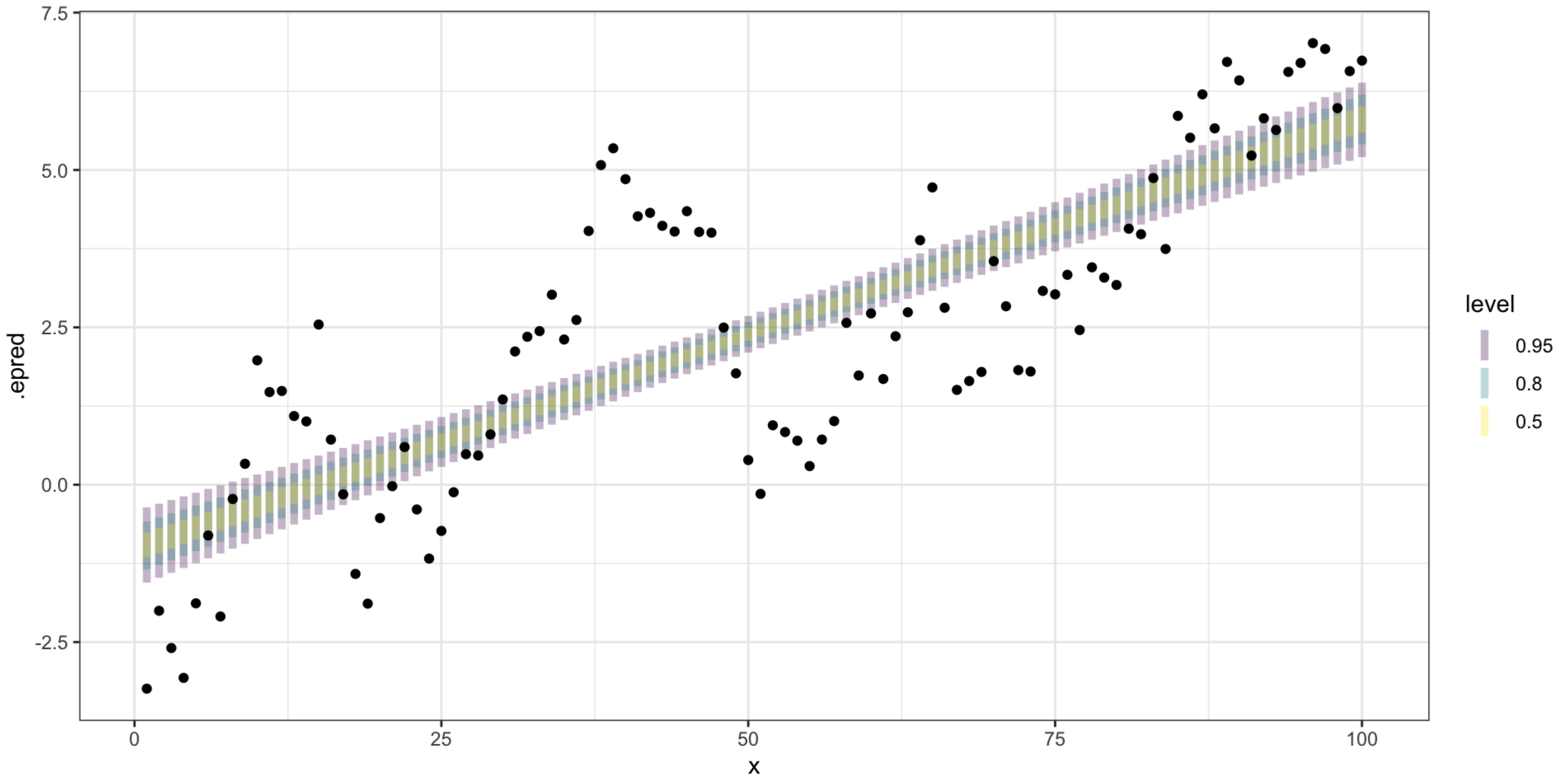
Where we left it - Empirical Coverage ($\hat{y}$)

```r
( dukestm::epred_draws_fix(b, newdata=d) |>
    group_by(x, y) |>
    tidybayes::mean_hdi(
      .epred, .width = c(0.5,0.9,0.95)
    ) |>
    mutate(contains = y >= .lower & y <= .upper) |>
    group_by(prob = .width) |>
    summarize(
      emp_cov = sum(contains)/n()
    )
)
```

```
# A tibble: 3 × 2
   prob emp_cov
  <dbl>   <dbl>
1  0.5     0.02
2  0.9     0.11
3  0.95    0.14
```

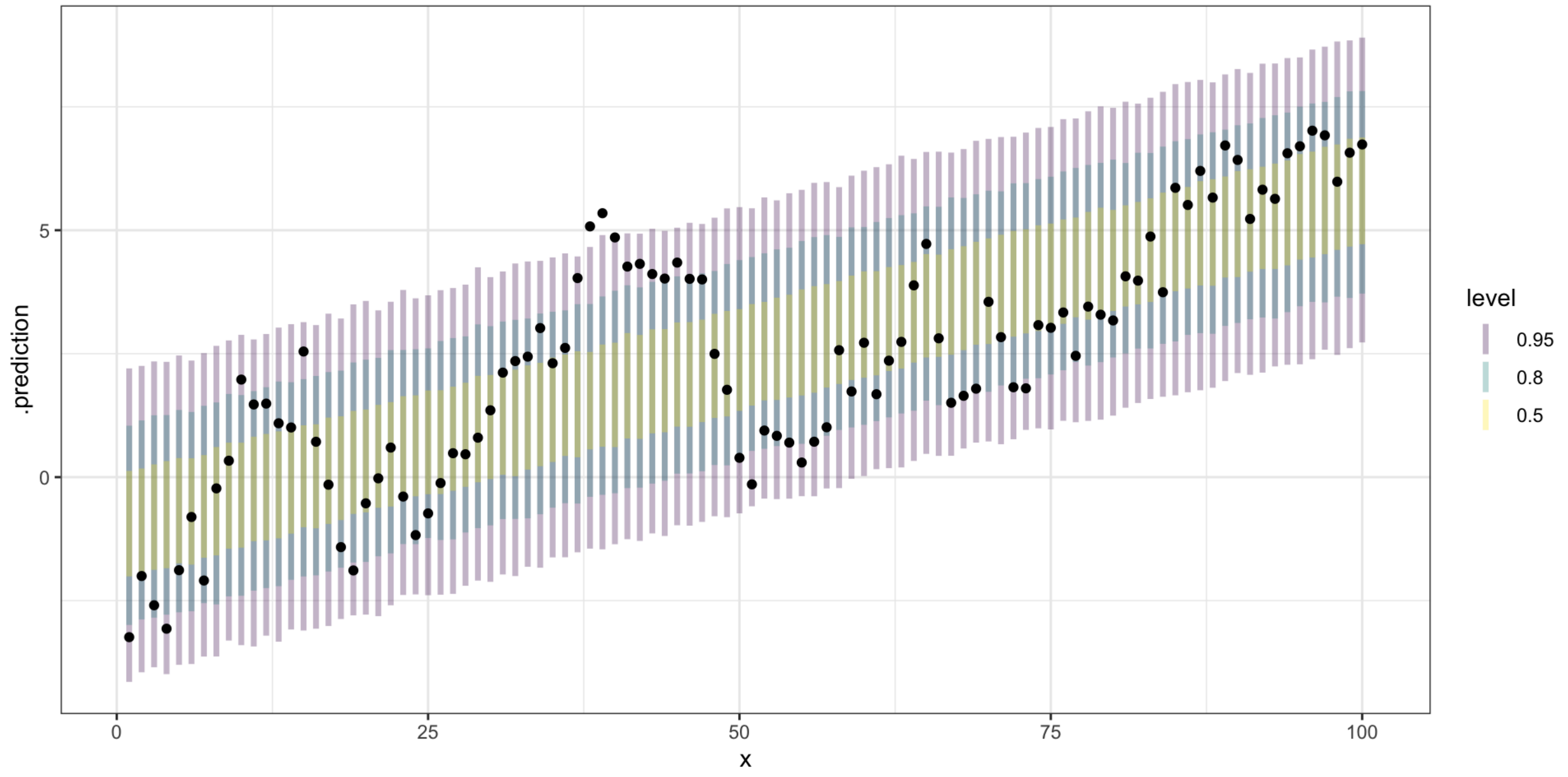
What went wrong?

```r
epred_draws_fix(b, newdata=d) |>
  ggplot(aes(x=x)) +
    ggdist::stat_interval(alpha=0.3, aes(y=.epred, group=x), linewidth=1.66) +
    geom_point(data=d, aes(y=y))
```



The right predictions

```r
predicted_draws_fix(b, newdata=d) |>
  ggplot(aes(x=x)) +
    ggdist::stat_interval(alpha=0.3, aes(y=.prediction, group=x), linewidth=1.25) +
    geom_point(data=d, aes(y=y))
```



Empirical Coverage (y)

```r
predicted_draws_fix(b, newdata=d) |>
  group_by(x, y) |>
  tidybayes::mean_hdi(
    .prediction, .width = c(0.5,0.8,0.9,0.95)
  ) |>
  mutate(contains = y >= .lower & y <= .upper) |>
  group_by(prob = .width) |>
  summarize(
    emp_cov = sum(contains)/n()
  )
```

```
# A tibble: 4 × 2
   prob emp_cov
  <dbl>   <dbl>
1  0.5     0.42
2  0.8     0.81
3  0.9     0.95
4  0.95    0.97
```

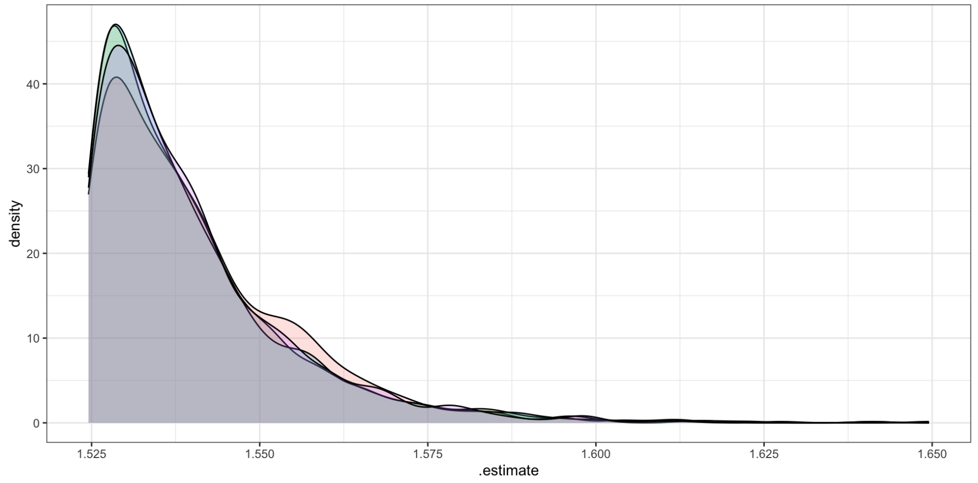
RMSE

$\hat{y}$

```
y_hat_rmse = epred_draws_fix(b, newdata=d) |>
  group_by(.iteration, .chain) |>
  yardstick::rmse(truth = y, estimate = .epre
```

```
summarize(y_hat_rmse, mean(.estimate), .by =
```

```
# A tibble: 4 × 2
  .chain `mean(.estimate)`
   <int>             <dbl>
1      1              1.54
2      2              1.54
3      3              1.54
4      4              1.54
```

