Model Complexity

STAT 4710

September 14, 2023

Rolling into Unit 2

✔ **Unit 1:** R for data mining

Unit 2: Prediction fundamentals

- **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

Unit 3: Regression-based methods

Unit 4: Tree-based methods

Unit 5: Deep learning

Lecture outline

Model complexity:
How flexibly a predictive model can fit its training data.

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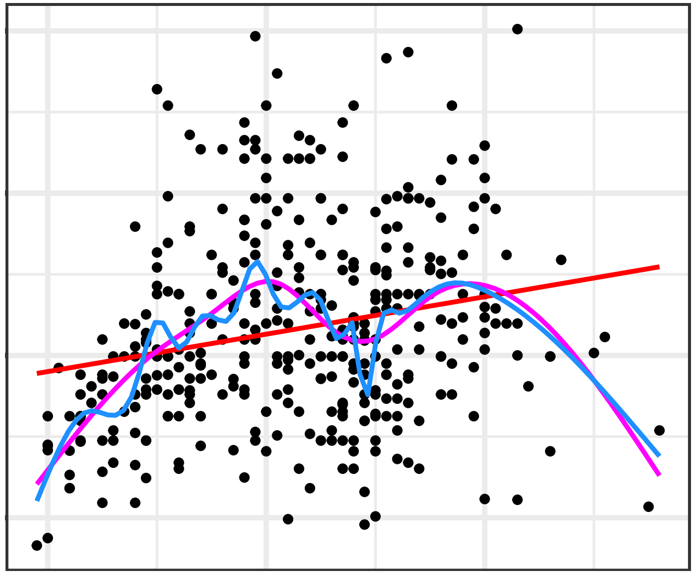
1. Case study: Fitting curves to scatter plots



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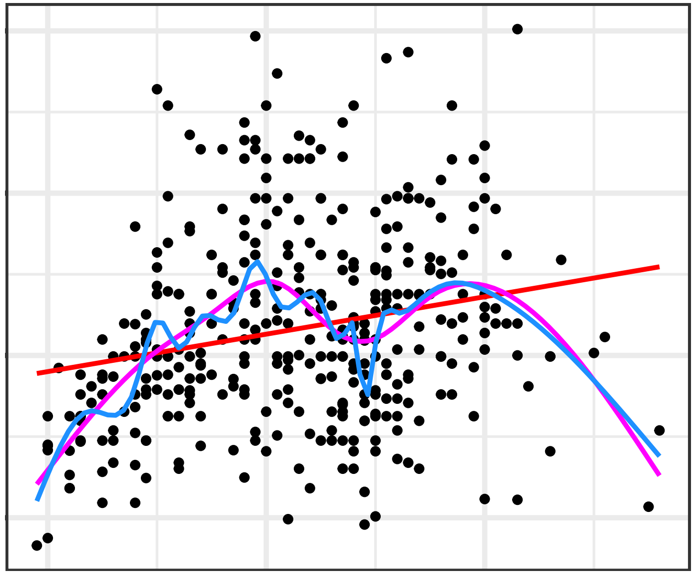
1. Case study: Fitting curves to scatter plots

2. Definition of model complexity



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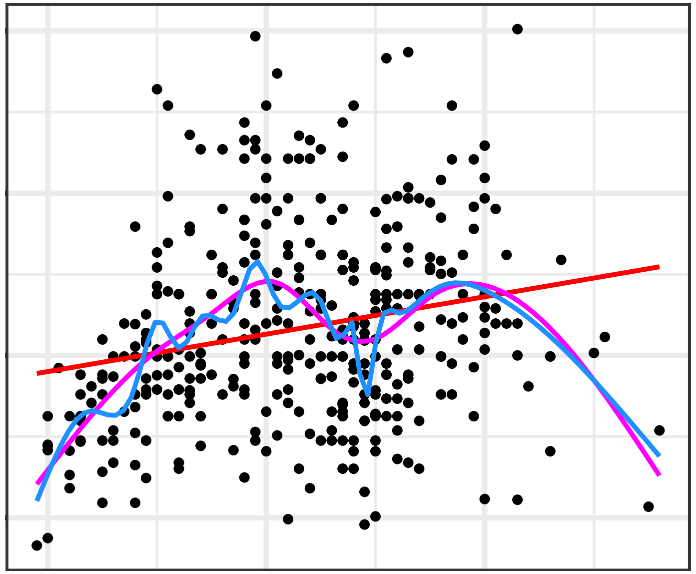
Model complexity:

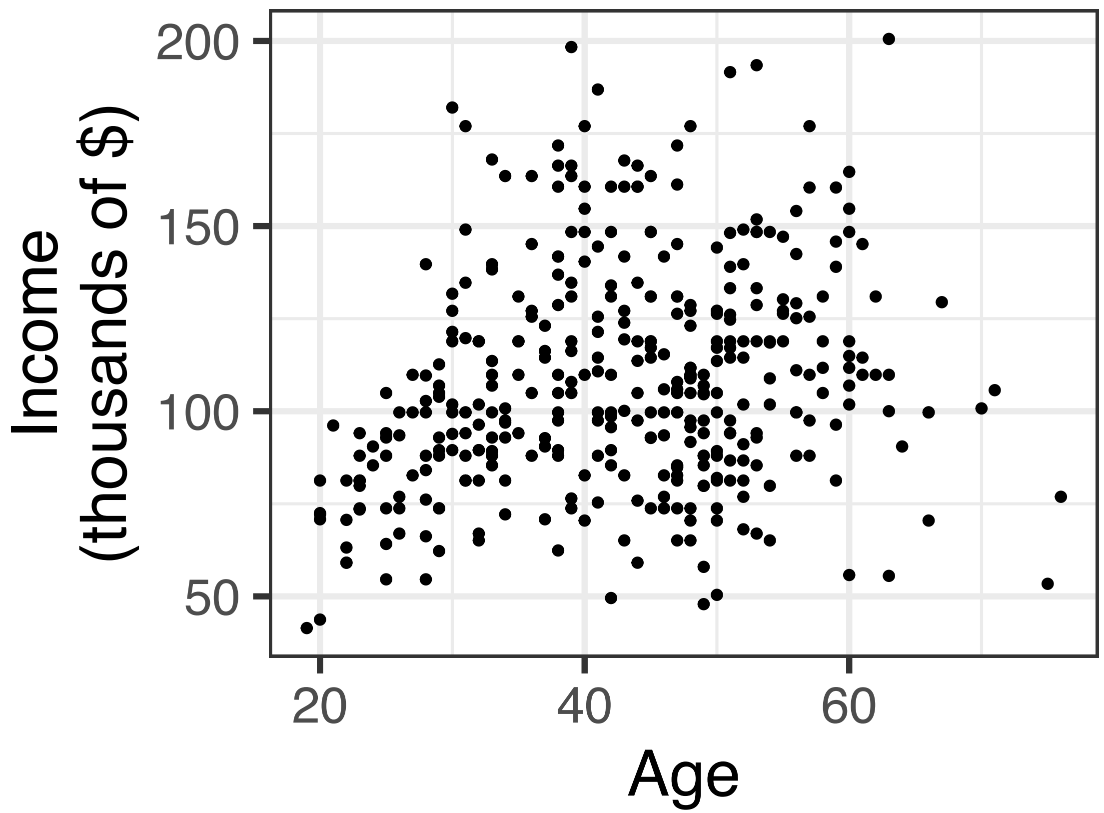
How flexibly a predictive model can fit its training data.

