Model Complexity

STAT 4710

September 15, 2022

Rolling into Unit 2

Unit 1: Intro to modern data mining

Unit 2: Tuning predictive models

Unit 3: Regression-based methods

Unit 4: Tree-based methods

Unit 5: Deep learning

Lecture 1: Model complexity

Lecture 2: Bias-variance trade-off

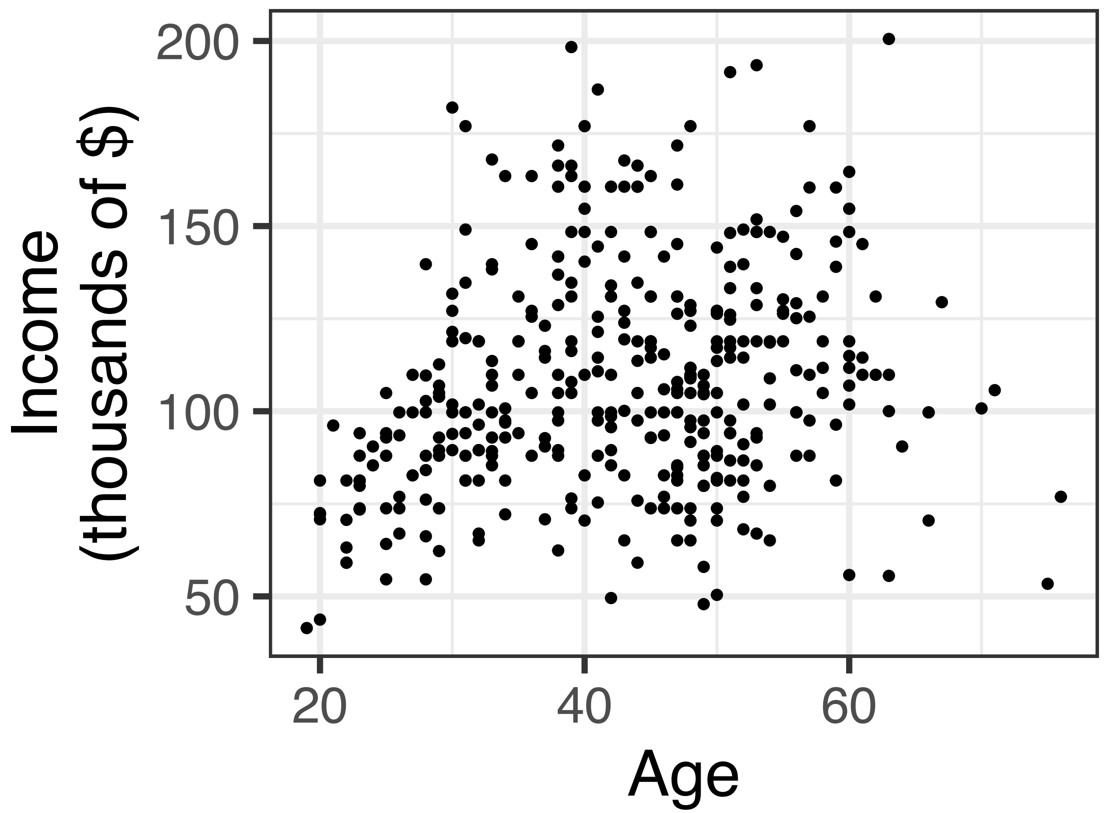
Lecture 3: Cross-validation

Lecture 4: Classification

Lecture 5: Unit review and quiz in class

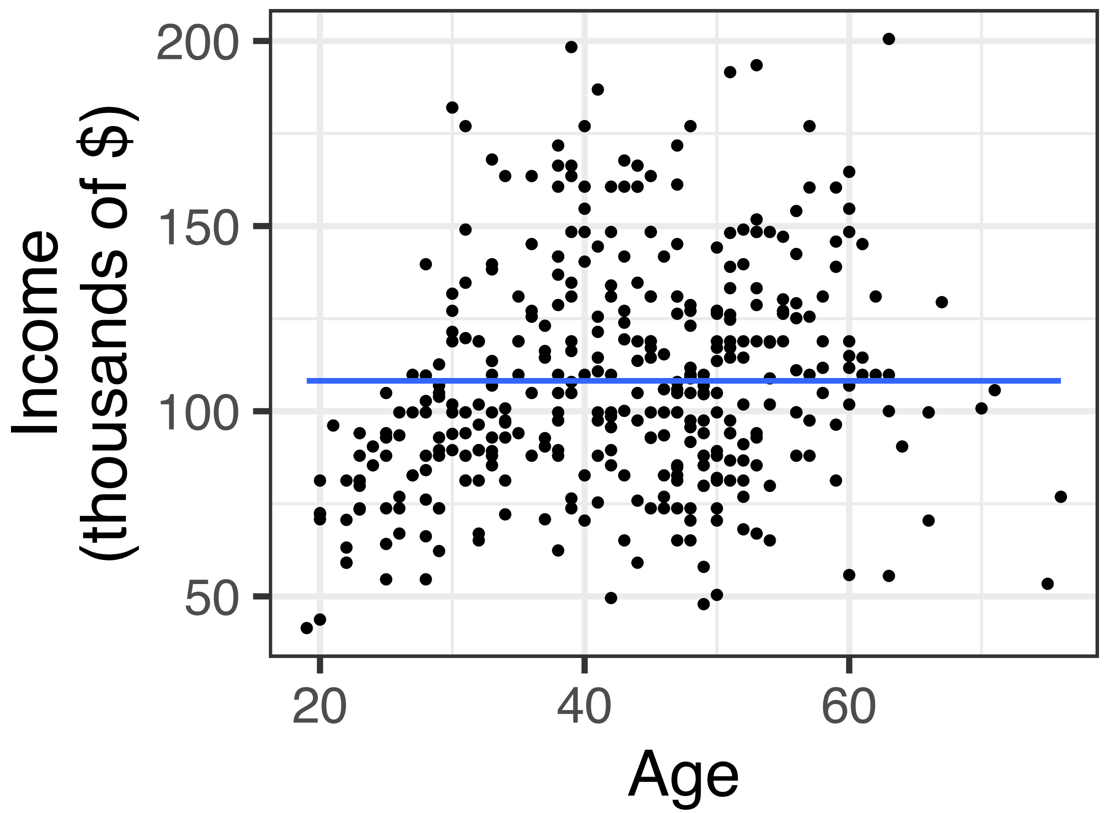
Example: Fit trend of income based on age

What does the trend look like?



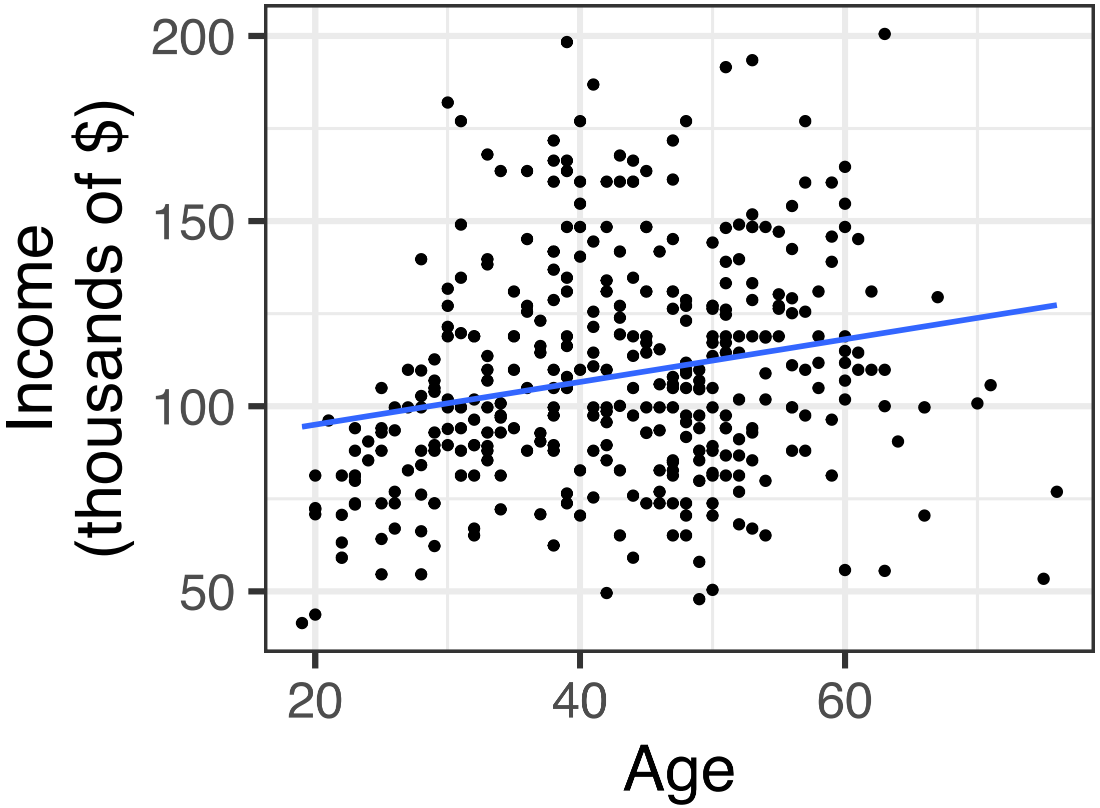
Intercept-only model (no trend)