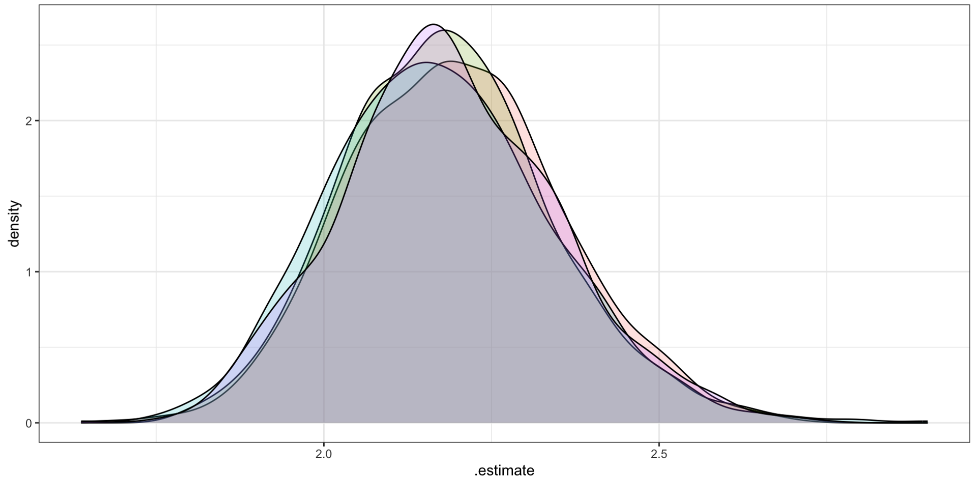


y

```
y_rmse = predicted_draws_fix(b, newdata=d) |>
  group_by(.iteration, .chain) |>
  yardstick::rmse(truth = y, estimate = .prec
```

```
summarize(y_rmse, mean(.estimate), .by = .cha
```

```
# A tibble: 4 × 2
  .chain `mean(.estimate)`
   <int>             <dbl>
1      1              2.20
2      2              2.18
3      3              2.18
4      4              2.19
```



CRPS

$\hat{y}$

```r
epred_draws_fix(b, newdata=d) |>
  group_by(.chain, x) |>
    summarise(
      crps = dukestm::calc_crps(.epred, obs=y
    ) |>
    summarize(
      mean(crps)
    )
```

```
# A tibble: 4 × 2
  .chain `mean(crps)`
   <int>        <dbl>
1      1         1.19
2      2         1.19
3      3         1.19
4      4         1.19
```

y

```r
predicted_draws_fix(b, newdata=d) |>
  group_by(.chain, x) |>
    summarise(
      crps = dukestm::calc_crps(.prediction,
    ) |>
    summarize(
      mean(crps)
    )
```

```
# A tibble: 4 × 2
  .chain `mean(crps)`
   <int>        <dbl>
1      1        0.885
2      2        0.878
3      3        0.882
4      4        0.884
```

Posterior sampling functions

$$\mathrm{E}(y_i)$$

$$y_i \sim \mathrm{Normal}(\mu_i, \sigma)$$

$$\mu_i = \alpha + \beta x_i$$

`posterior_epred()` gives the draws from the expected value of the posterior predictive distribution, or the average of each draw from `posterior_predict()`.

In Gaussian regression, this is the **same as the linear predictor μ**.

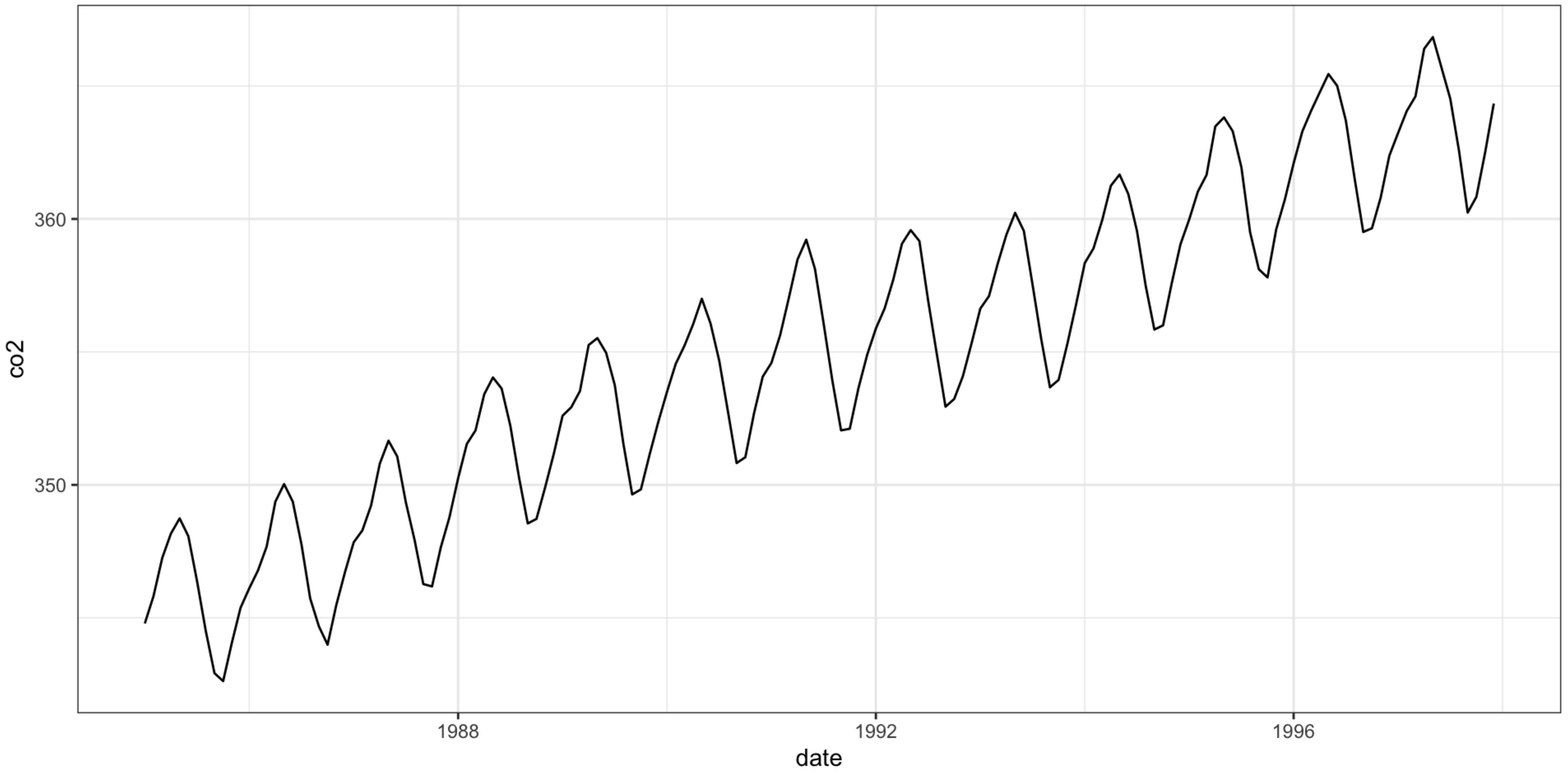
`posterior_linpred()` gives the posterior draws of the linear model.

`posterior_predict()` gives the draws from a random normal distribution with draws from the posterior distributions of μ and σ.

From Andrew Heiss' blog post Visualizing the differences between Bayesian posterior predictions, linear

Residual Analysis

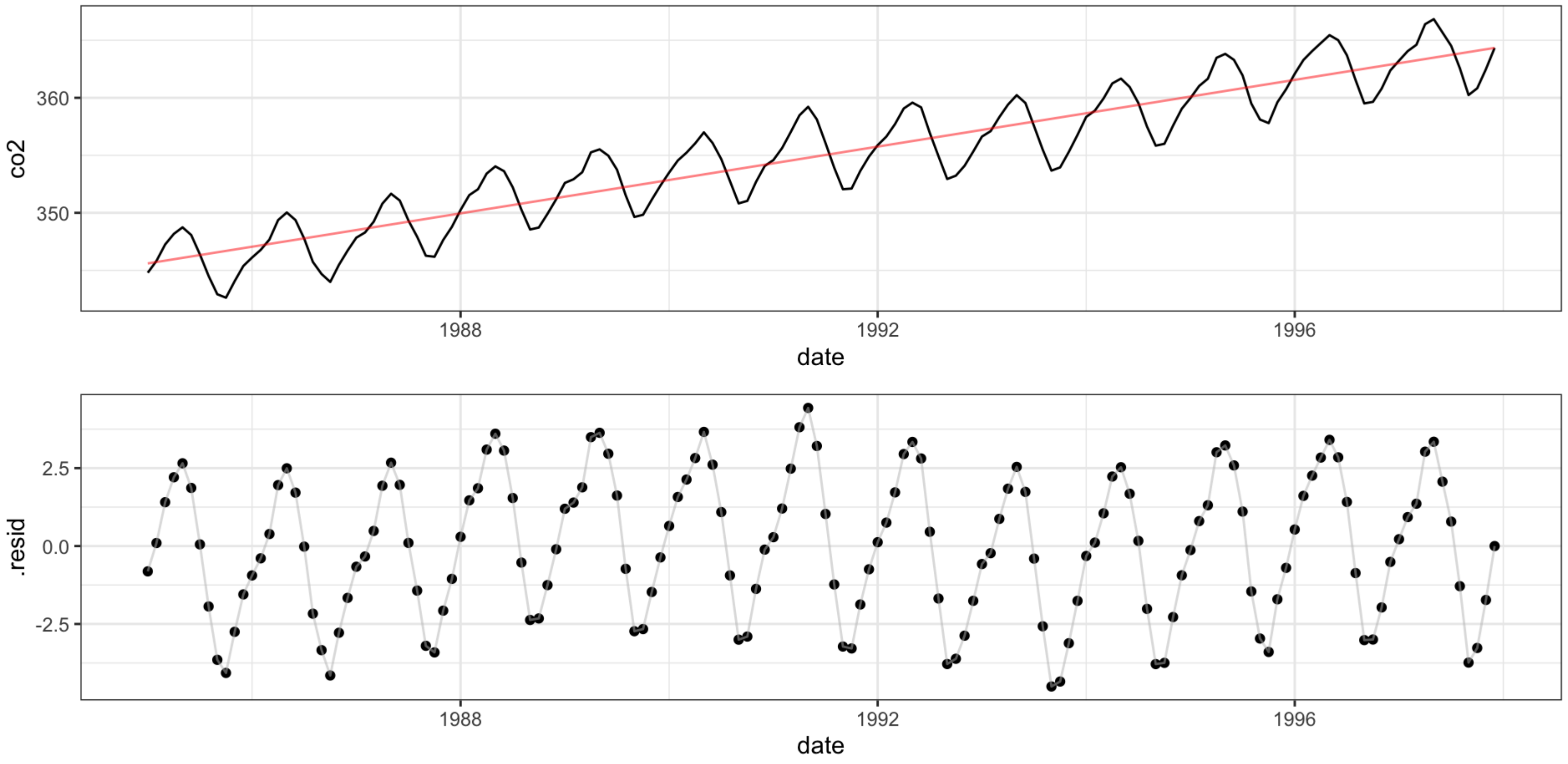
Atmospheric CO_2 (ppm) from Mauna Loa



Where to start?