1. Case study: Fitting curves to scatter plots
2. Definition of model complexity
3. How model complexity impacts predictive performance



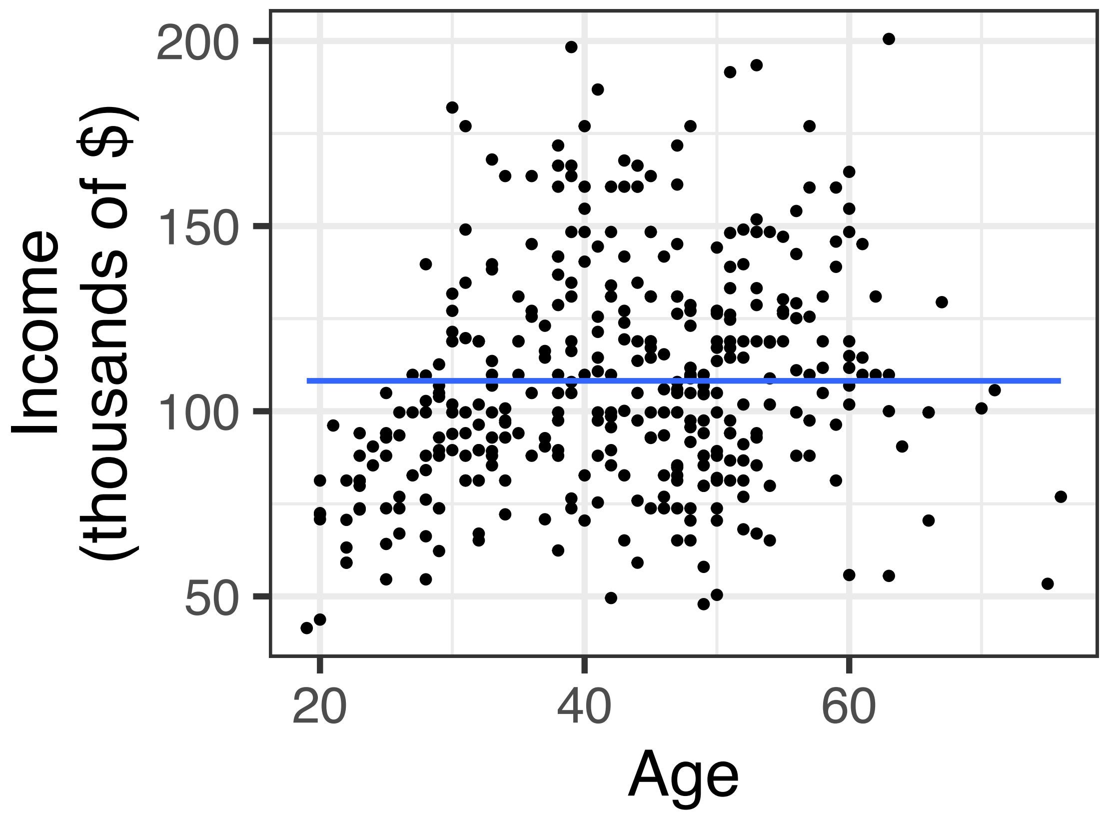
Example: Fit trend of income based on age

What does the trend look like?



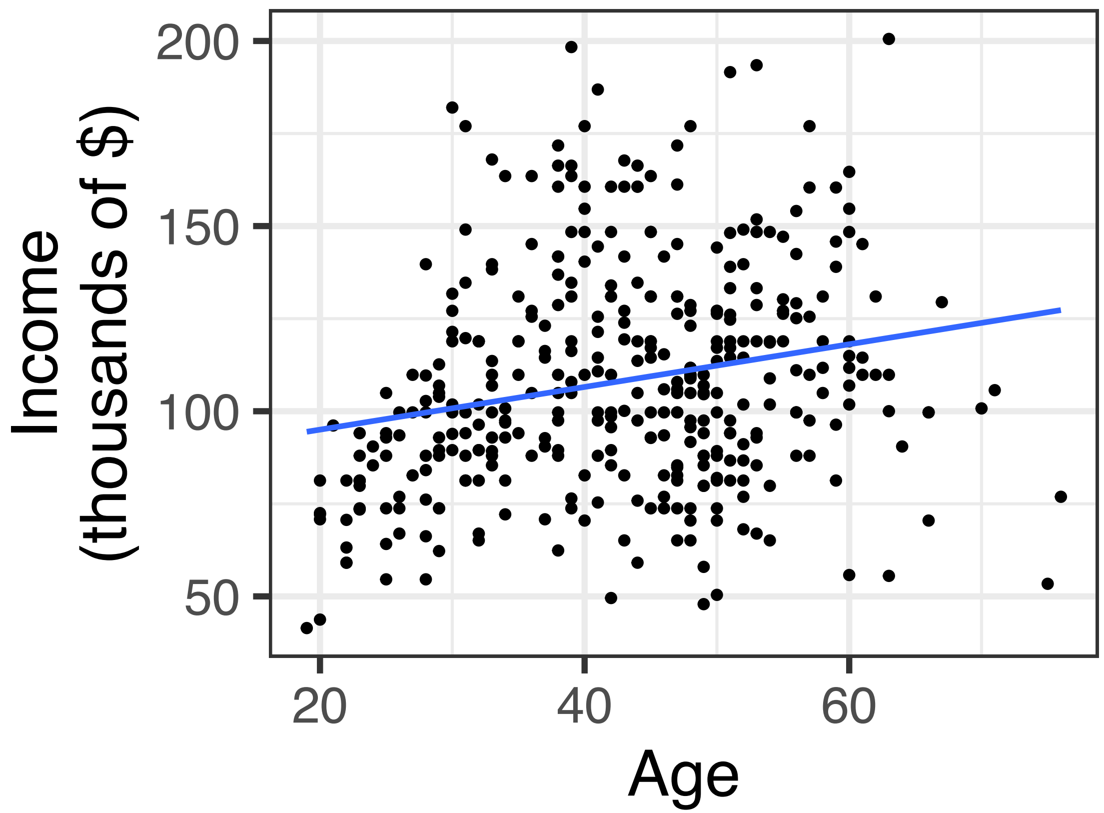
Intercept-only model (no trend)

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



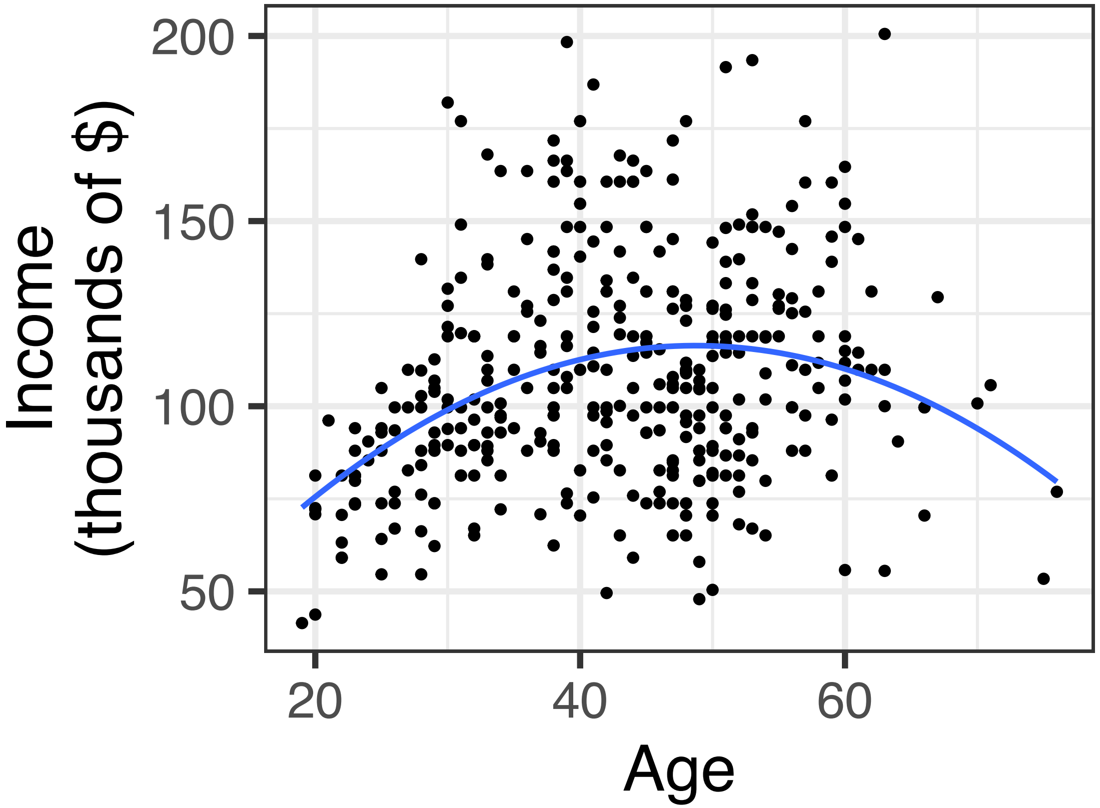
Linear model (linear trend)