$$\text{income} = \beta_0 + \epsilon$$



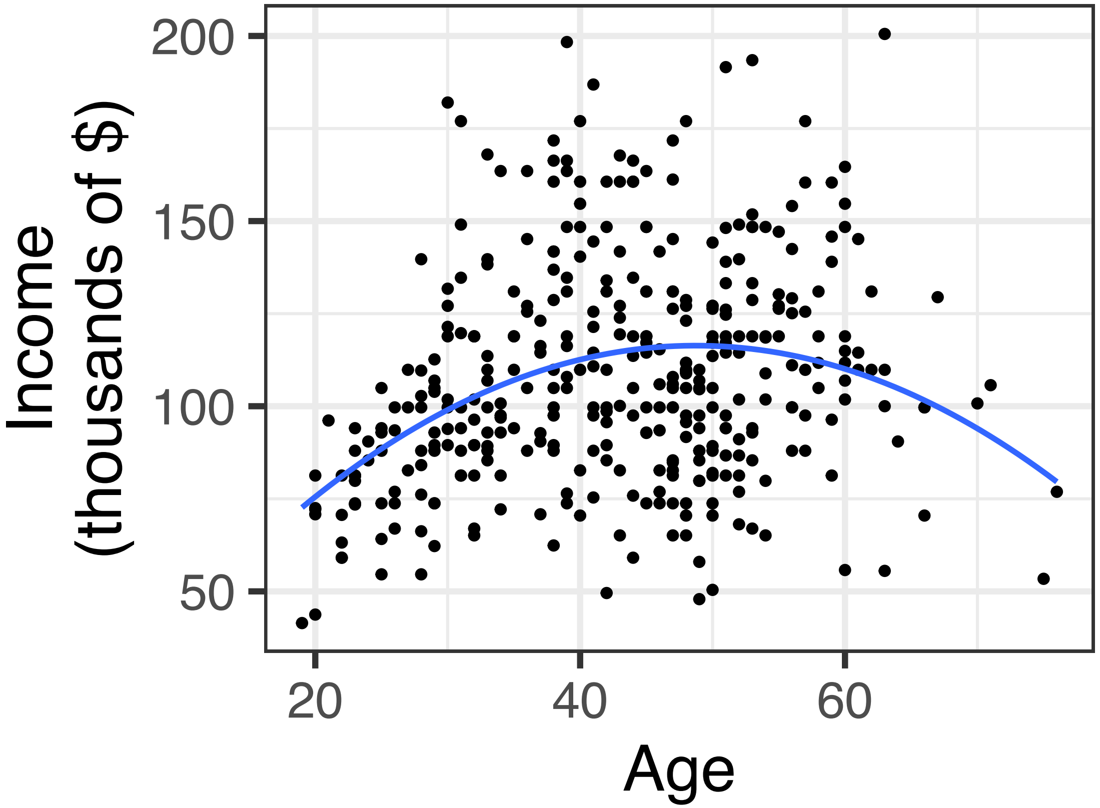
Linear model (linear trend)

$$\text{income} = \beta_0 + \beta_1 \cdot \text{age} + \epsilon$$



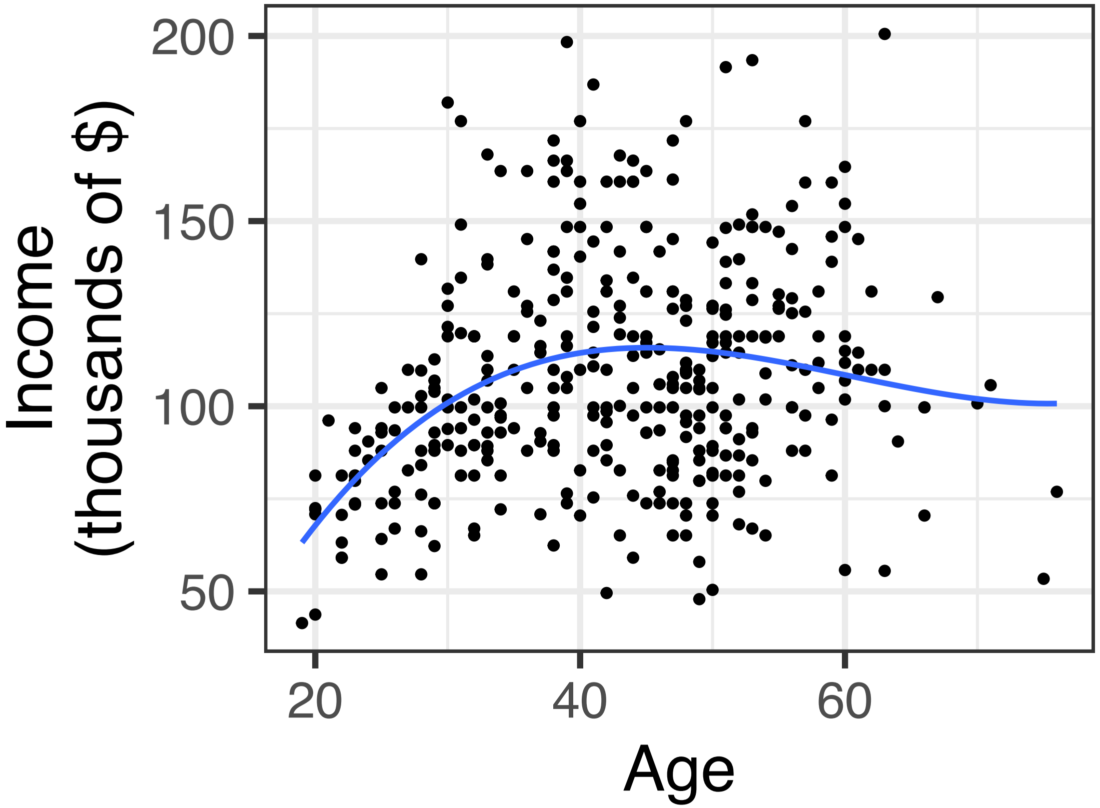
Polynomial model (quadratic trend)

$$\text{income} = \beta_0 + \beta_1 \cdot \text{age} + \beta_2 \cdot \text{age}^2 + \epsilon$$



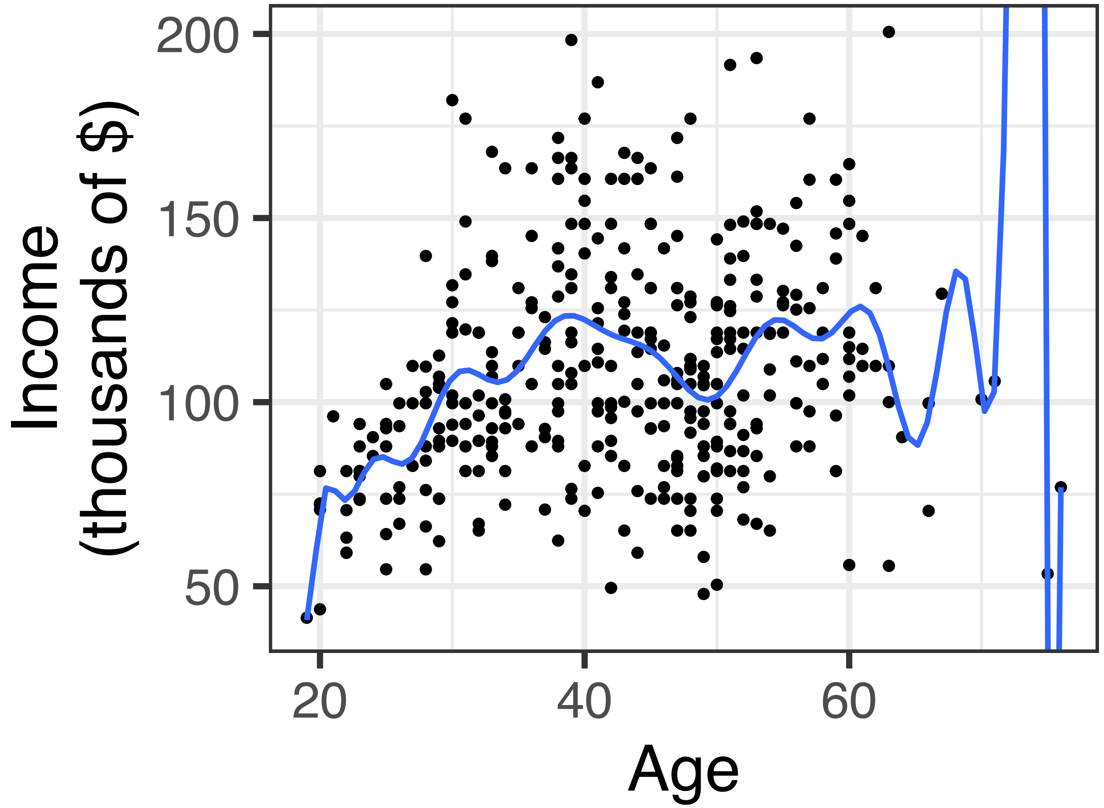
Polynomial model (cubic trend)

$$\text{income} = \beta_0 + \beta_1 \cdot \text{age} + \beta_2 \cdot \text{age}^2 + \beta_3 \cdot \text{age}^3 + \epsilon$$