Well, it looks like stuff is going up on average …

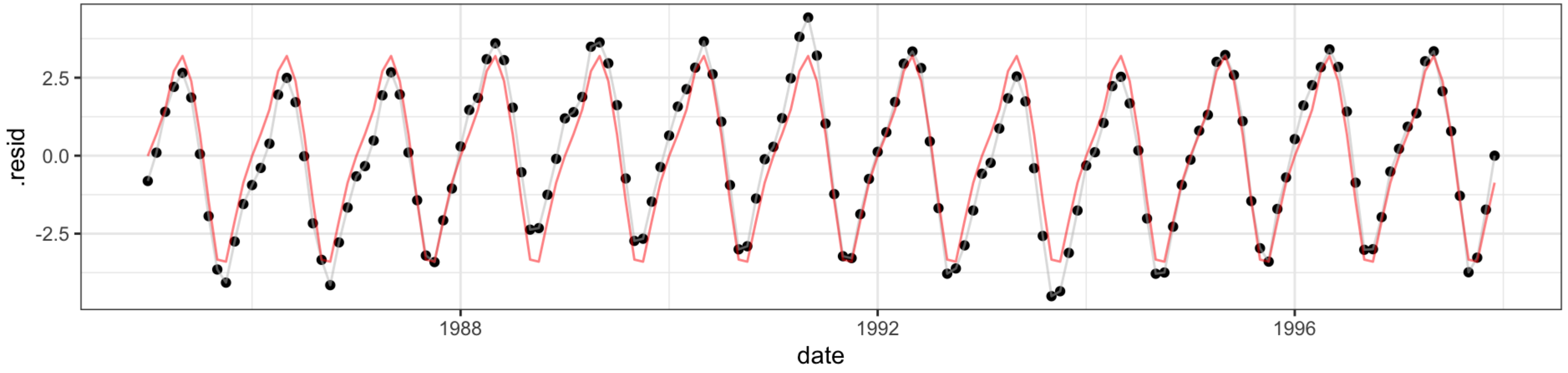
```r
l = lm(co2~date, data=mauna_loa)
```

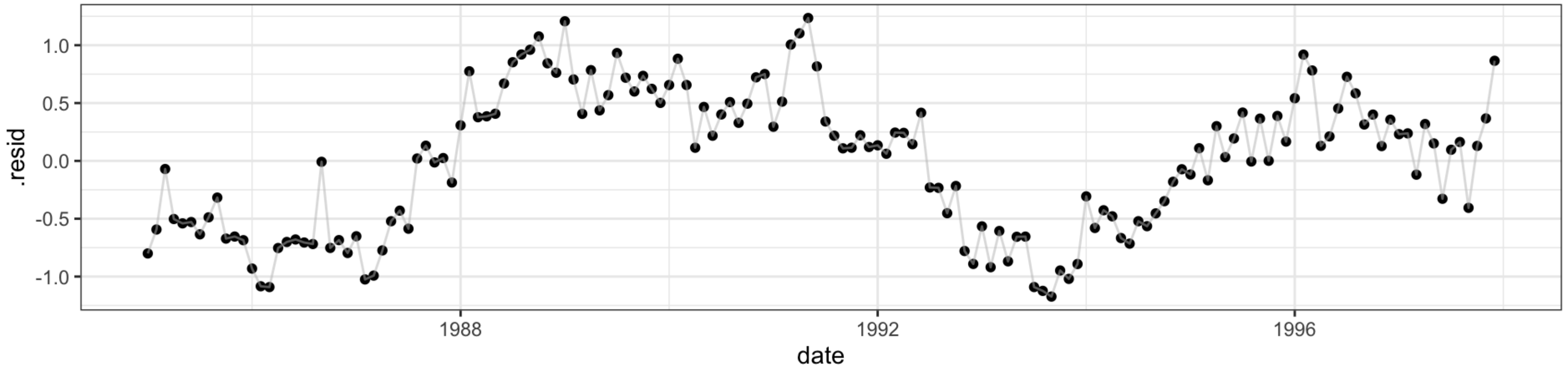


and then?

Well there is some periodicity lets add the month (as a factor) …

```r
ls = lm(.resid~month, data=mauna_loa_l)
```

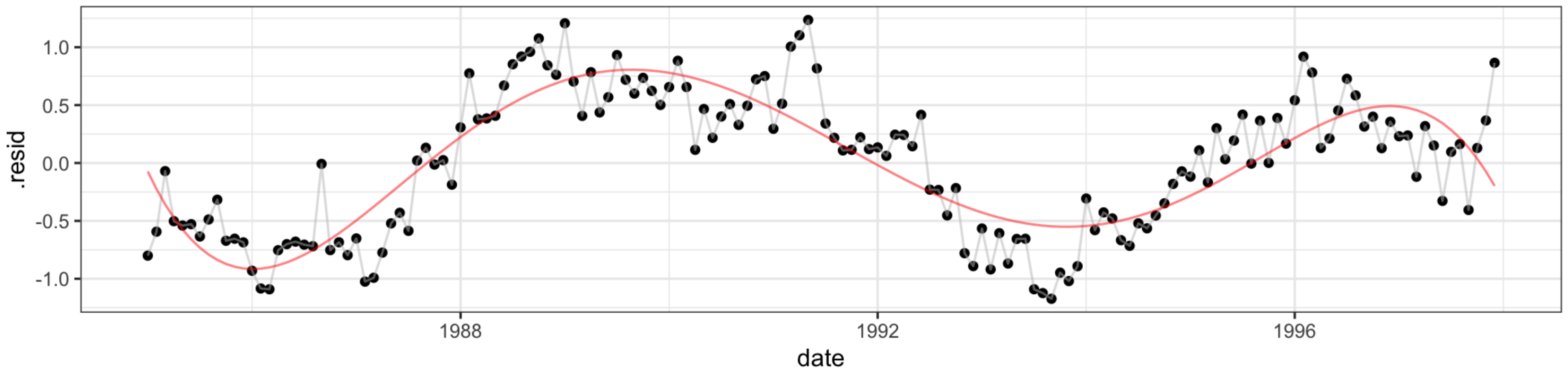


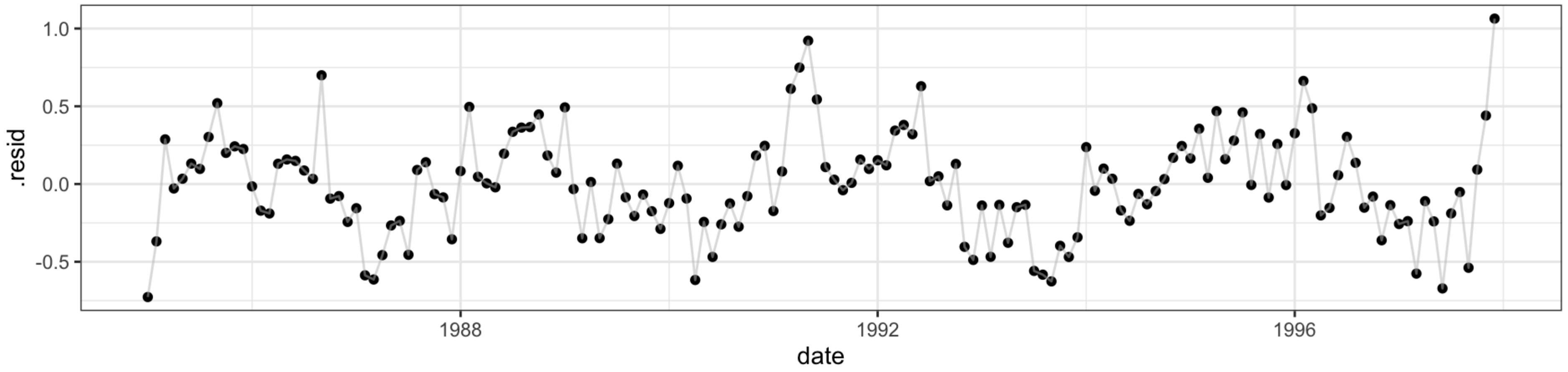


and then and then?

There is still some long term trend in the data, maybe a fancy polynomial can help …

```r
lsy = lm(.resid~poly(date,5), data=mauna_loa_ls)
```