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



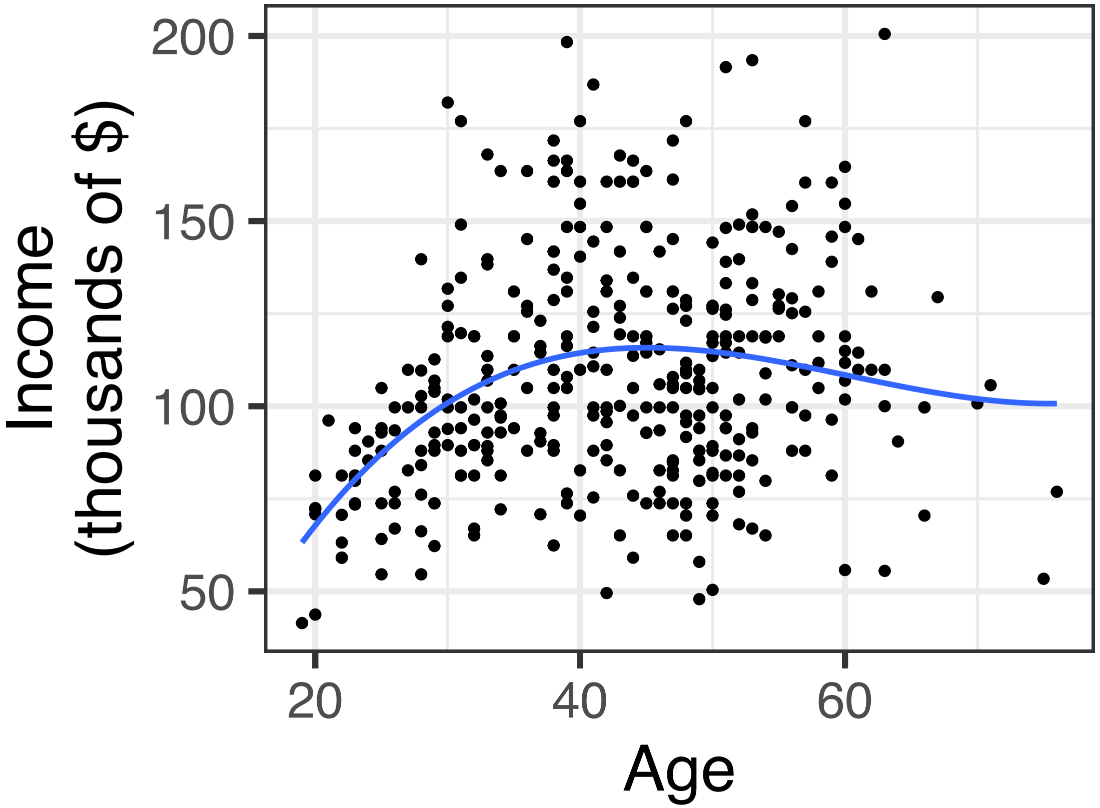
Polynomial model (quadratic trend)

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



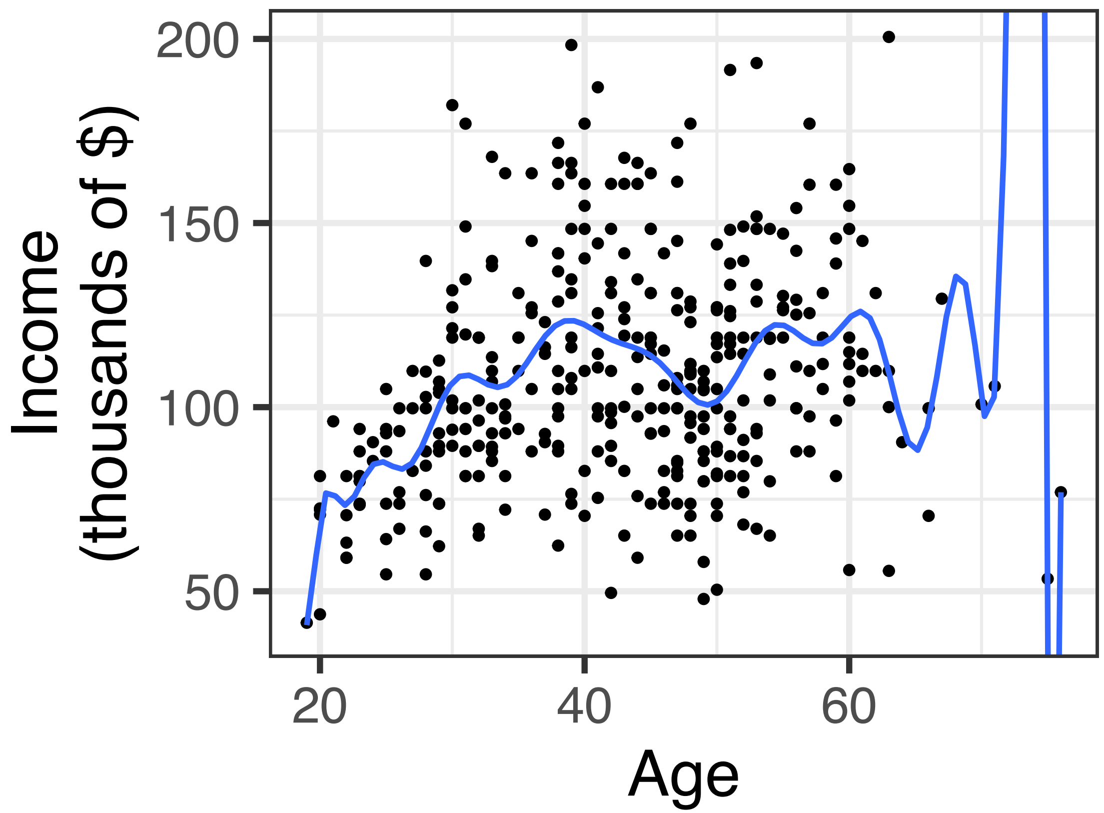
Polynomial model (cubic trend)