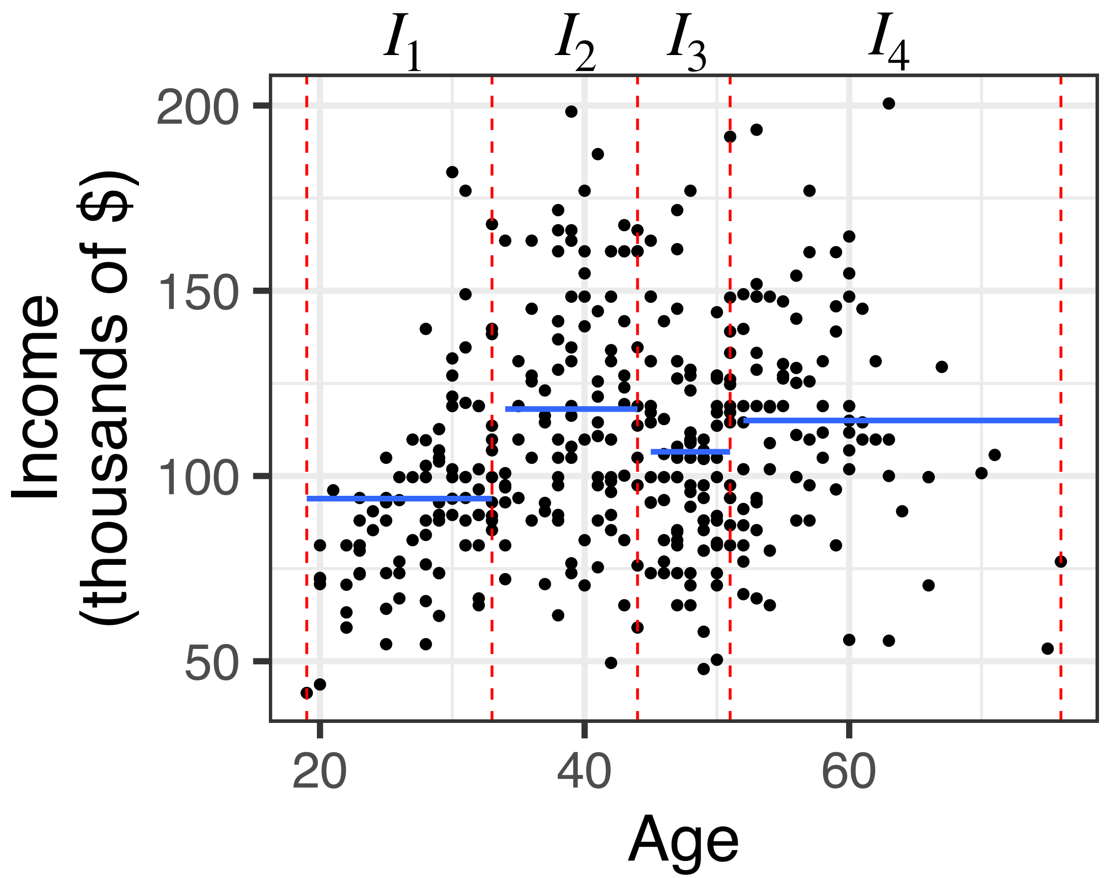
20th degree polynomial model

$$\text{income} = \beta_0 + \beta_1 \cdot \text{age} + \beta_2 \cdot \text{age}^2 + \cdots + \beta_{20} \cdot \text{age}^{20} + \epsilon$$



Piece-wise polynomial (piece-wise constant)

$$\text{income} = \beta_1 \cdot 1(\text{age} \in I_1) + \cdots + \beta_4 \cdot 1(\text{age} \in I_4) + \epsilon$$



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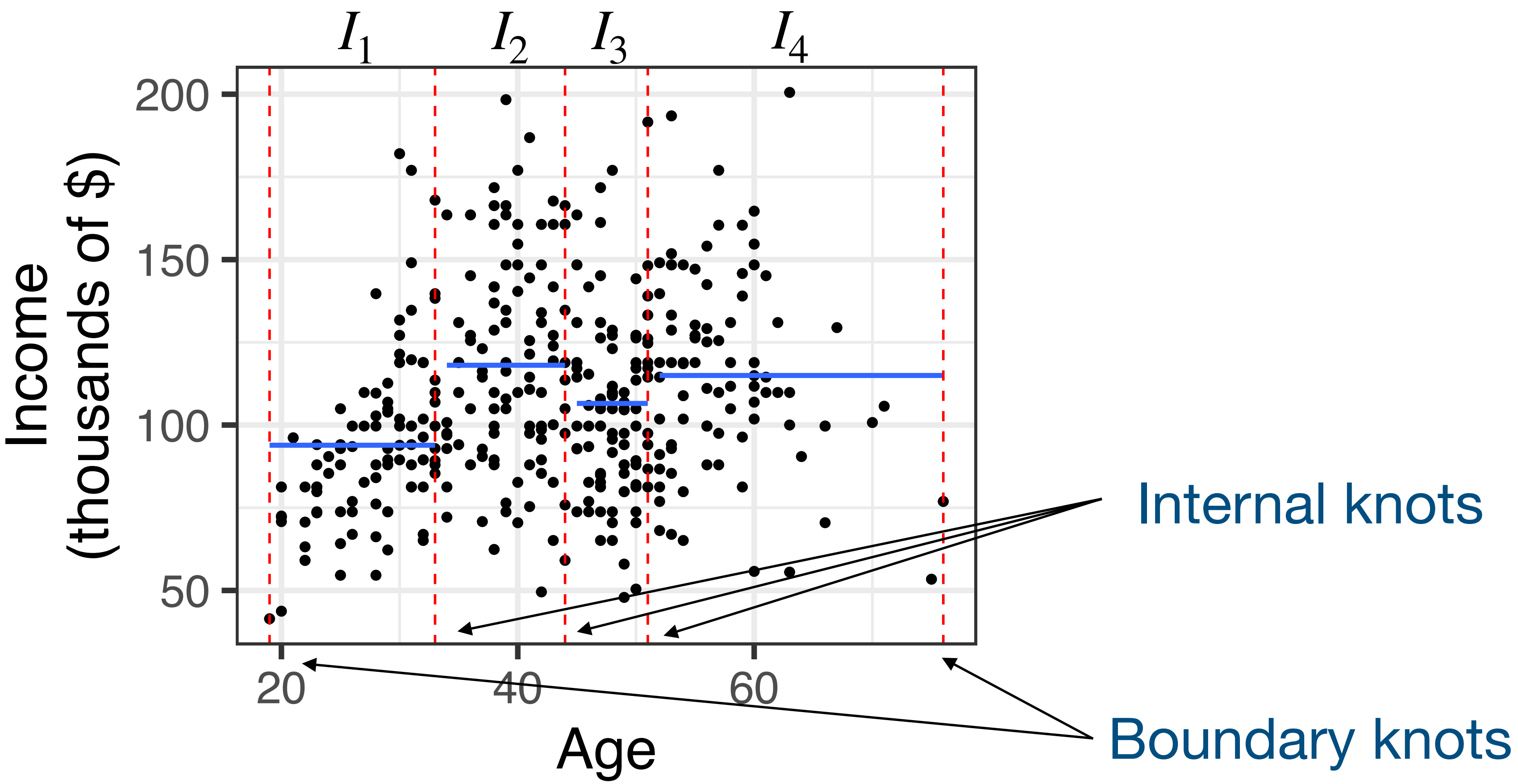
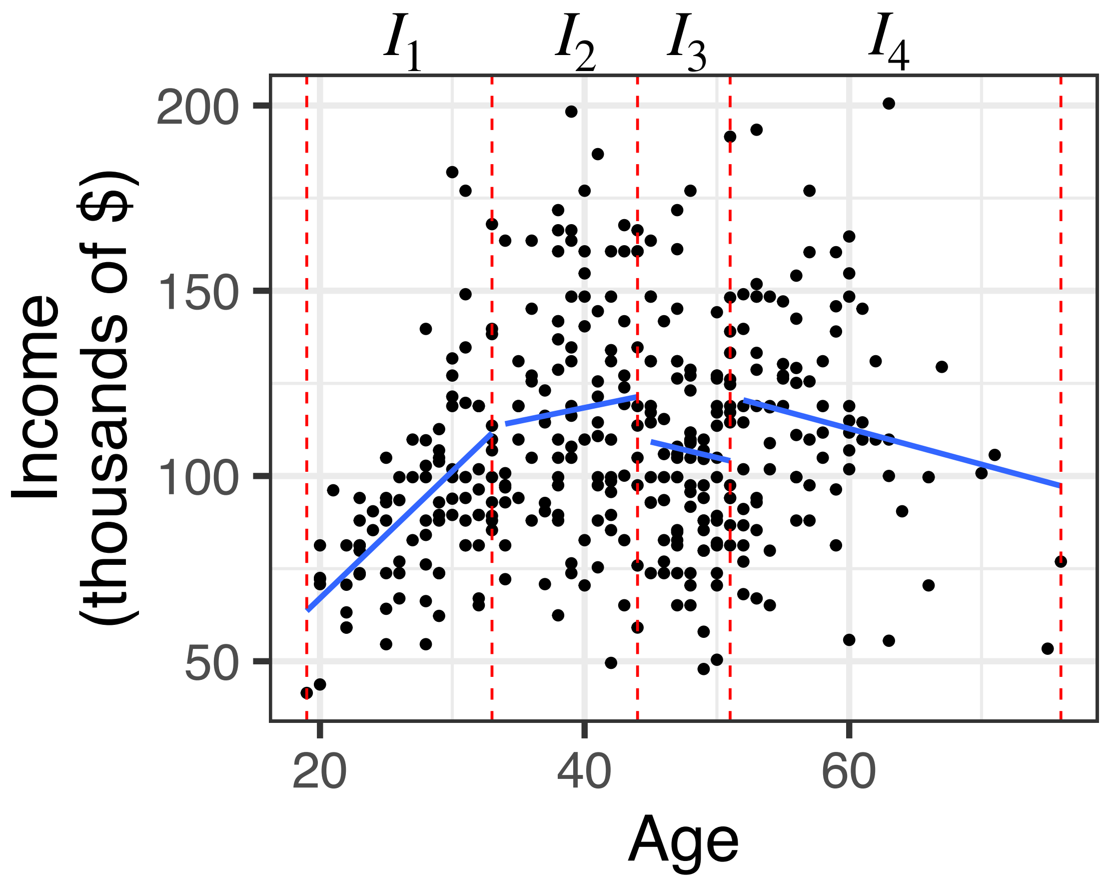