1.0
0.5
0.0
-0.5
-1.0
.resid
1988
1992
1996
date

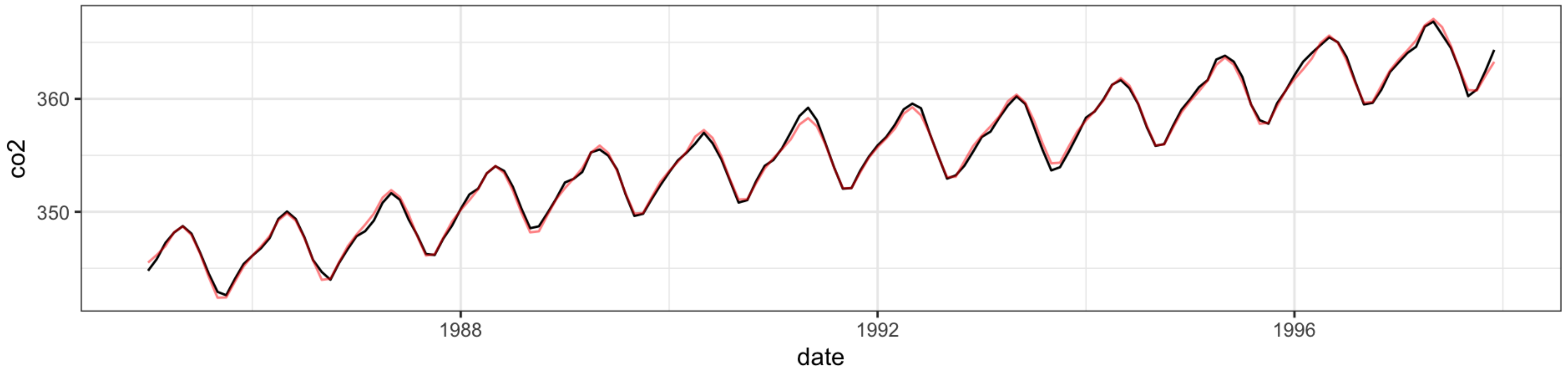

1.0
0.5
0.0
-0.5
.resid
1988
1992
1996
date

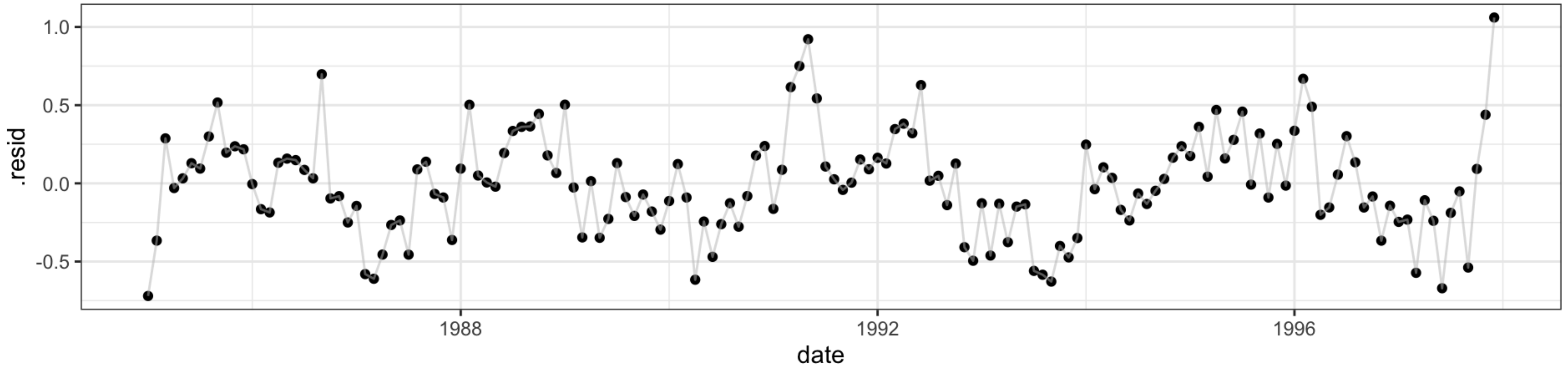
Putting it all together ...

```r
l_comb = lm(co2~date + month + poly(date,5), data=mauna_loa)
summary(l_comb)
```

```

Call:
lm(formula = co2 ~ date + month + poly(date, 5), data = mauna_loa)

Residuals:
     Min       1Q   Median       3Q      Max 
-0.72022 -0.19169 -0.00638  0.17565  1.06026 

Coefficients: (1 not defined because of singularities)
                 Estimate Std. Error  t value Pr(>|t|)    
(Intercept)    -2.587e+03  1.460e+01 -177.174  < 2e-16 ***
date            1.479e+00  7.334e-03  201.649  < 2e-16 ***
monthAug       -4.155e+00  1.346e-01  -30.880  < 2e-16 ***
monthDec       -3.566e+00  1.350e-01  -26.404  < 2e-16 ***
monthFeb       -2.022e+00  1.345e-01  -15.041  < 2e-16 ***
monthJan       -2.729e+00  1.345e-01  -20.286  < 2e-16 ***
monthJul       -2.018e+00  1.345e-01  -15.003  < 2e-16 ***
monthJun       -3.136e-01  1.345e-01   -2.332 0.021117 *  
monthMar       -1.233e+00  1.344e-01   -9.175 5.54e-16 ***
monthMay        4.881e-01  1.344e-01    3.631 0.000396 ***
monthNov       -4.799e+00  1.349e-01  -35.577  < 2e-16 ***
monthOct       -6.102e+00  1.348e-01  -45.283  < 2e-16 ***
```

Combined fit + Residuals





Model performance

Model	rmse
`co2 ~ date`	2.248
`co2 ~ month`	5.566
`co2 ~ date+month`	0.594
`co2 ~ poly(date,5)`	2.171
`co2 ~ month+poly(date,5)`	0.323
`co2 ~ date+month+poly(date,5)`	0.323

Generalized Linear Models

Background

A generalized linear model has three key components:

1. a probability distribution (from the exponential family) that describes your response variable
2. a linear predictor $\boldsymbol{\eta} = \boldsymbol{X}\boldsymbol{\beta}$,
3. and a link function g such that $\mathrm{g}(\mathrm{E}(\boldsymbol{Y}|\boldsymbol{X})) = \boldsymbol{\eta}$ (or $\mathrm{E}(\boldsymbol{Y}|\boldsymbol{X}) = \mathrm{g}^{-1}(\boldsymbol{\eta})$).

Poisson Regression

This is a special case of a generalized linear model for count data where we assume the outcome variable follows a poisson distribution (mean = variance).

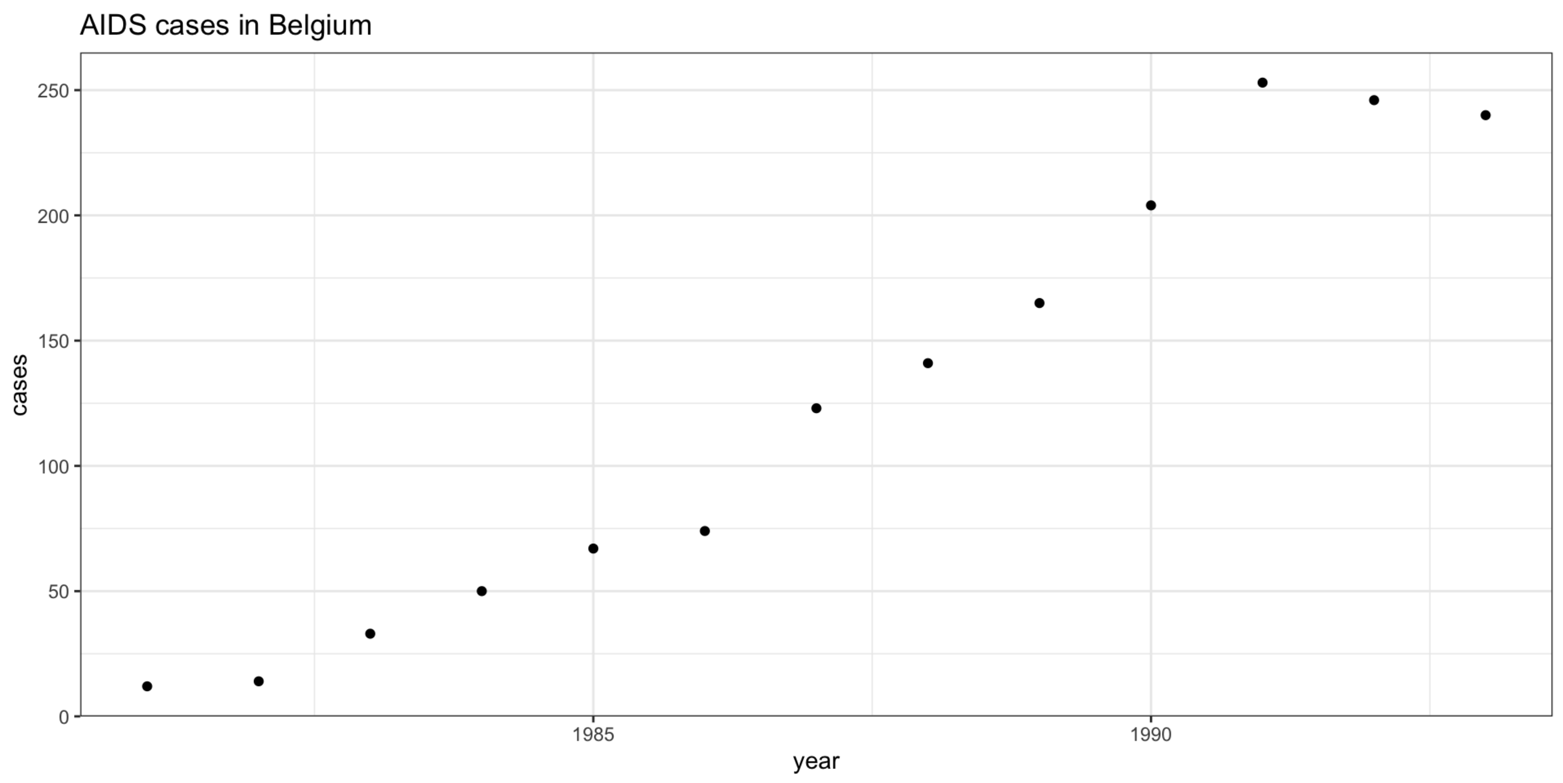
$$Y_i \sim \text{Poisson}(\lambda_i)$$
$$\log E(Y_i | \boldsymbol{X}_{i\cdot}) = \log \lambda_i = \underset{1\times p}{\boldsymbol{X}_{i\cdot}} \underset{p\times 1}{\boldsymbol{\beta}}$$

Example - AIDS in Belgium

These data represent the total number of new AIDS cases reported in Belgium during the early stages of the epidemic.

```r
aids
```

```
# A tibble: 13 × 2
    year cases
   <int> <int>
 1  1981    12
 2  1982    14
 3  1983    33
 4  1984    50
 5  1985    67
 6  1986    74
 7  1987   123
 8  1988   141
 9  1989   165
10  1990   204
11  1991   253
12  1992   246
13  1993   240
```