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



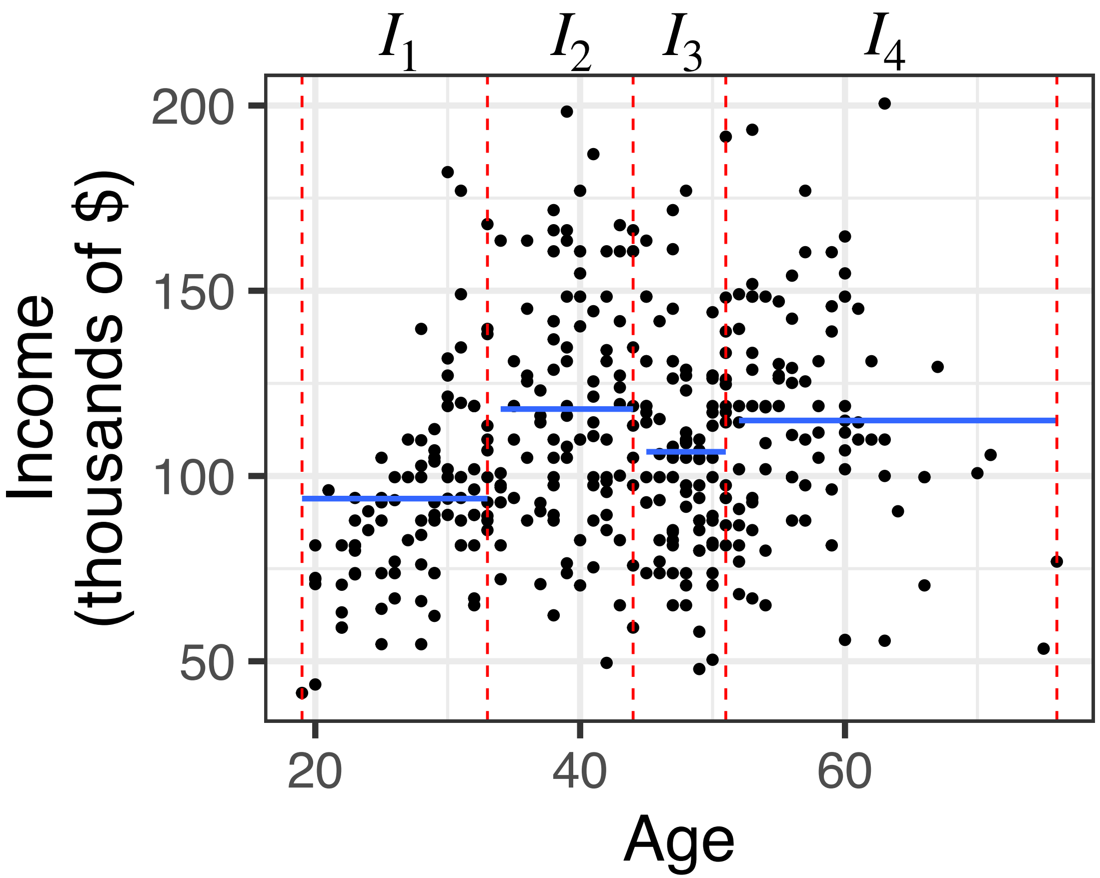
20th degree polynomial model

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



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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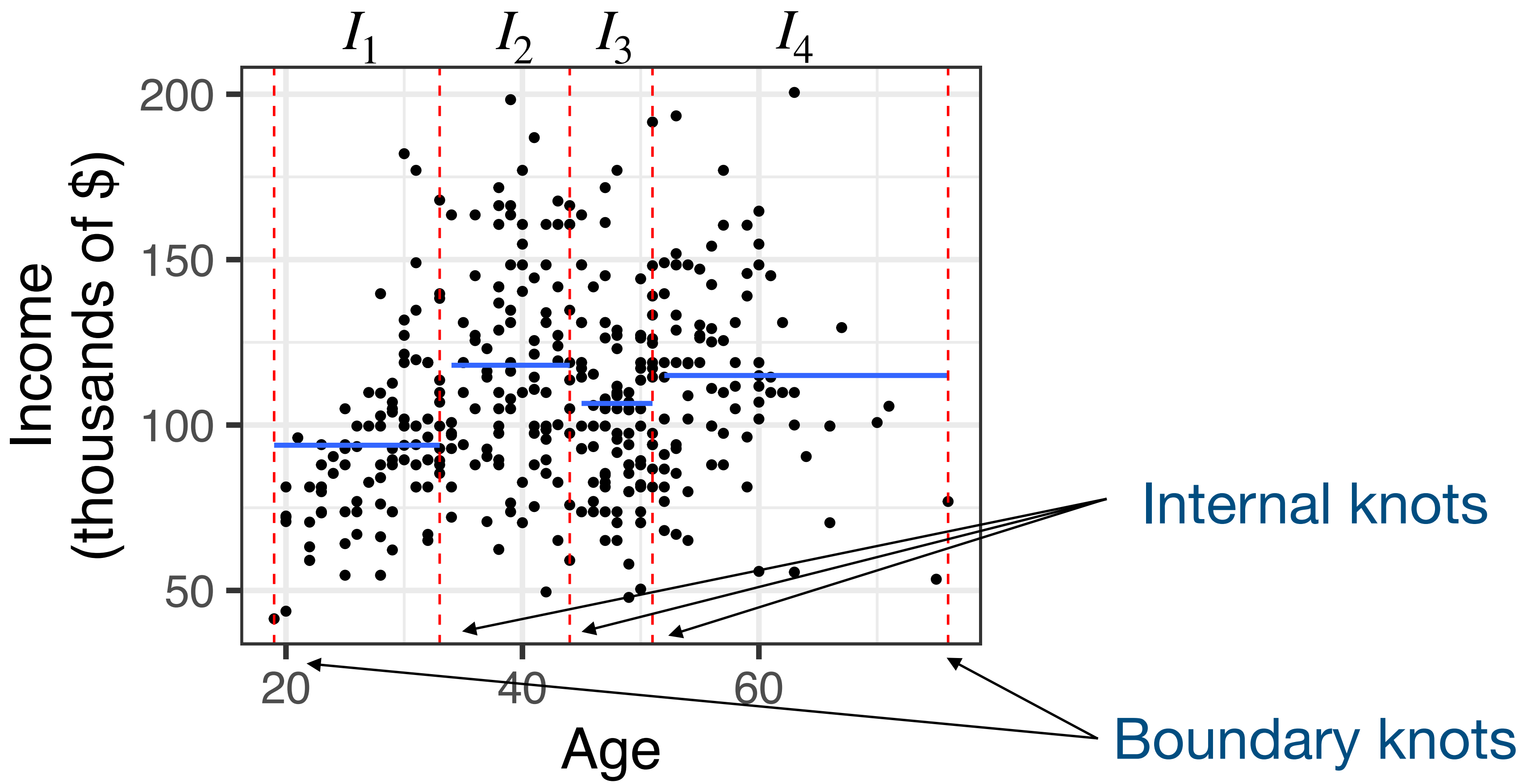
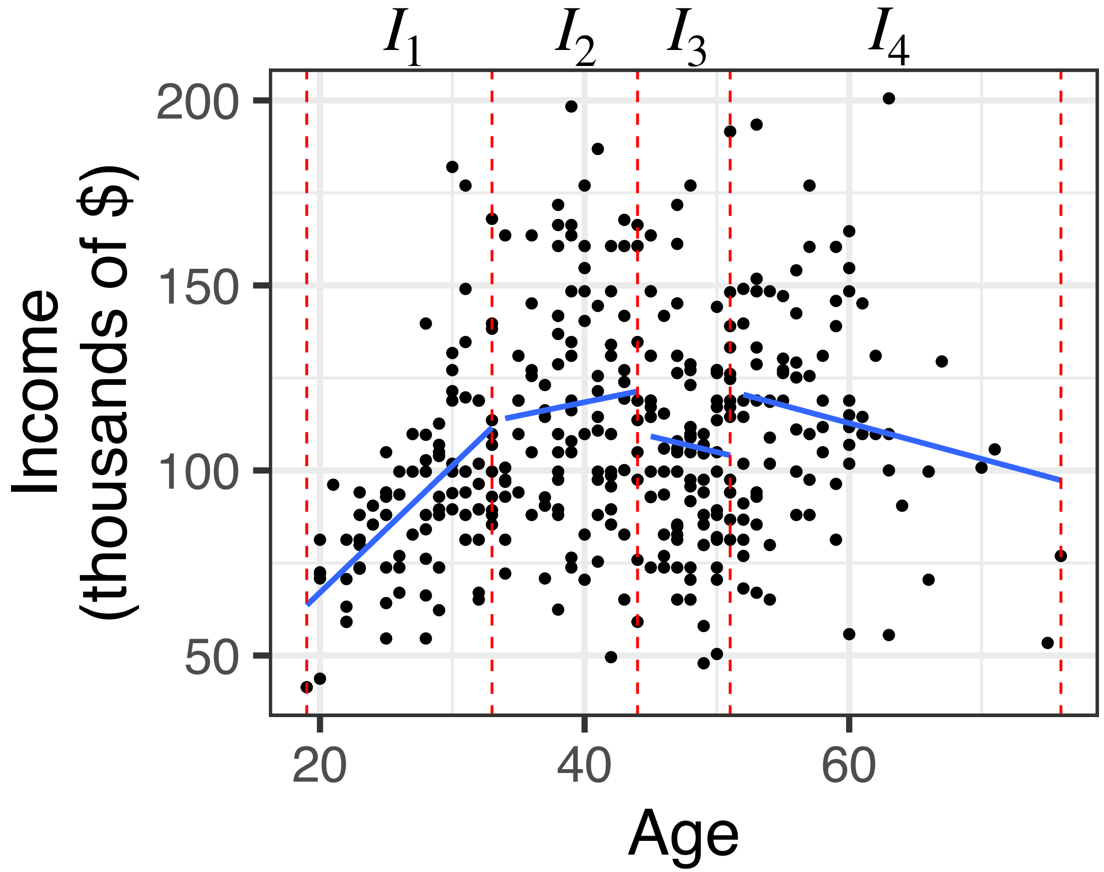