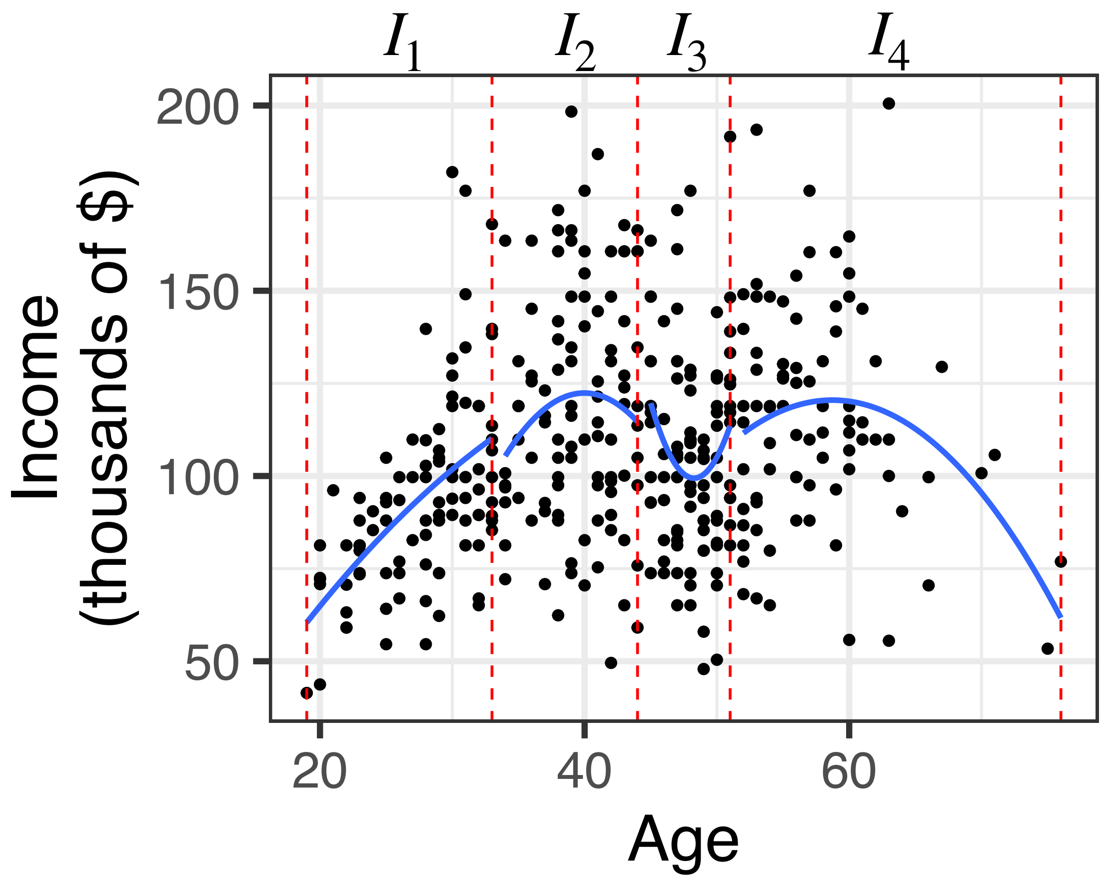
Piece-wise polynomial (piece-wise linear)

$$\text{income} = (\beta_{01} + \beta_{11}\text{age}) \cdot 1(\text{age} \in I_1) + \cdots + (\beta_{04} + \beta_{14}\text{age}) \cdot 1(\text{age} \in I_4) + \epsilon$$



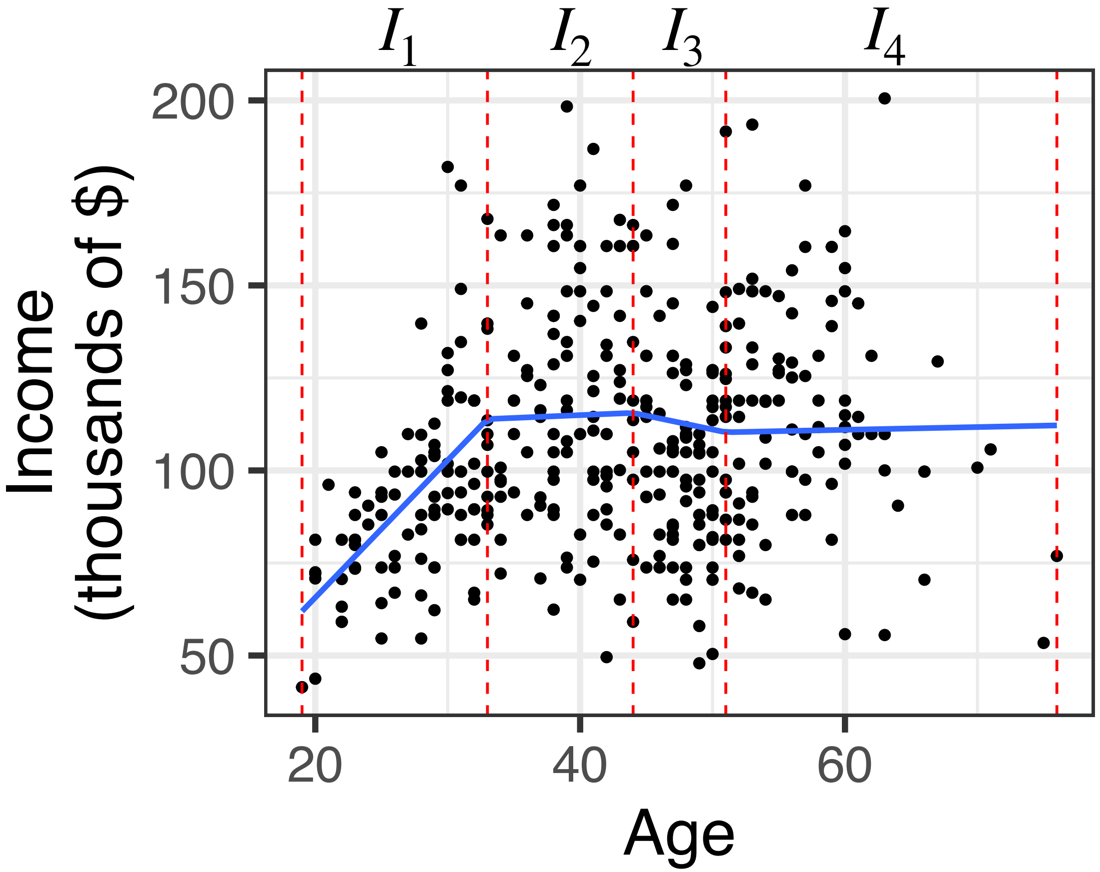
Piece-wise polynomial (piece-wise quadratic)

$$\text{income} = (\beta_{01} + \beta_{11}\text{age} + \beta_{21}\text{age}^2) \cdot 1(\text{age} \in I_1) + \cdots + (\ldots) \cdot 1(\text{age} \in I_4) + \epsilon$$