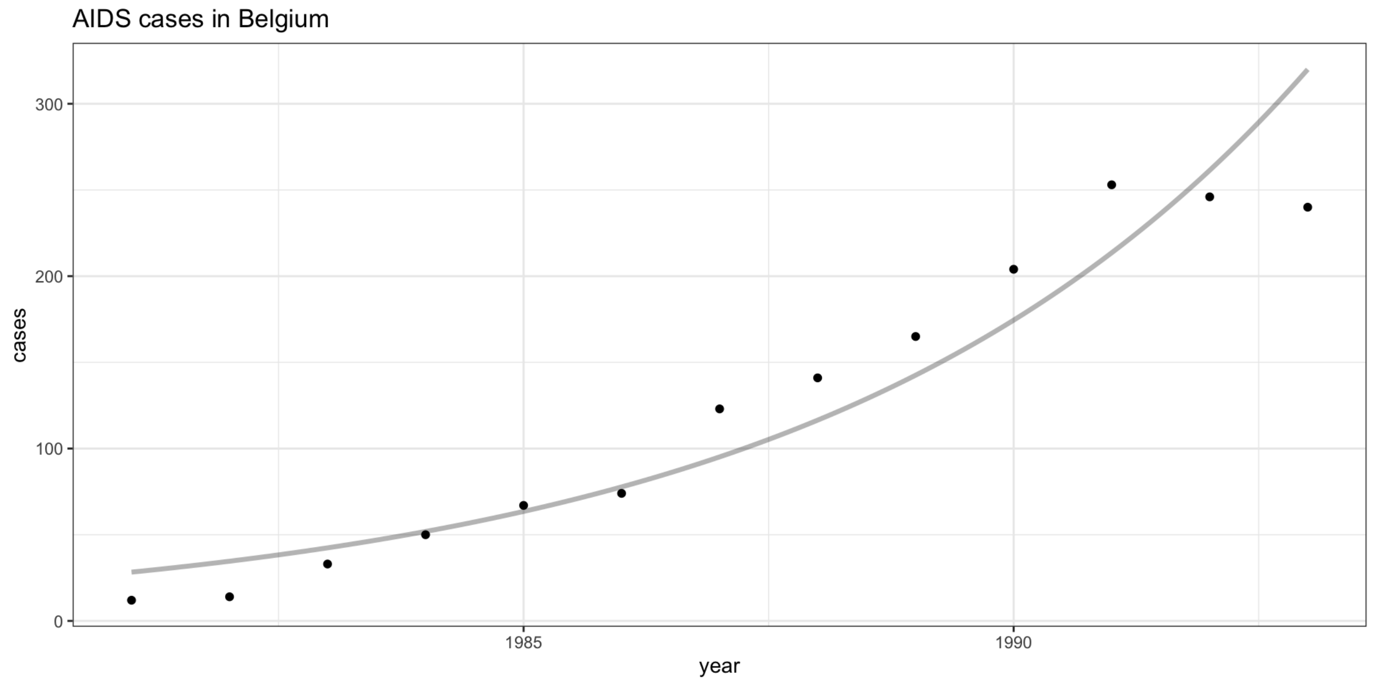
Frequentist glm fit

```r
( g = glm(cases~year, data=aids, family=poisson) )
```

```
Call:  glm(formula = cases ~ year, family = poisson, data = aids)

Coefficients:
(Intercept)         year  
  -397.0594       0.2021  

Degrees of Freedom: 12 Total (i.e. Null);  11 Residual
Null Deviance:	    872.2 
Residual Deviance: 80.69 	AIC: 166.4
```

Model Fit

```r
g_pred = broom::augment(
  g, type.predict = "response",
  newdata = tibble(year=seq(1981,1993,by=0.1))
)

aids_base +
  geom_line(data=g_pred, aes(y=.fitted), size=1.2, alpha=0.3)
```

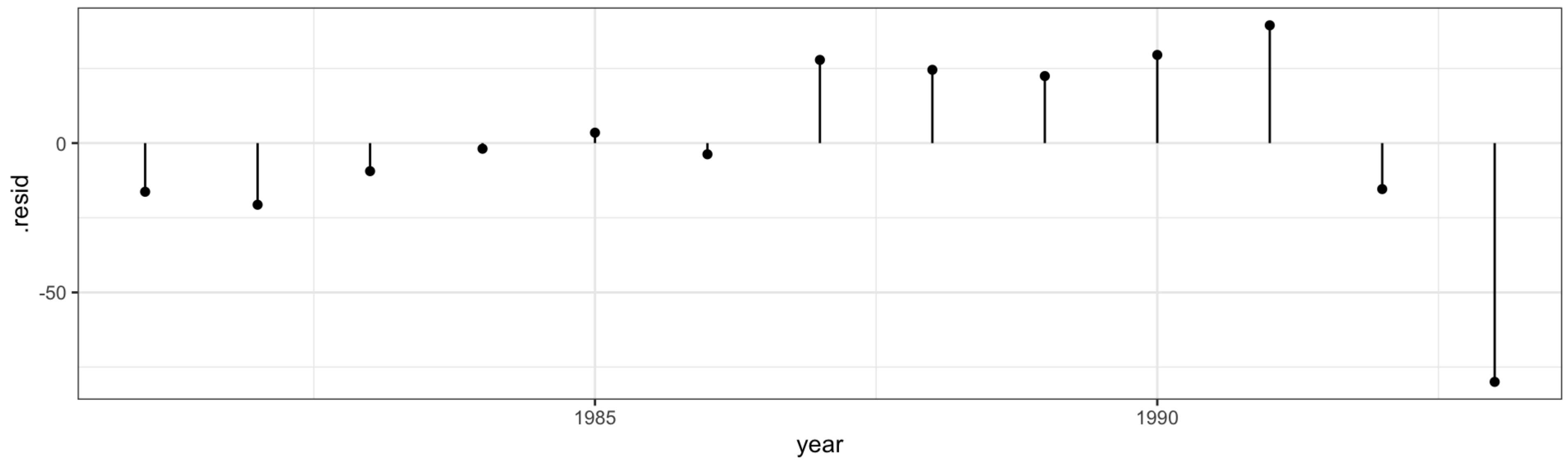


Residuals?

The naive approach is to use standard residuals,

$$r_i = Y_i - E(Y_i|X) = Y_i - \hat{\lambda}_i$$

```r
g_pred_std = broom::augment(
  g, type.predict = "response"
) |>
  mutate(.resid = cases - .fitted)
```

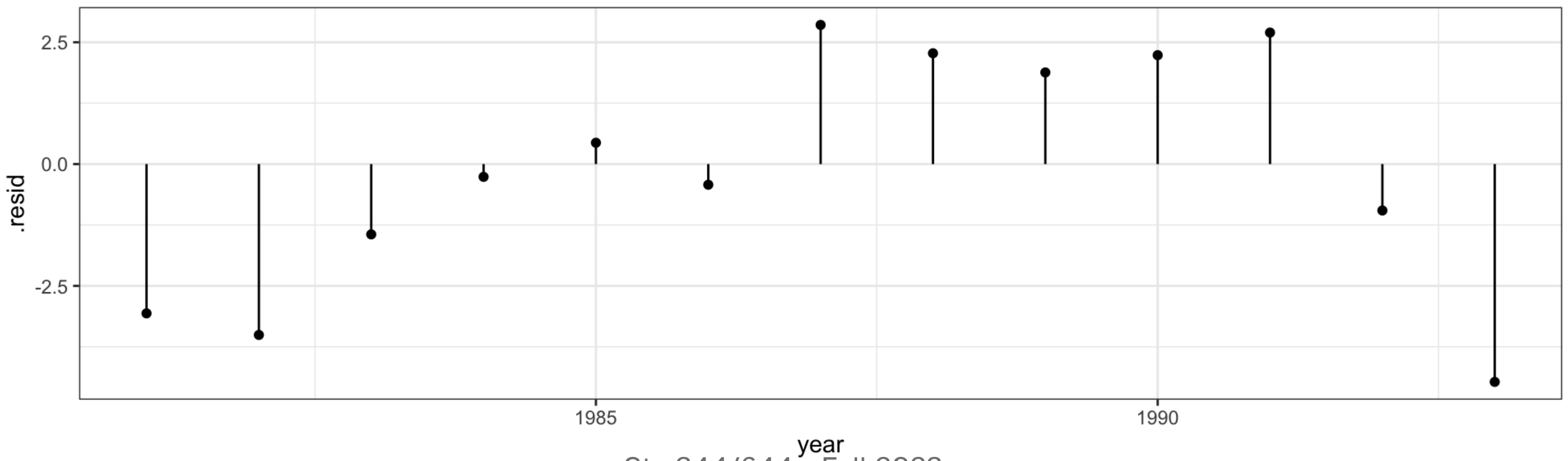


Accounting for variability

Pearson residuals:

$$r_i = \frac{Y_i - E(Y_i|X)}{\sqrt{Var(Y_i|X)}} = \frac{Y_i - \hat{\lambda}_i}{\sqrt{\hat{\lambda}_i}}$$

```r
g_pred_pearson = broom::augment(
  g, type.predict = "response", type.residuals = "pearson"
)
```



Deviance

Deviance is a way of measuring the difference between a GLM's fit and the fit of the perfect model (i.e. where $\theta_{best} = E(Y_i|X) = Y_i$).

It is defined as twice the log of the ratio between the likelihood of the perfect model and the likelihood of the given model,

$$
\begin{aligned}
D &= 2\log\left(\frac{\square(\theta_{best}|Y)}{\square(\hat{\theta}|Y)}\right) \\
&= 2\left(l(\theta_{best}|Y) - l(\hat{\theta}|Y)\right)
\end{aligned}
$$

Derivation - Normal

Derivation - Poisson

glm output

```r
summary(g)
```

```

Call:
glm(formula = cases ~ year, family = poisson, data = aids)

Coefficients:
              Estimate Std. Error z value Pr(>|z|)    
(Intercept) -3.971e+02  1.546e+01  -25.68   <2e-16 ***
year         2.021e-01  7.771e-03   26.01   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for poisson family taken to be 1)

    Null deviance: 872.206  on 12  degrees of freedom
Residual deviance:  80.686  on 11  degrees of freedom
AIC: 166.37
```

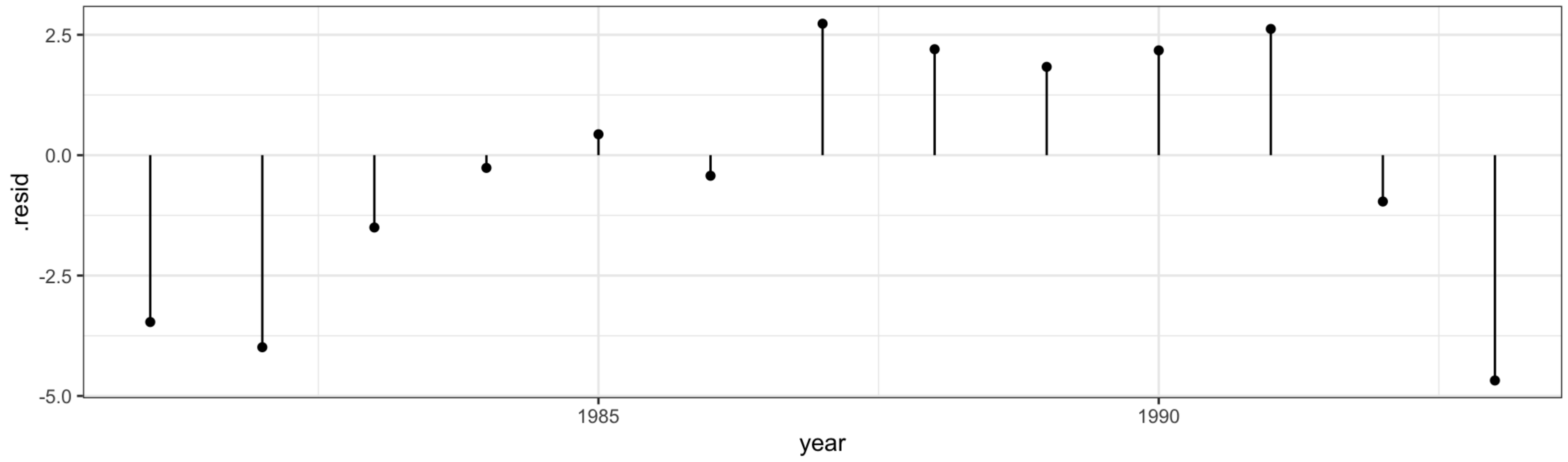
Deviance residuals

We can therefore think of deviance as $D = \sum_{i=1}^{n} d_i^2$ where d_i is a generalized residual.