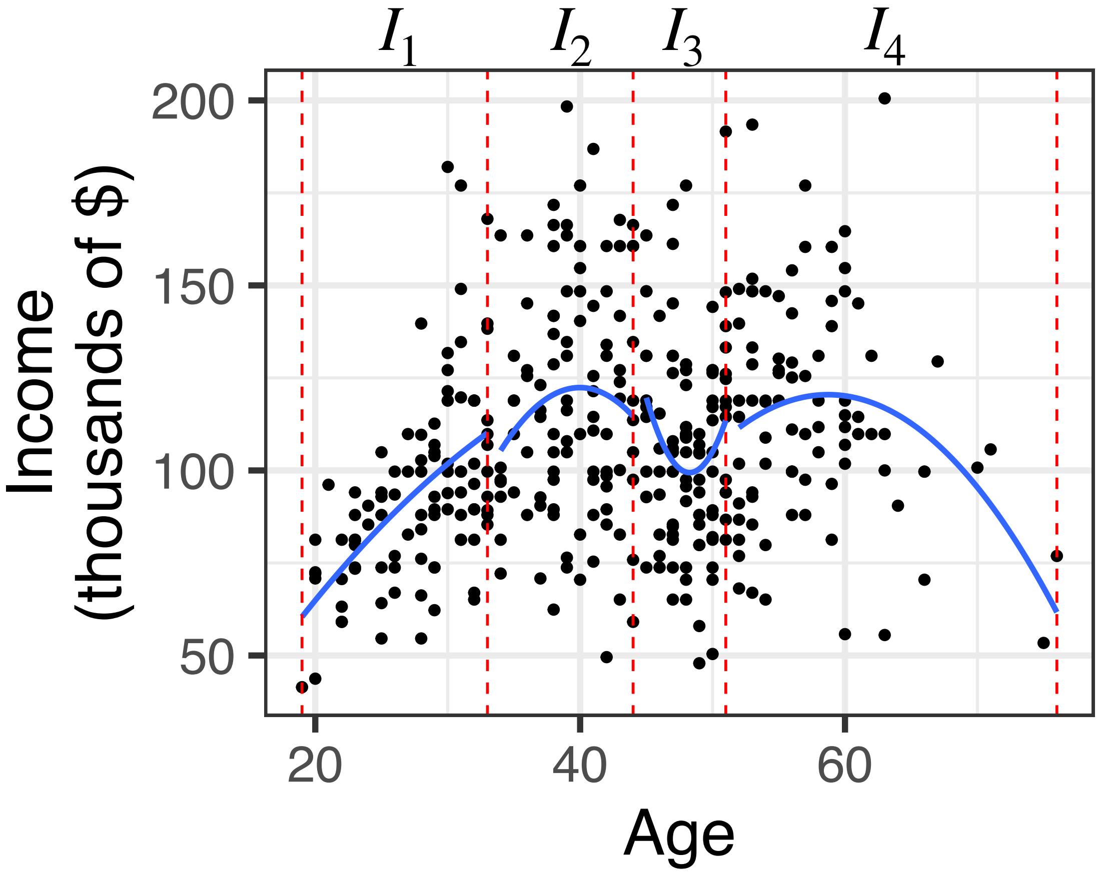
Piece-wise polynomial (piece-wise linear)

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



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)

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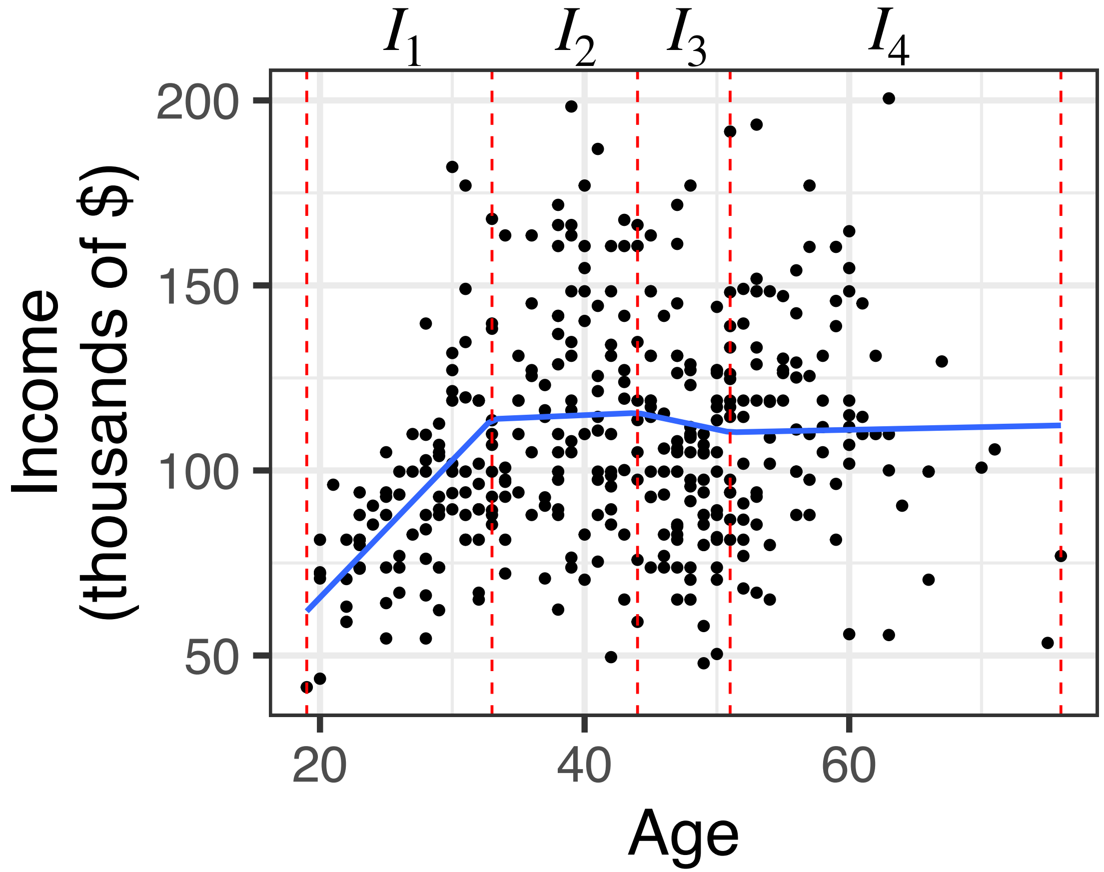

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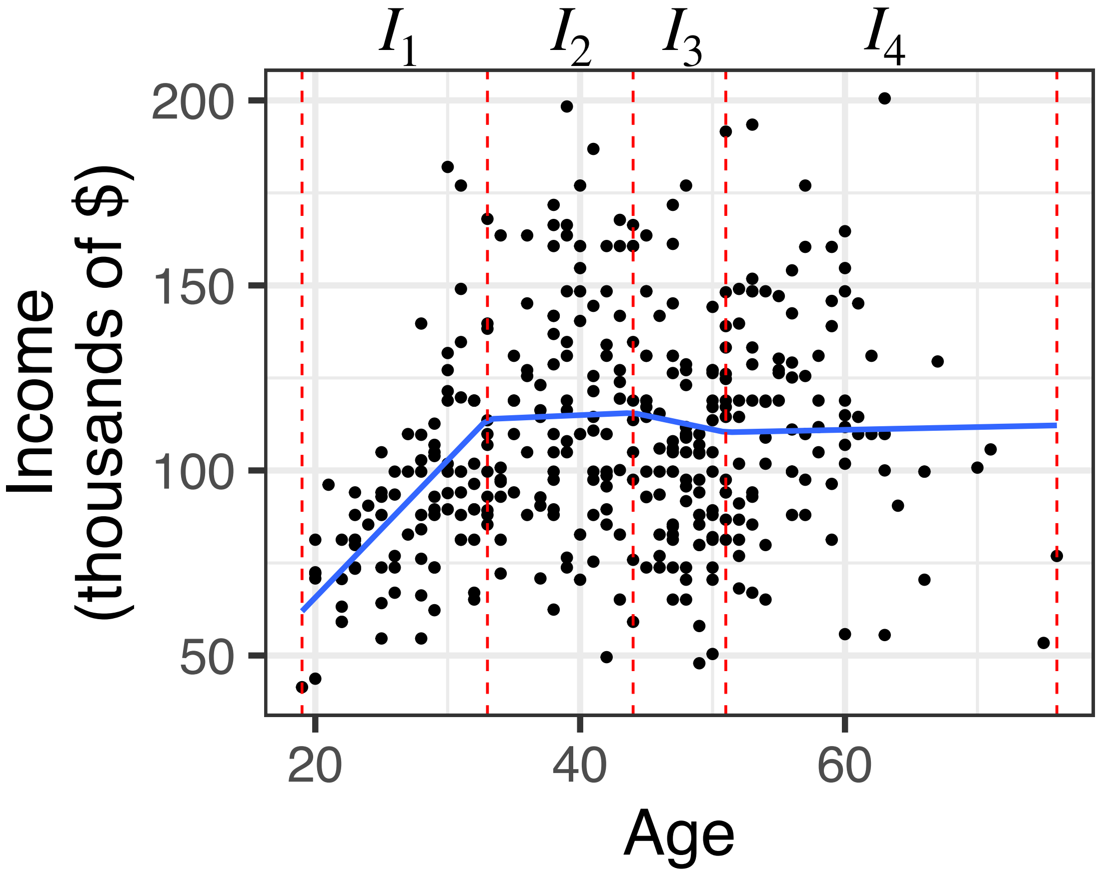