Spline (piece-wise linear)

$$\text{income} = (\beta_{01} + \beta_{11}\text{age}) \cdot 1(\text{age} \in I_1) + \cdots + (\beta_{04} + \beta_{14}\text{age}) \cdot 1(\text{age} \in I_4) + \epsilon$$



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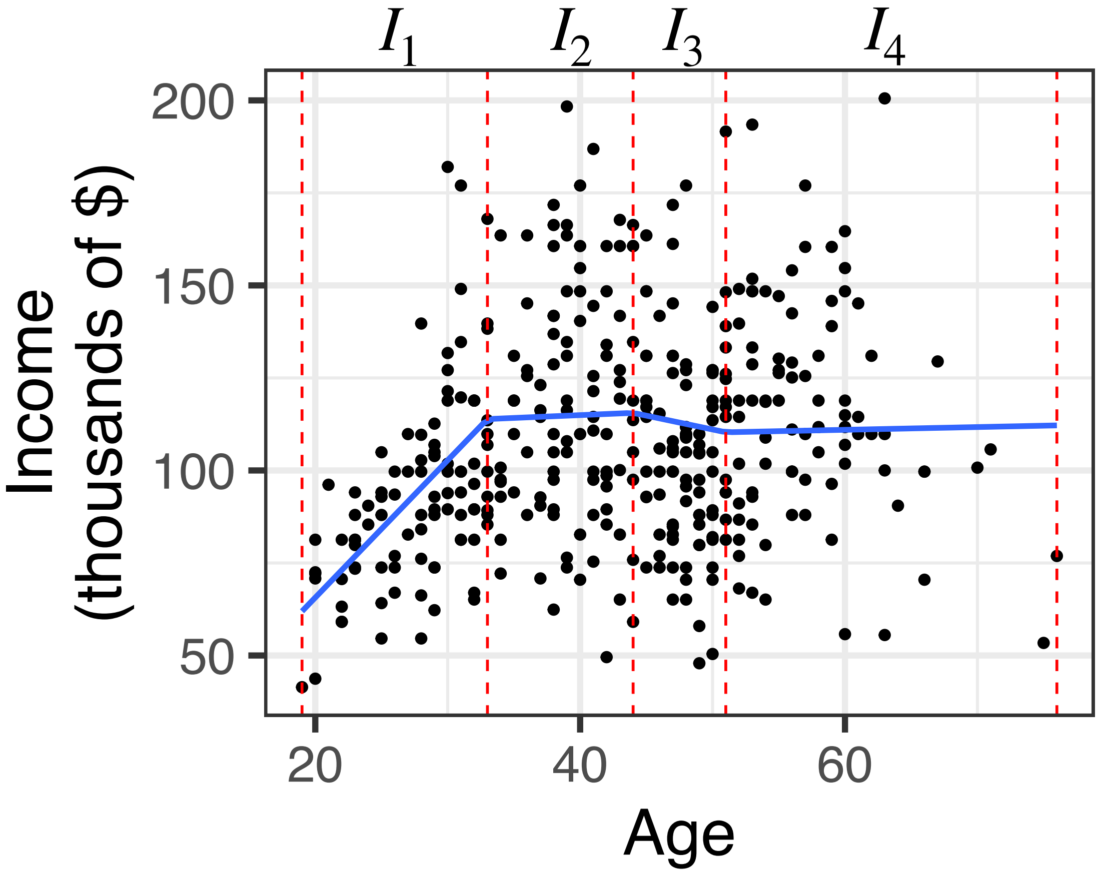
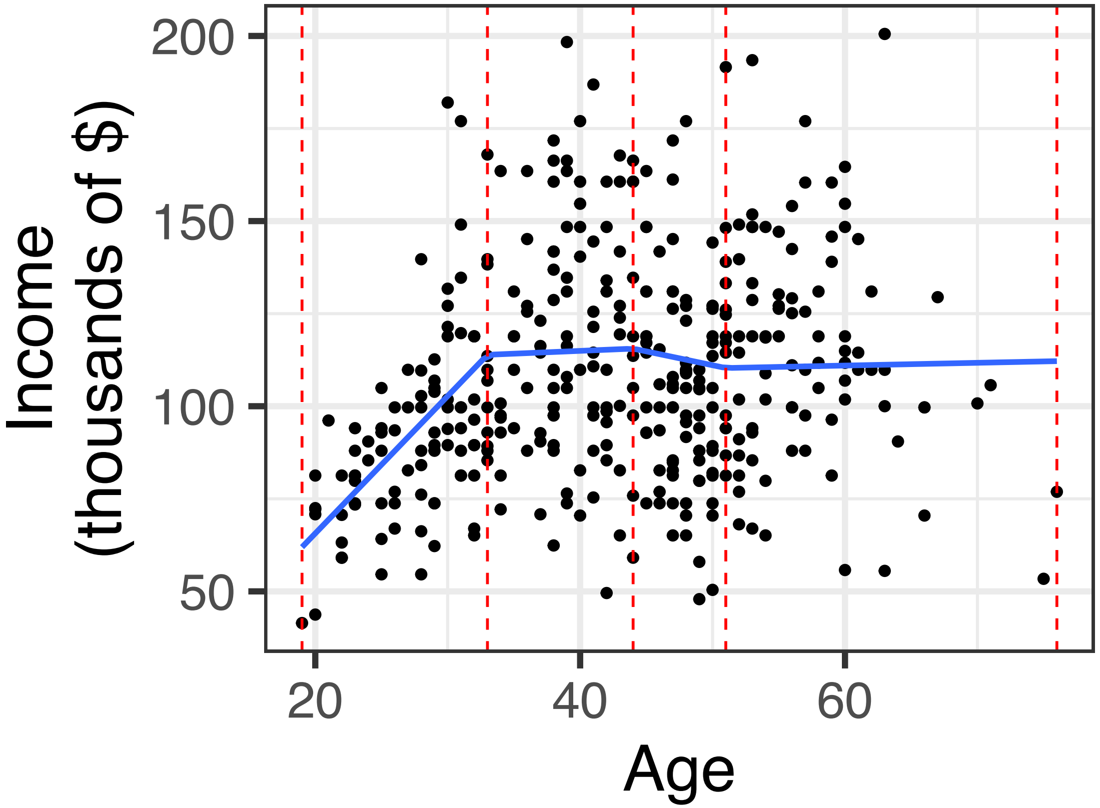


Spline (piece-wise linear)

$$\text{income} = \beta_0 + \beta_1 \cdot f_1(\text{age}) + \cdots + \beta_{p-1} f_{p-1}(\text{age}) + \epsilon$$