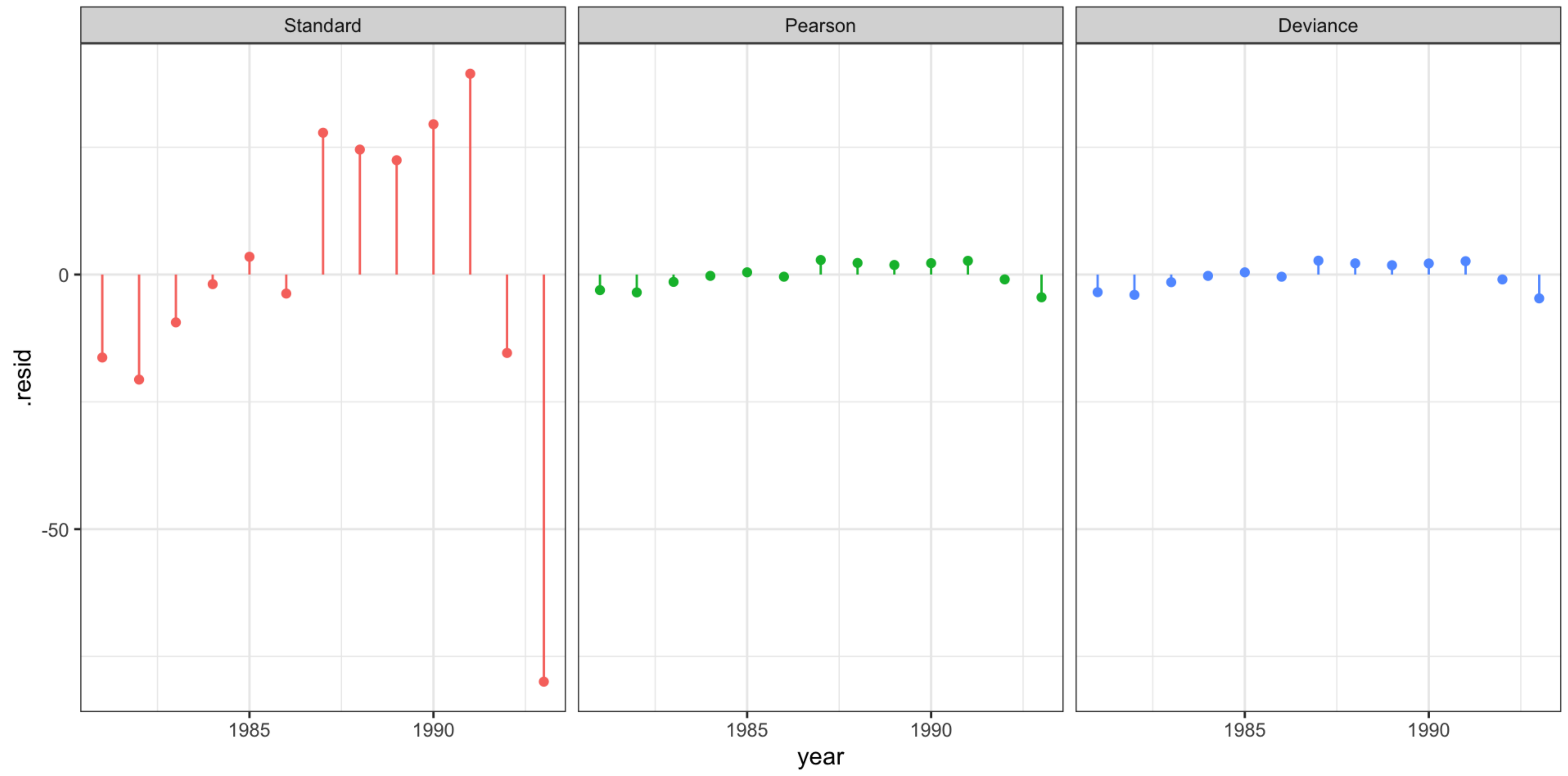
In the Poisson case we have,

$$d_i = \text{sign}(y_i - \lambda_i)\sqrt{2(y_i \log(y_i/\hat{\lambda}_i) - (y_i - \hat{\lambda}_i))}$$

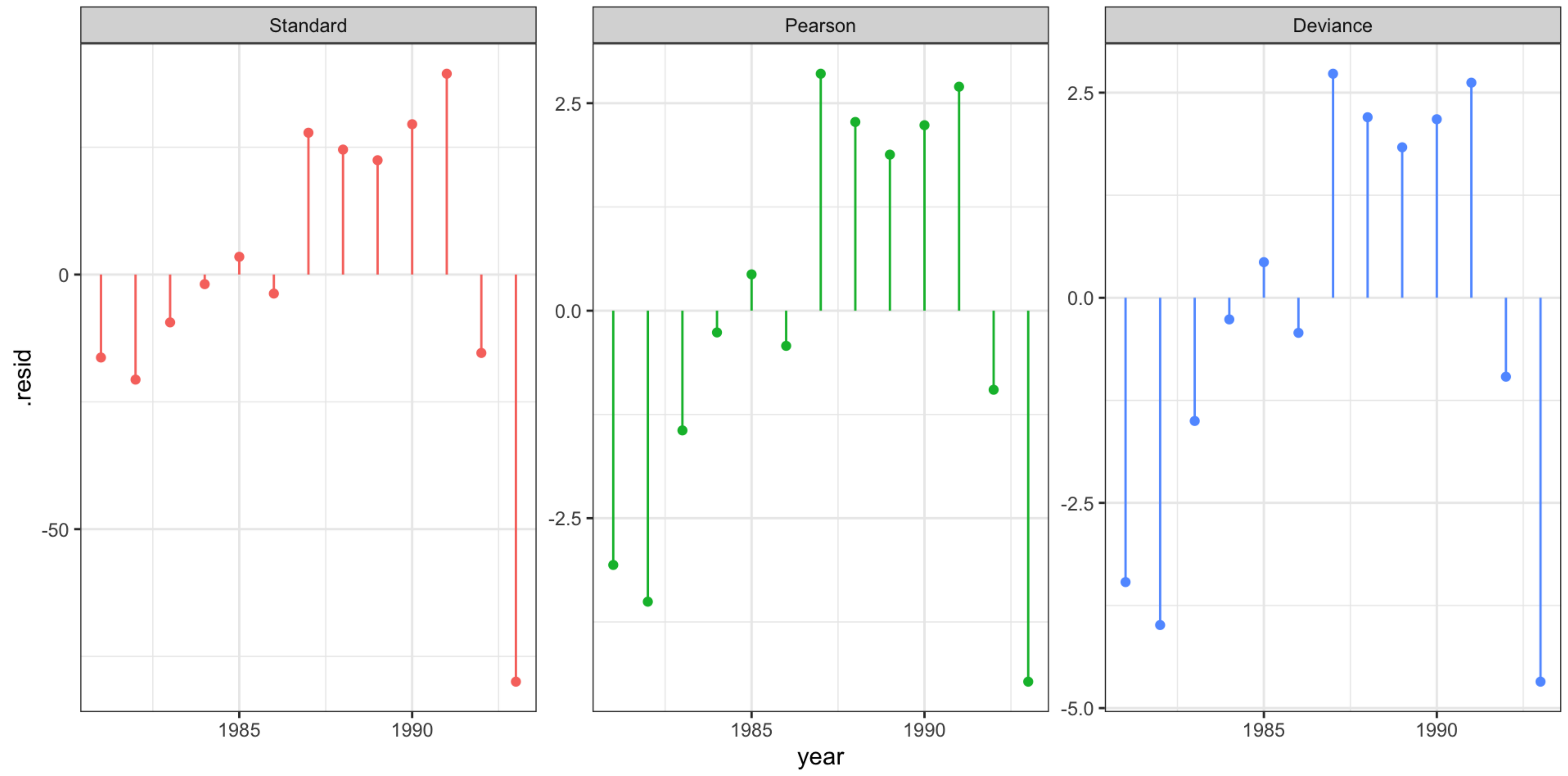
```r
g_pred_dev = broom::augment(
  g, type.predict = "response", type.residuals = "deviance"
)
```