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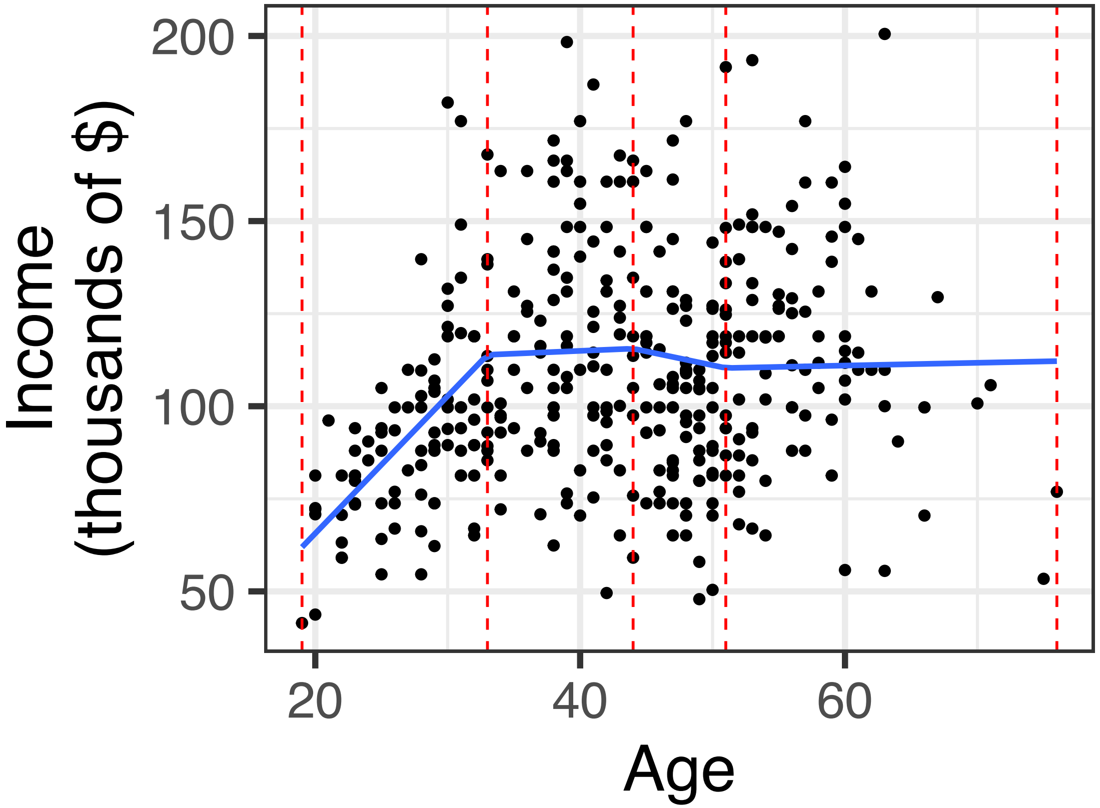

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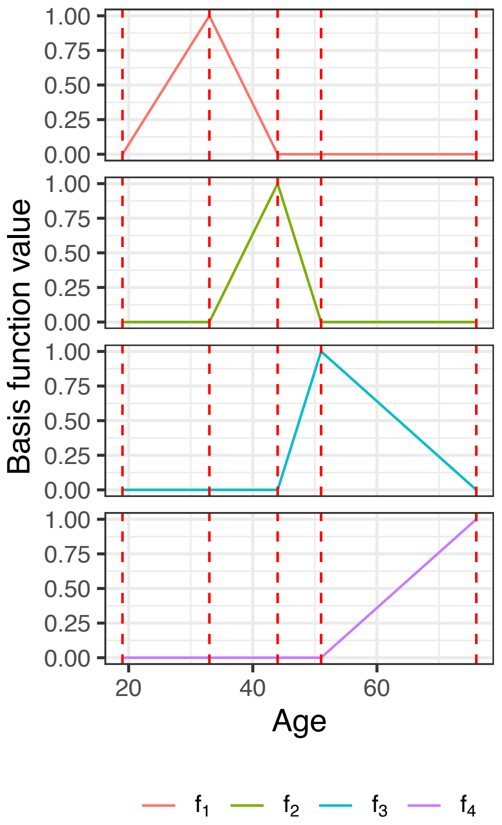
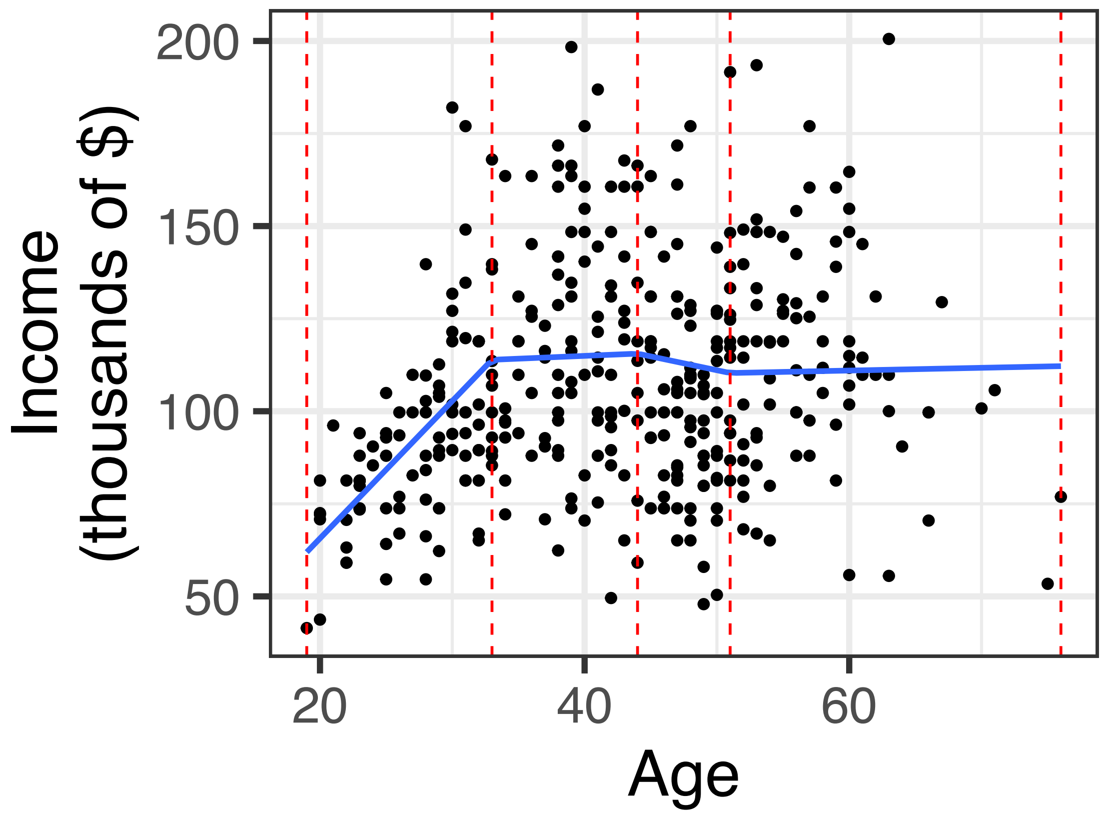
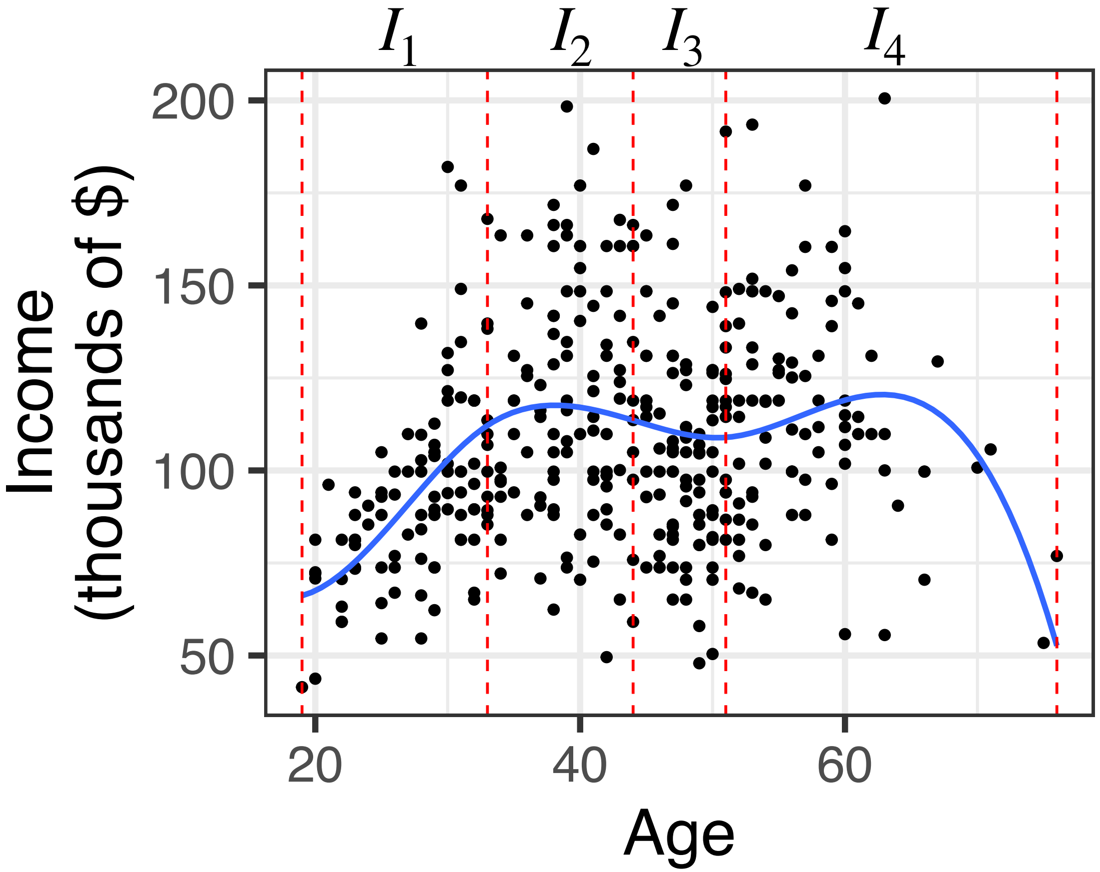