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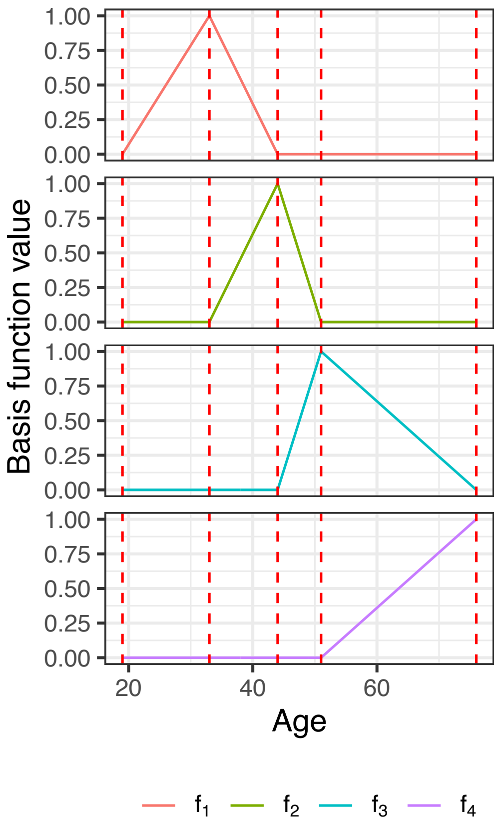
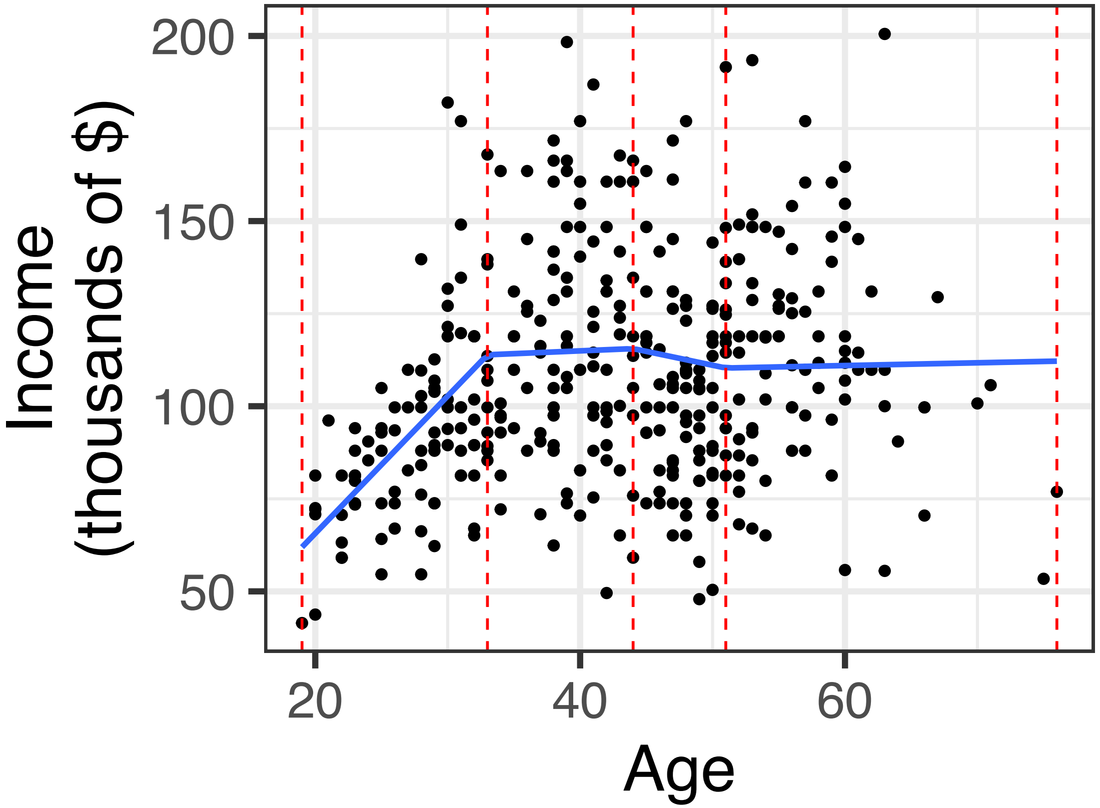
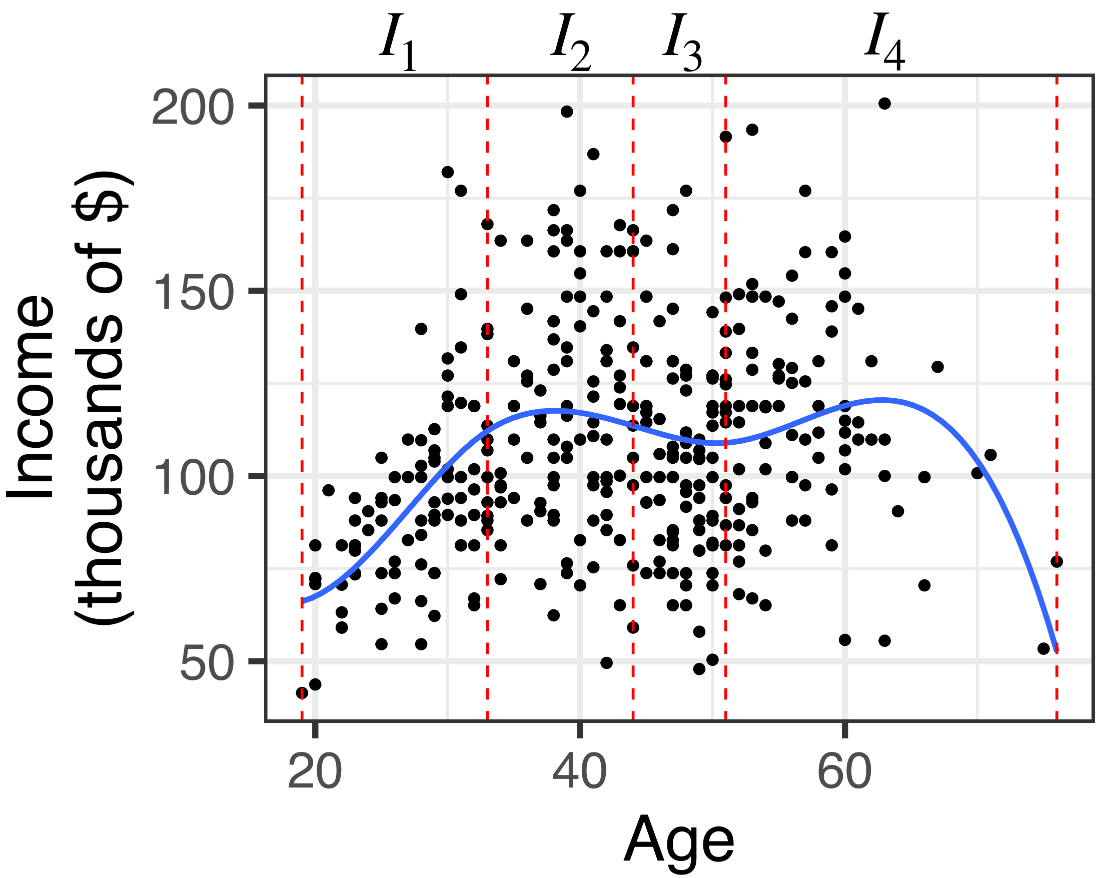




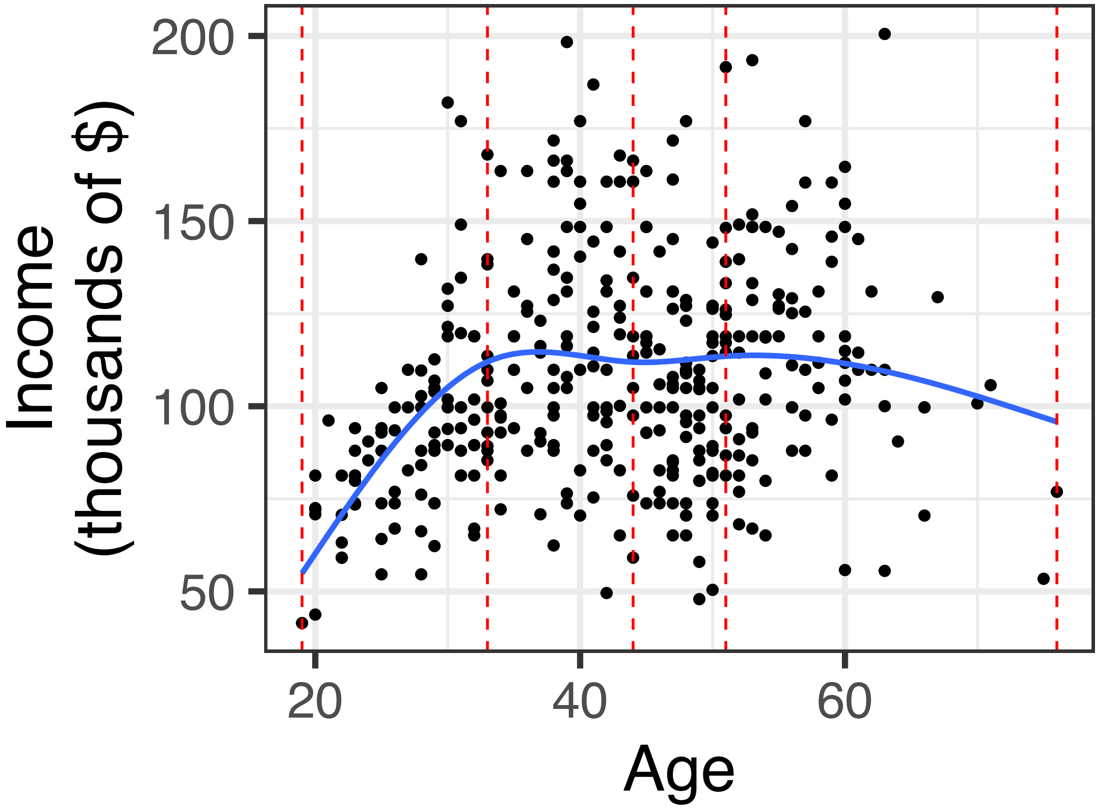
Spline (piece-wise cubic)

$$\text{income} = \beta_0 + \beta_1 \cdot f_1(\text{age}) + \cdots + \beta_{p-1} f_{p-1}(\text{age}) + \epsilon$$



Natural cubic spline (with 5 total knots)

$$\text{income} = \beta_0 + \beta_1 \cdot f_1(\text{age}) + \cdots + \beta_{p-1} f_{p-1}(\text{age}) + \epsilon$$