Comparing Residuals



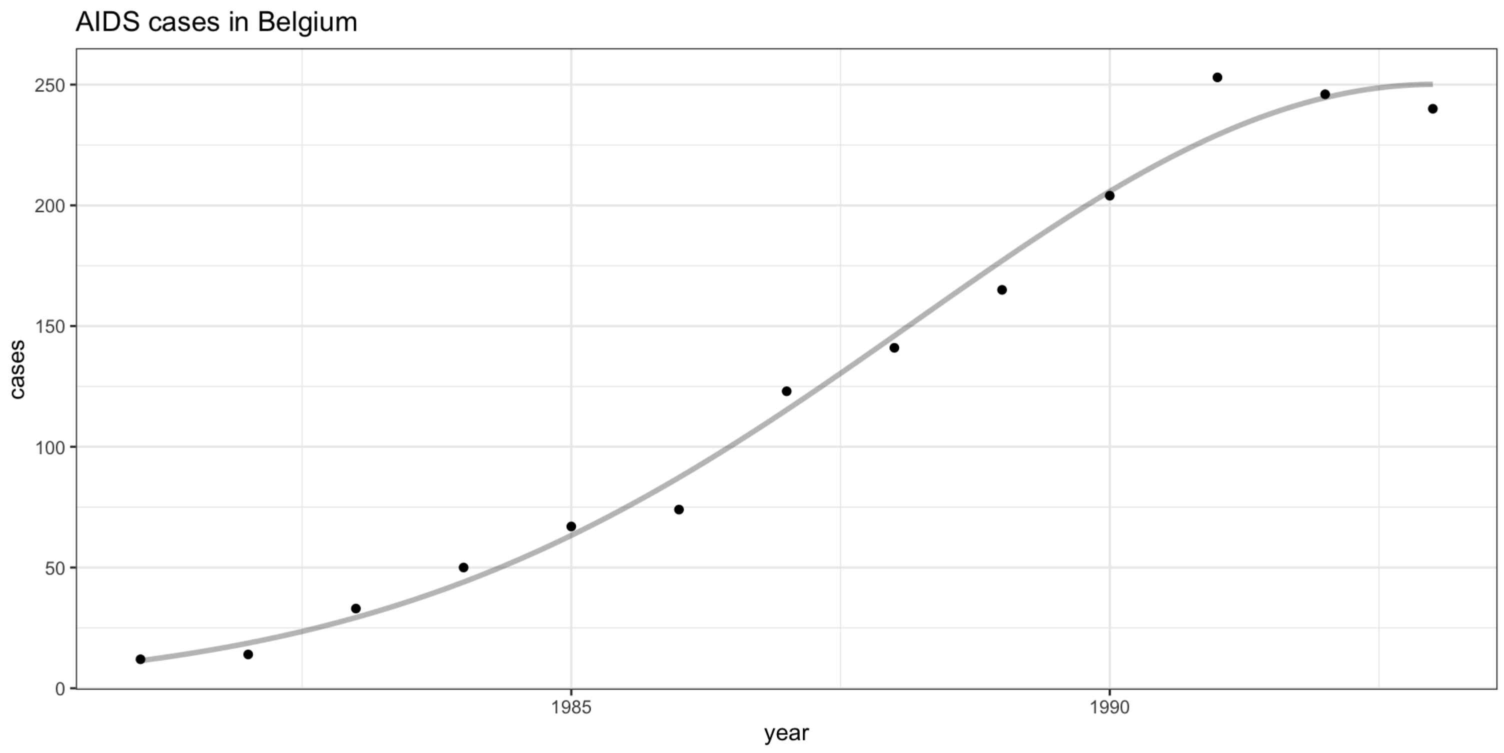
Comparing Residuals - scale free



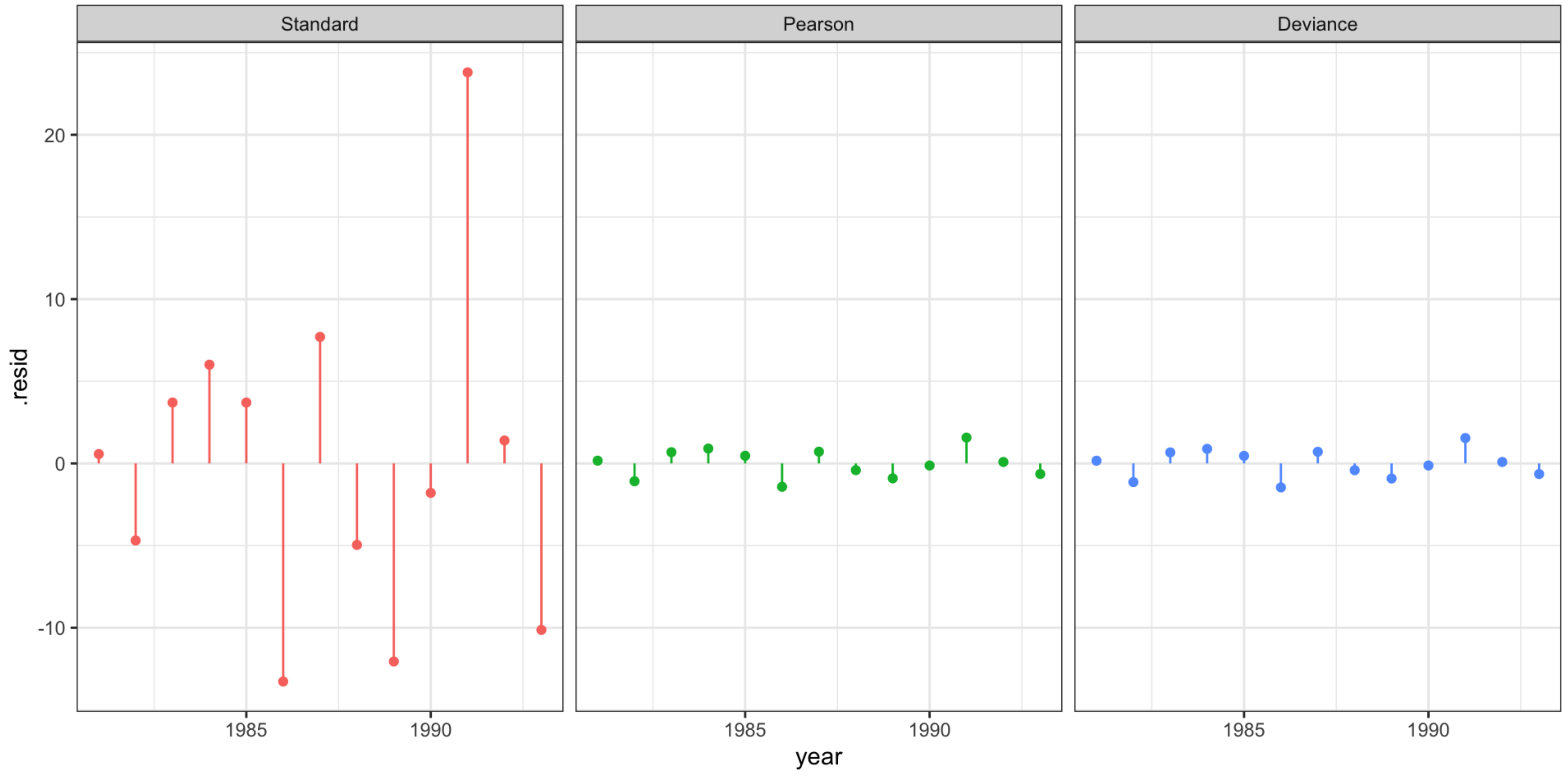
Updating the model

Quadratic fit

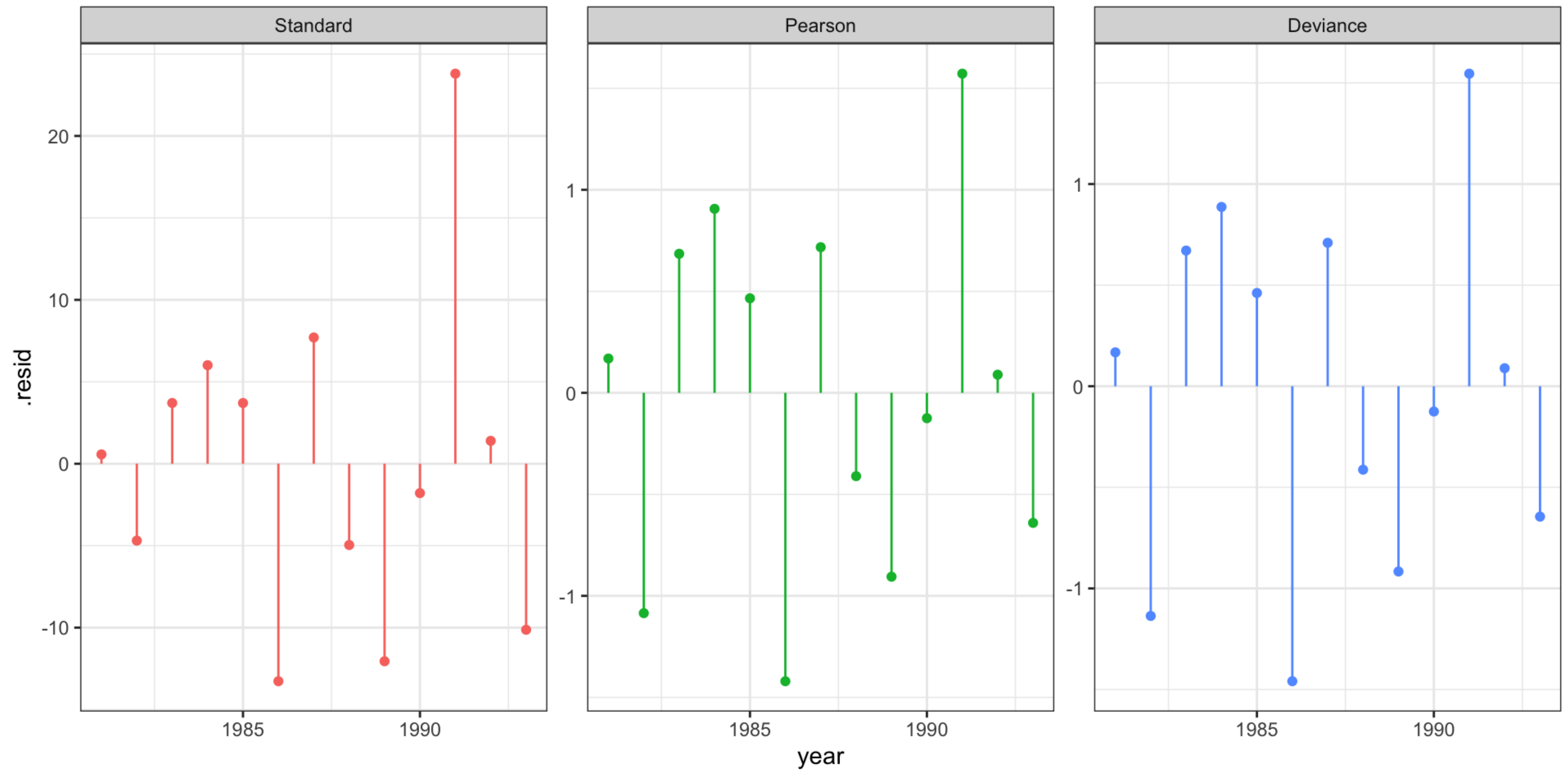
```r
g2 = glm(cases~year+I(year^2), data=aids, family=poisson)

g2_pred = broom::augment(
  g2, type.predict = "response",
  newdata=tibble(year=seq(1981,1993,by=0.1))
)
```



Quadratic fit - residuals



Quadratic fit - residuals (scale free)



Bayesian Model

Bayesian Poisson Regression Model

```r
( g_bayes = brms::brm(
    cases~year, data=aids, family=poisson,
    silent=2, refresh=0
) )
```

```
 Family: poisson
  Links: mu = log
Formula: cases ~ year
   Data: aids (Number of observations: 13)
  Draws: 4 chains, each with iter = 2000; warmup = 1000; thin = 1;
         total post-warmup draws = 4000

Population-Level Effects:
          Estimate Est.Error l-95% CI u-95% CI Rhat Bulk_ESS Tail_ESS
Intercept  -396.93     15.47  -427.20  -366.60 1.00     1502     2091
year          0.20      0.01     0.19     0.22 1.00     1504     2091

Draws were sampled using sampling(NUTS). For each parameter, Bulk_ESS
and Tail_ESS are effective sample size measures, and Rhat is the potential
scale reduction factor on split chains (at convergence, Rhat = 1).
```