Spline (piece-wise cubic)

$$\text{income} = \beta_0 + \beta_1 \cdot g_1(\text{age}) + \cdots + \beta_{p-1} \cdot g_{p-1}(\text{age}) + \epsilon$$



Natural cubic spline (with 5 total knots)

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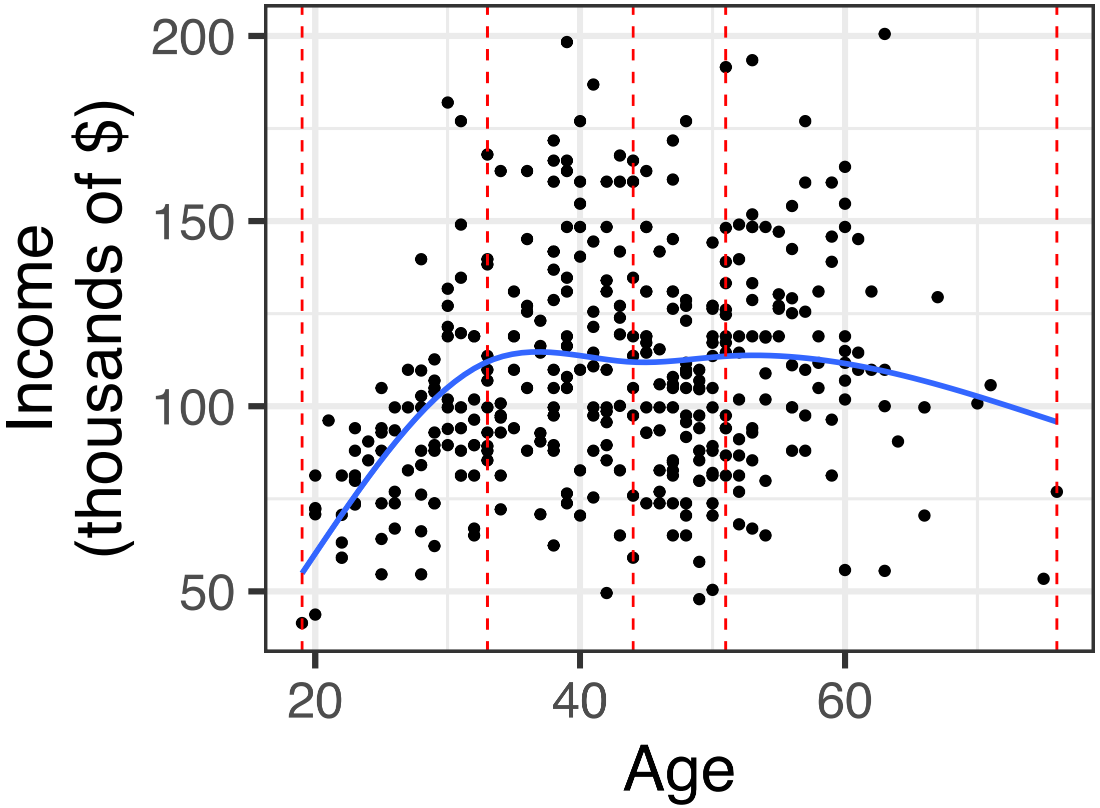

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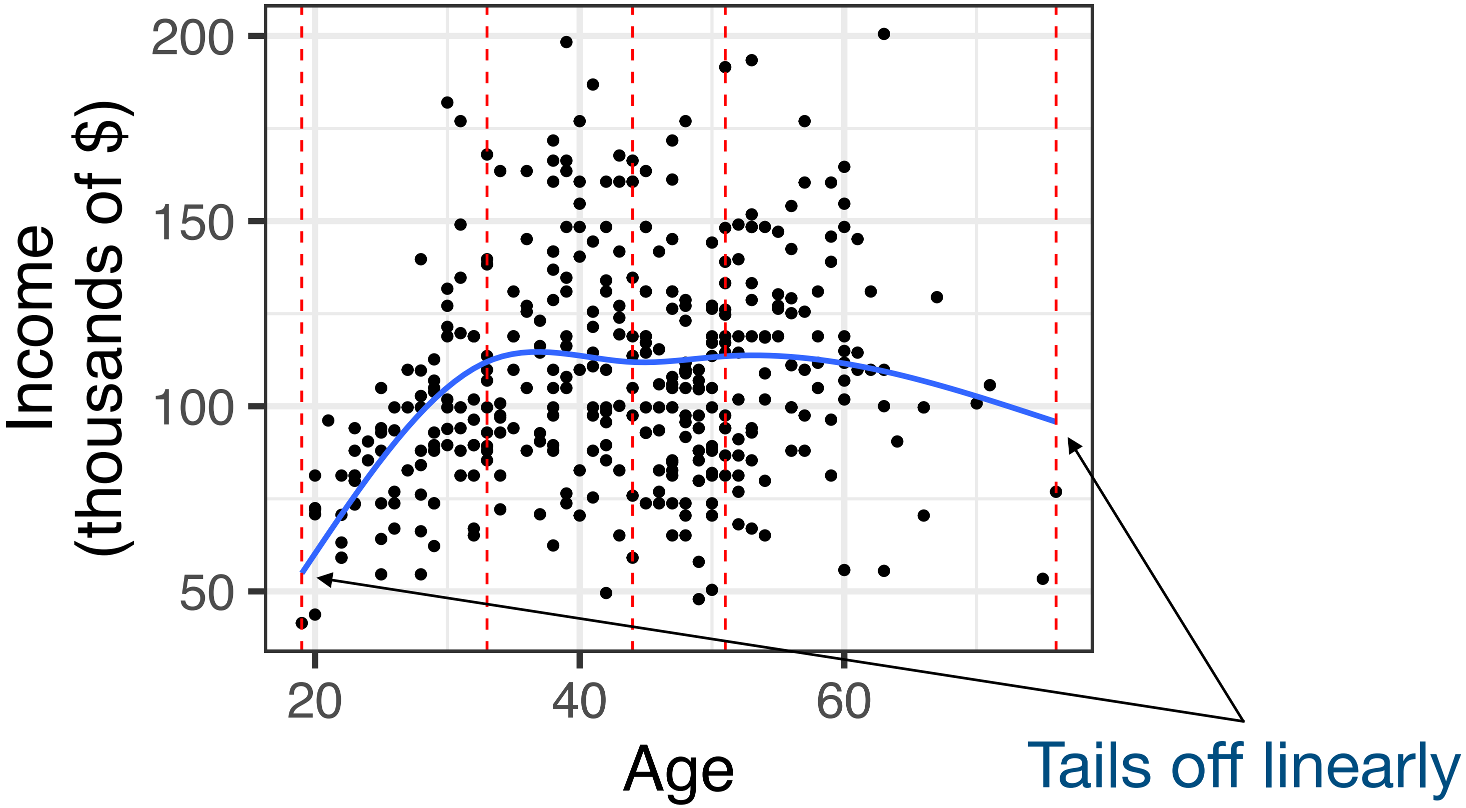