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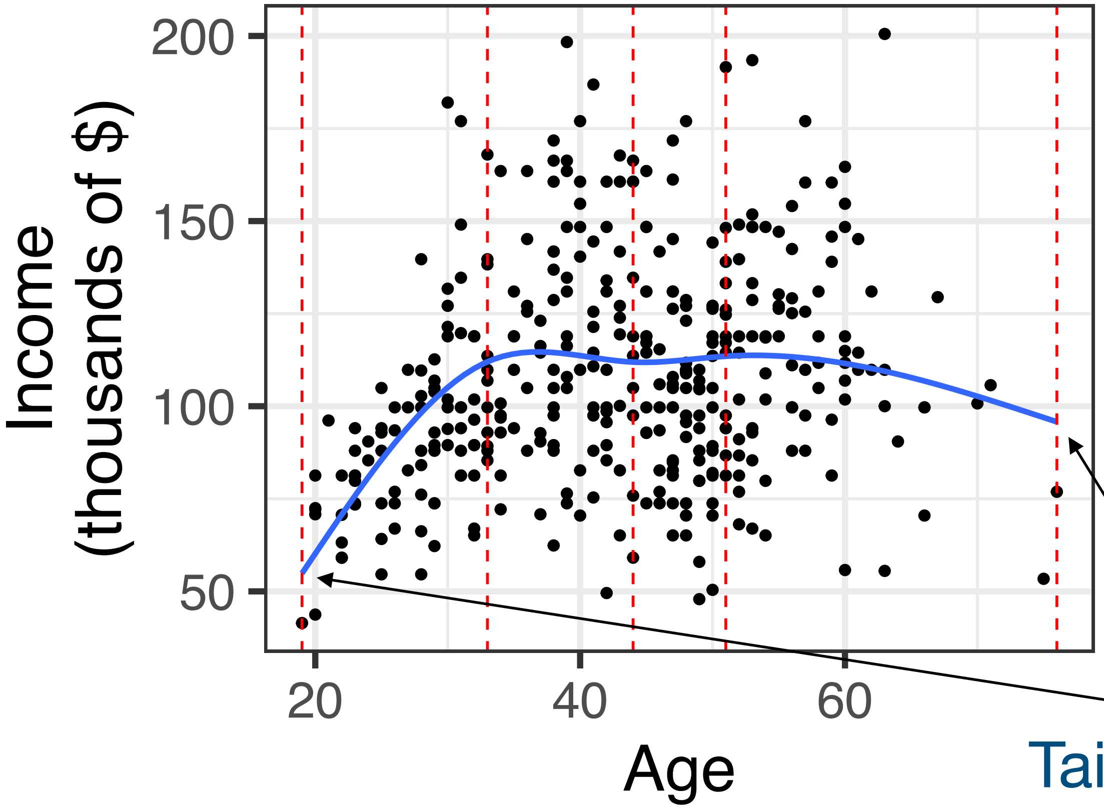
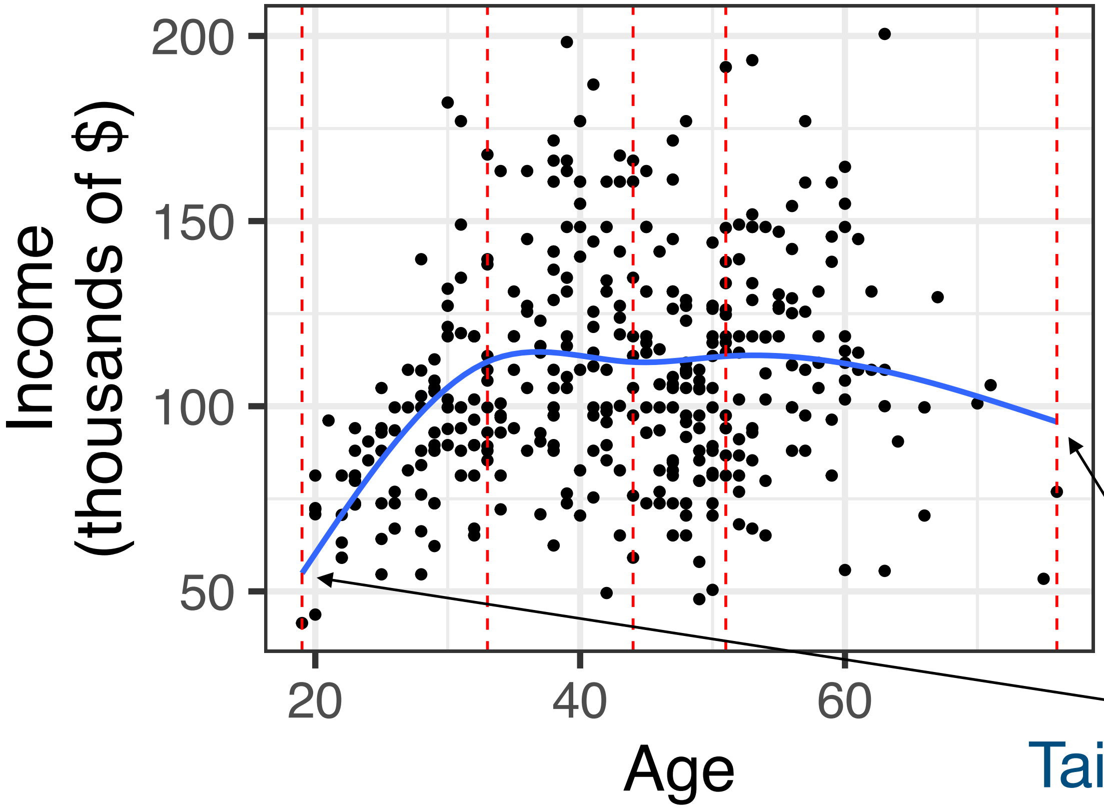


Tails off linearly

Natural cubic spline (with 5 total knots)

$$\text{income} = \beta_0 + \beta_1 \cdot f_1(\text{age}) + \cdots + \beta_{p-1} f_{p-1}(\text{age}) + \epsilon$$

The preferred way to fit smooth curves to data.

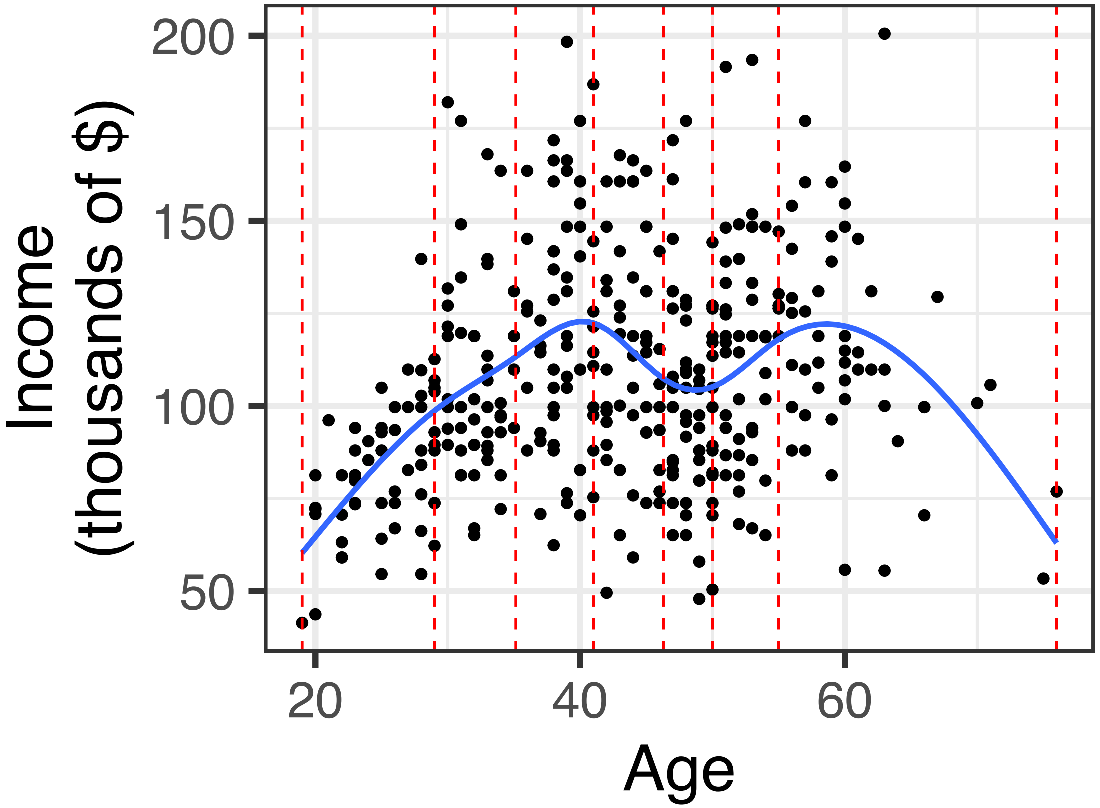


Tails off linearly

Natural cubic spline (with 8 total knots)

$$\text{income} = \beta_0 + \beta_1 \cdot f_1(\text{age}) + \cdots + \beta_{p-1} f_{p-1}(\text{age}) + \epsilon$$