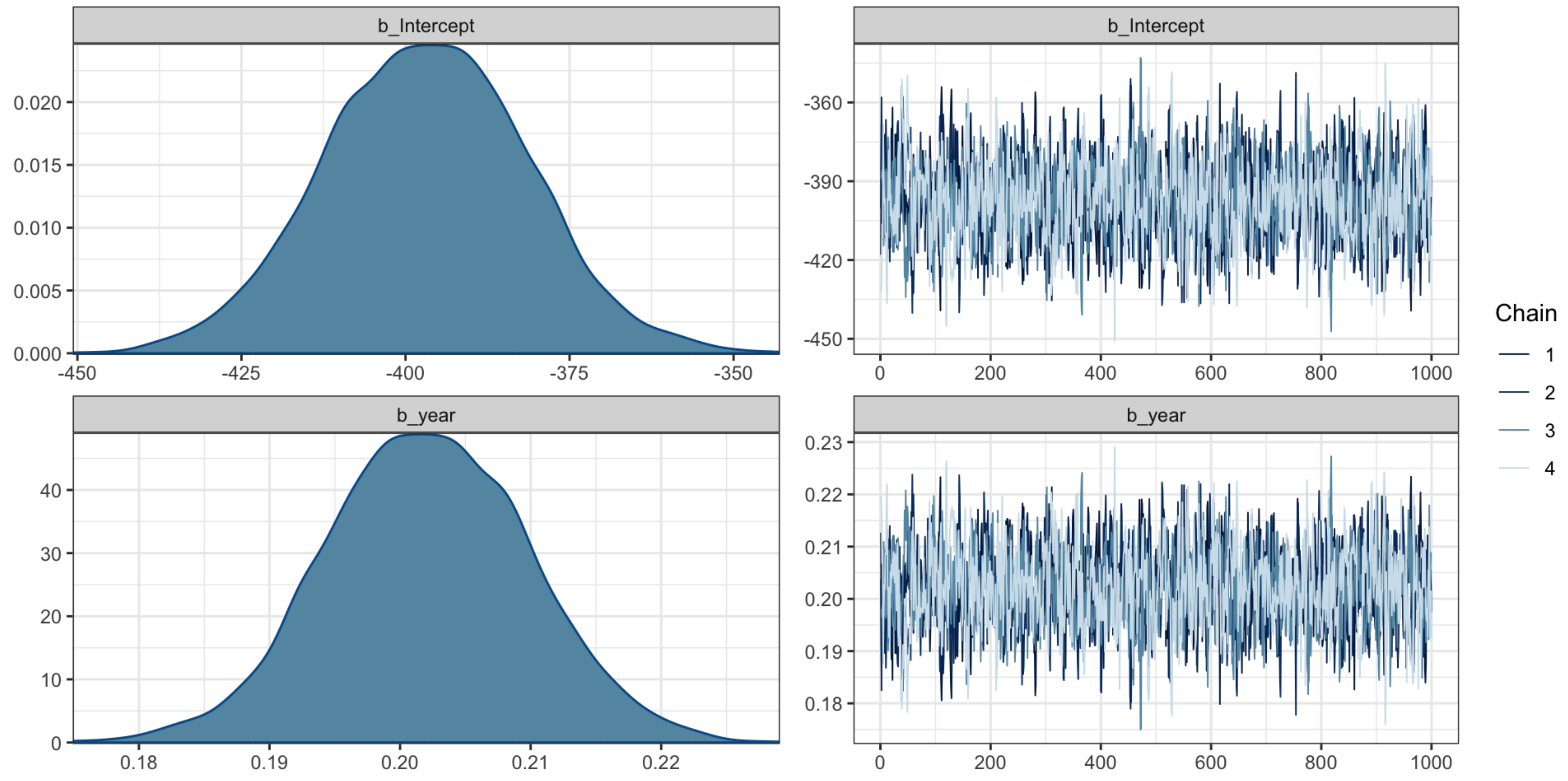
Model priors

```r
brms::prior_summary(g_bayes)
```

```
                  prior     class coef group resp dpar nlpar lb ub
source
                 (flat)         b
default
                 (flat)         b year
(vectorized)
 student_t(3, 4.8, 2.5) Intercept
default
```

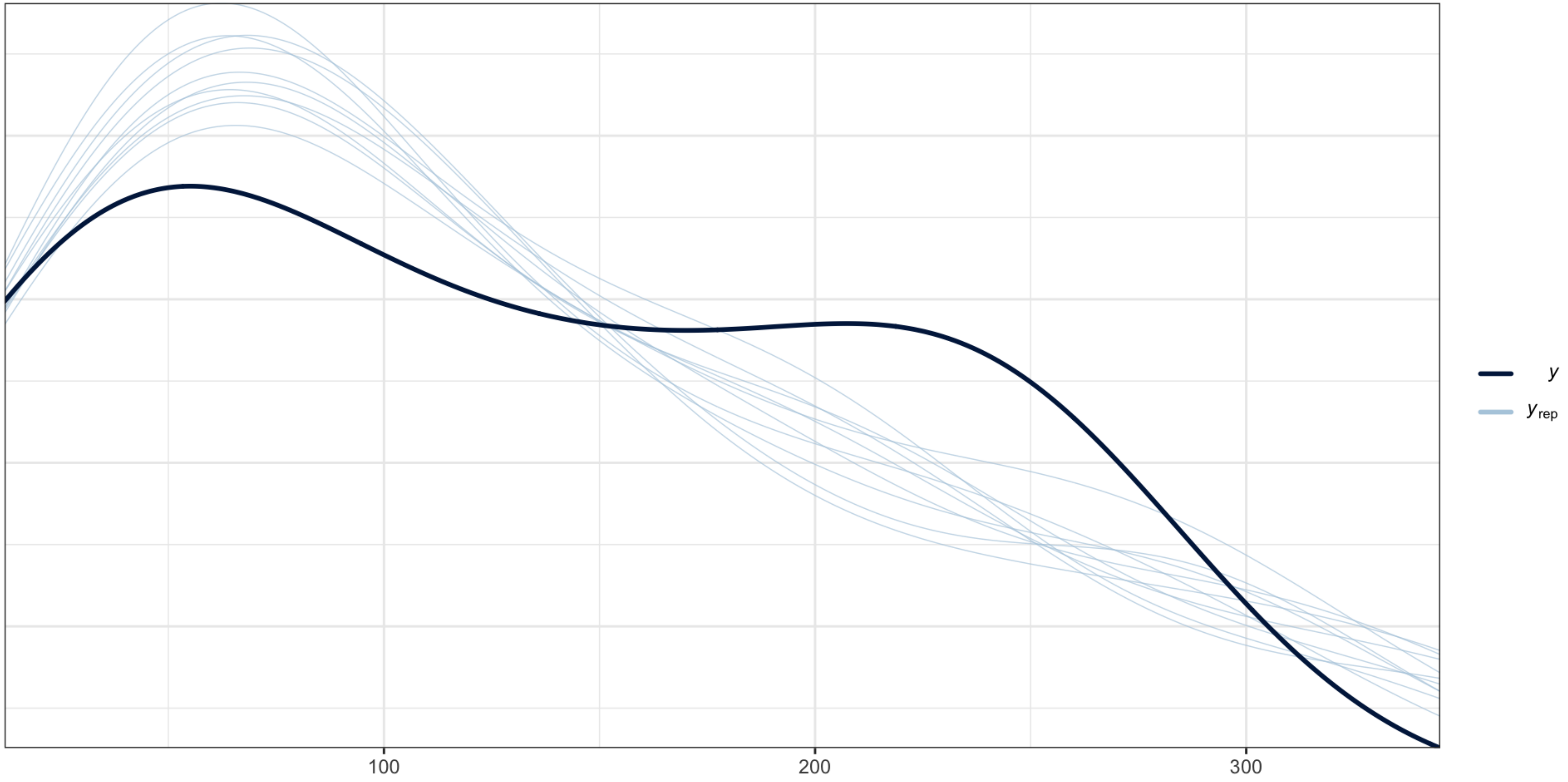
MCMC Diagnostics

```r
plot(g_bayes)
```



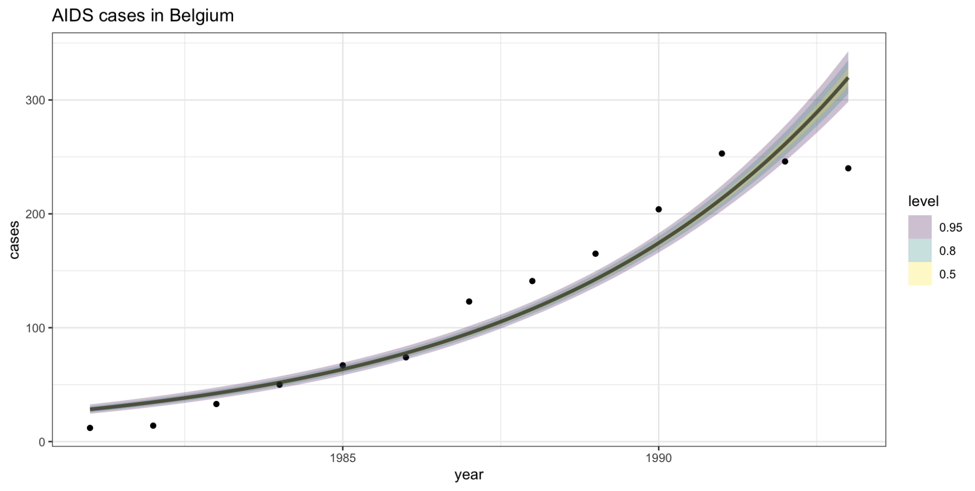
Posterior Predictive Check

```r
brms::pp_check(g_bayes)
```



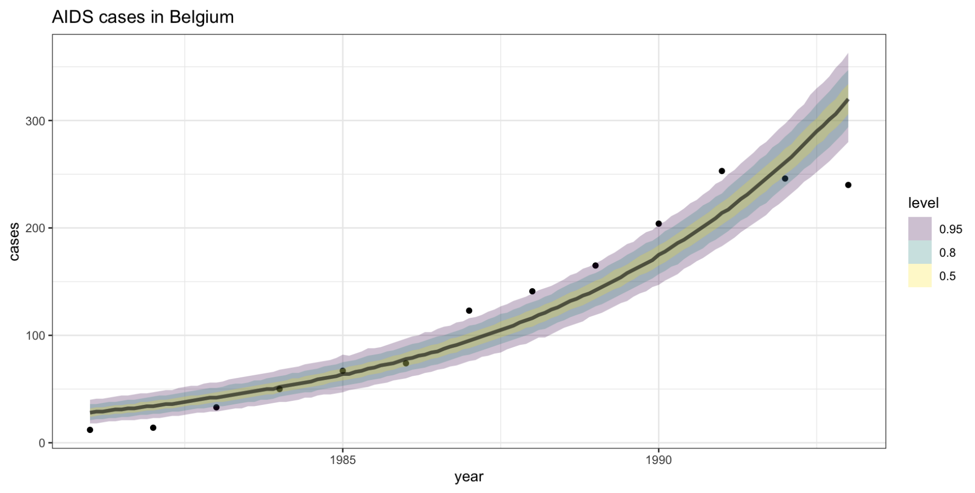
Model fit - λ CI

```r
aids_base +
  ggdist::stat_lineribbon(
    data = tidybayes::epred_draws(
      g_bayes,
      newdata = tibble(year=seq(1981,1993,by=
    ),
    aes(y=.epred),
    alpha=0.25
  )
```



Model fit - Y CI

```r
aids_base +
  ggdist::stat_lineribbon(
    data = tidybayes::predicted_draws(
      g_bayes,
      newdata = tibble(year=seq(1981,1993,by=
    ),
    aes(y=.prediction),
    alpha=0.25
  )
```


AIDS cases in Belgium
cases
year
level