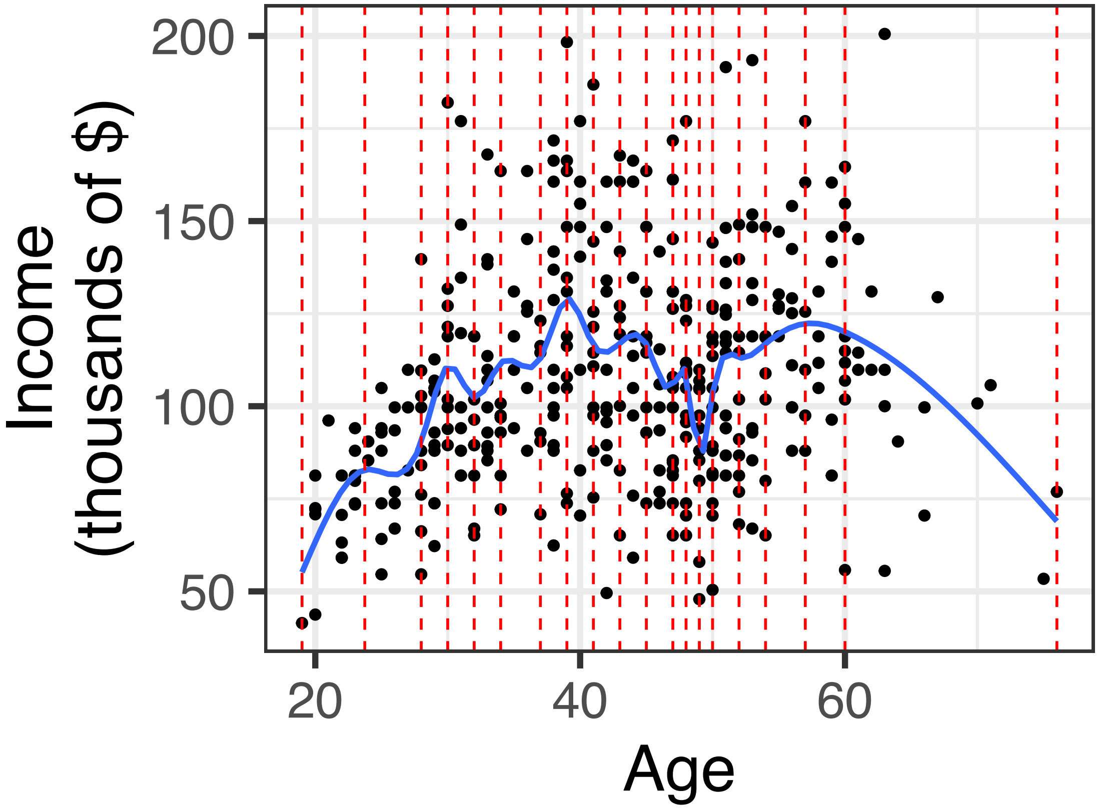
The preferred way to fit smooth curves to data.



Natural cubic spline (with 20 total knots)

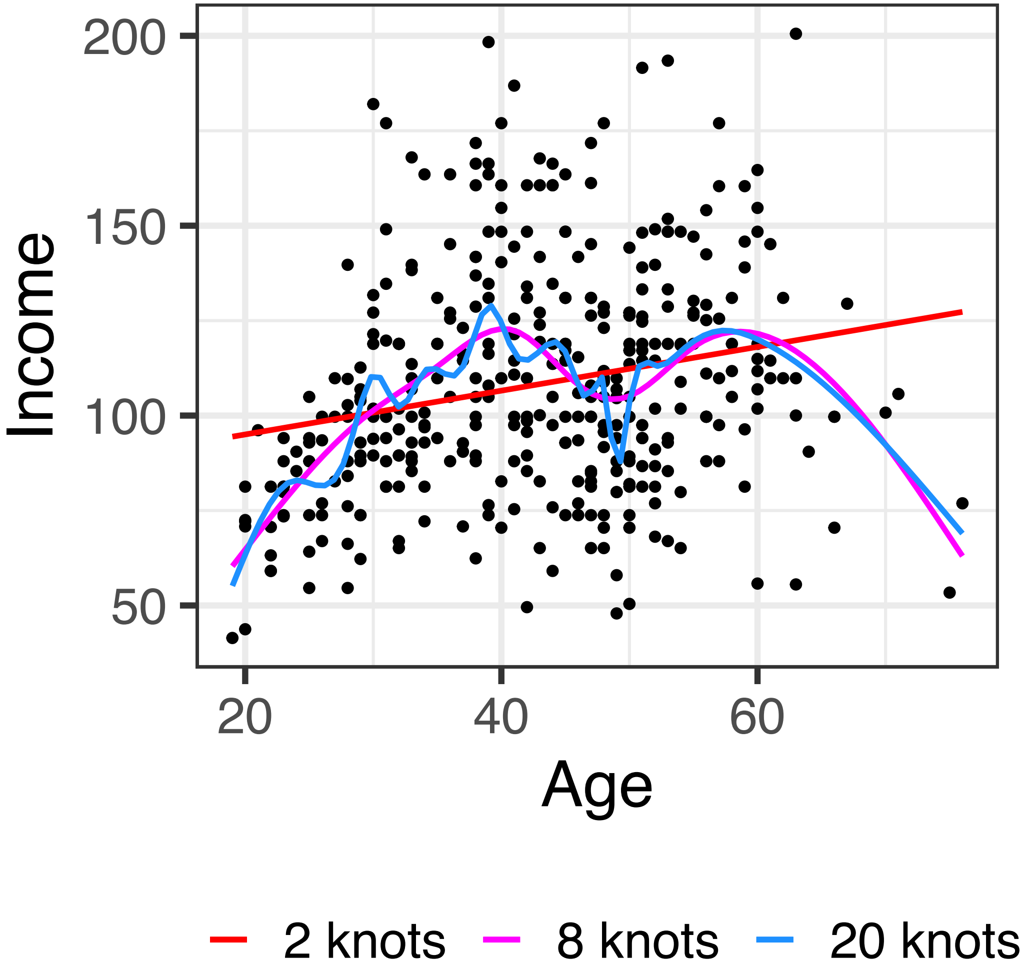
$$\text{income} = \beta_0 + \beta_1 \cdot f_1(\text{age}) + \cdots + \beta_{p-1} f_{p-1}(\text{age}) + \epsilon$$

The preferred way to fit smooth curves to data.



Model complexity

- The same data can be fit with models of varying degrees of *flexibility* or *complexity*.
- Example: Natural cubic splines with more knots are more flexible.
- Model complexity has an important effect on predictive performance:
    - Too flexible →
      too sensitive to noise in training data
    - Not flexible enough →
      can’t capture the underlying trend



Quantifying model complexity for linear regression

Complexity for linear regression models of the form

$$y = \beta_0 + \beta_1 \cdot f_1(x) + \cdots + \beta_{p-1} f_{p-1}(x) + \epsilon$$

is quantified via *degrees of freedom (df),* the number of free parameters β_j. In particular, the model above has p degrees of freedom.

Important examples:

- Polynomials of degree p have $p + 1$ degrees of freedom.
- Natural cubic splines with K total knots have K degrees of freedom.

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Important examples:

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- Natural cubic splines with K total knots have K degrees of freedom.*

*Caution: Sometimes the intercept is excluded from the spline definition, so a spline with K total knots is sometimes considered to have df = $K - 1$.

Recall: Prediction performance

You have training data $(X_1^{\text{train}}, Y_1^{\text{train}}), \dots, (X_n^{\text{train}}, Y_n^{\text{train}})$, based on which you construct a predictive model $\hat{f}$ such that, hopefully, $Y \approx \hat{f}(X)$.

Will deploy $\hat{f}$ on test data $X_1^{\text{test}}, \dots, X_N^{\text{test}}$ to guess $\hat{Y}_i^{\text{test}} = \hat{f}(X_i^{\text{test}})$ for each i.

Each X_i^{test} comes with a response Y_i^{test}, unknown to the predictive model.

Prediction quality: extent to which $Y_i^{\text{test}} \approx \hat{Y}_i^{\text{test}}$, e.g. mean squared test error:

$$\text{Test error of } \hat{f} = \frac{1}{N}\sum_{i=1}^{N}(Y_i^{\text{test}} - \hat{Y}_i^{\text{test}})^2.$$

Model complexity impacts prediction performance

Model complexity: how closely the model $\hat{f}$ fits the training data:

$$Y_i^{\text{train}} = f(X_i^{\text{train}}) + \epsilon_i.$$

During training, $\hat{f}$ picks up on patterns in both f (the signal) and ϵ_i (the noise).

Training error of $\hat{f}$ decreases as we increase model complexity, but test error will be high if model complexity is too low or too high.

Training error is an underestimate of the test error, especially as the model complexity increases (overfitting).