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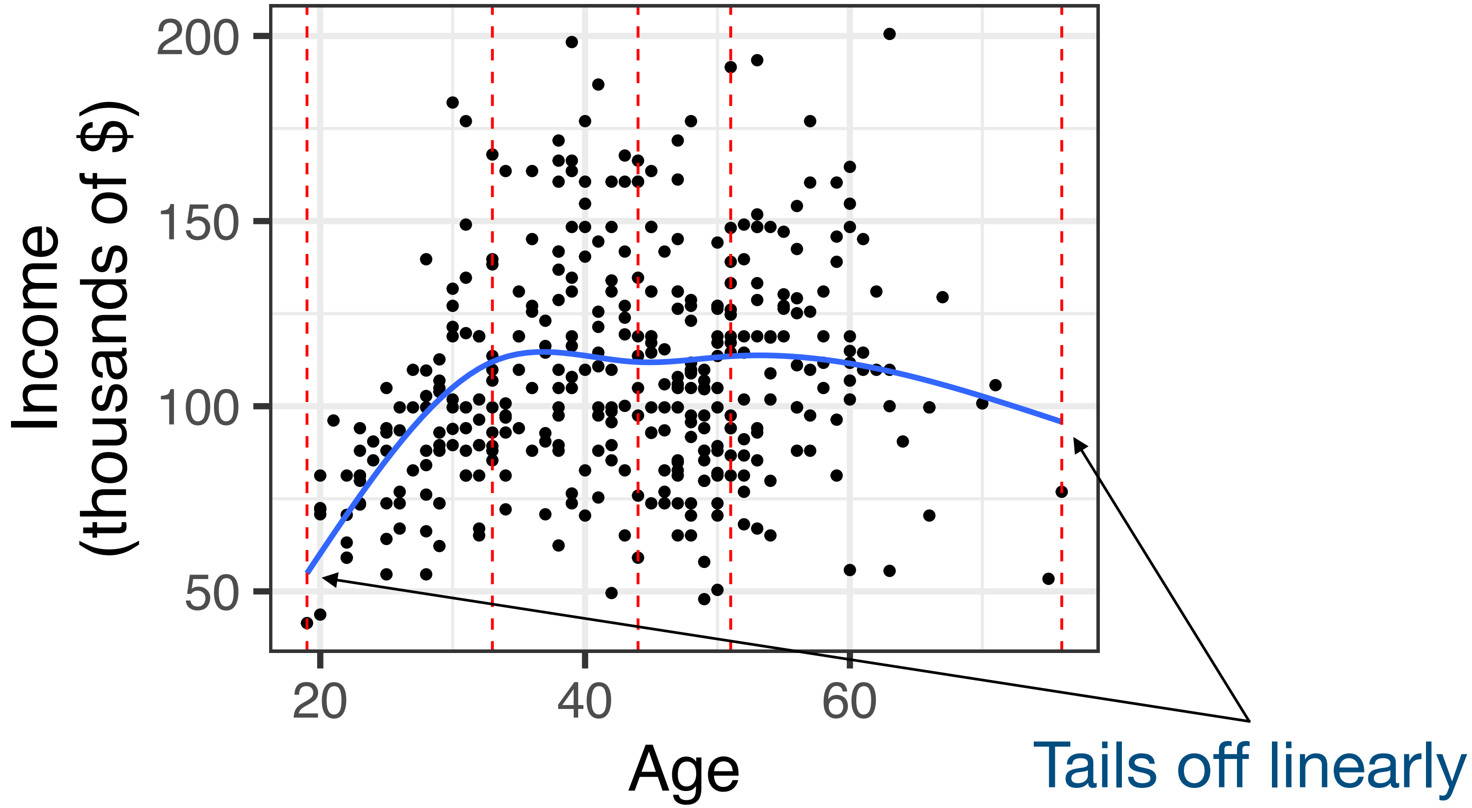
The preferred way to fit smooth curves to data.



Natural cubic spline (with 8 total knots)

$$\text{income} = \beta_0 + \beta_1 \cdot g_1(\text{age}) + \cdots + \beta_{p-1} \cdot g_{p-1}(\text{age}) + \epsilon$$

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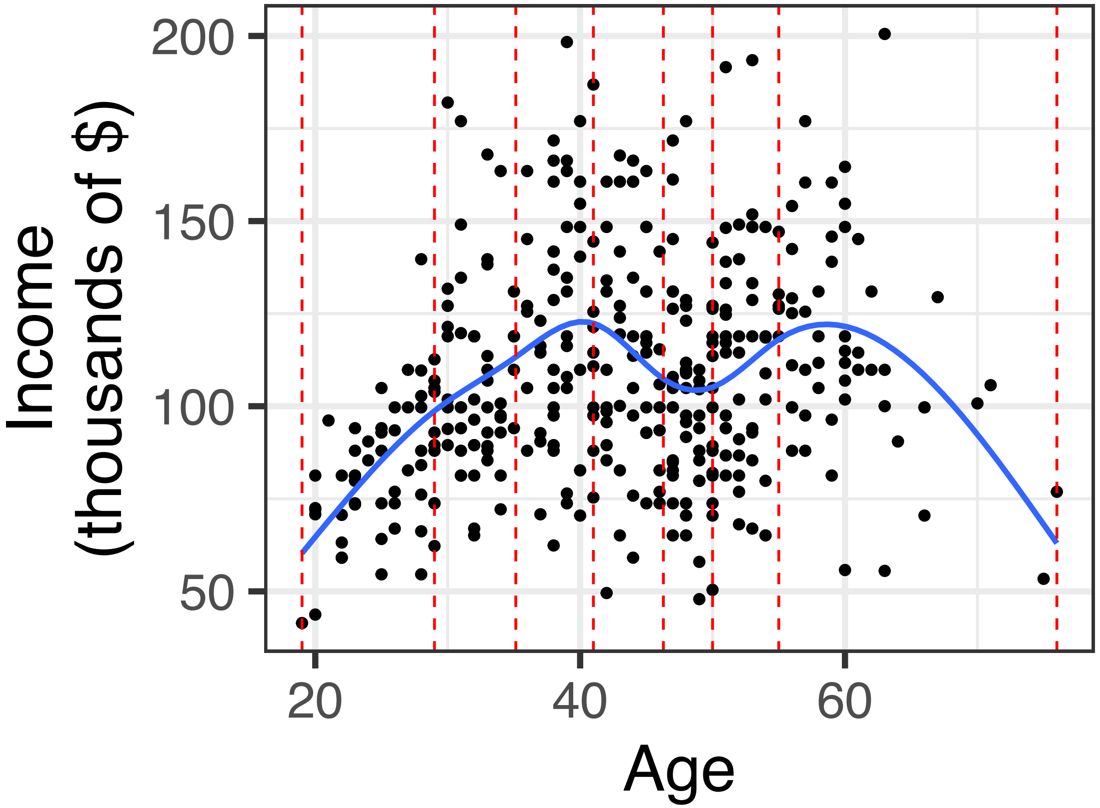

Natural cubic spline (with 20 total knots)

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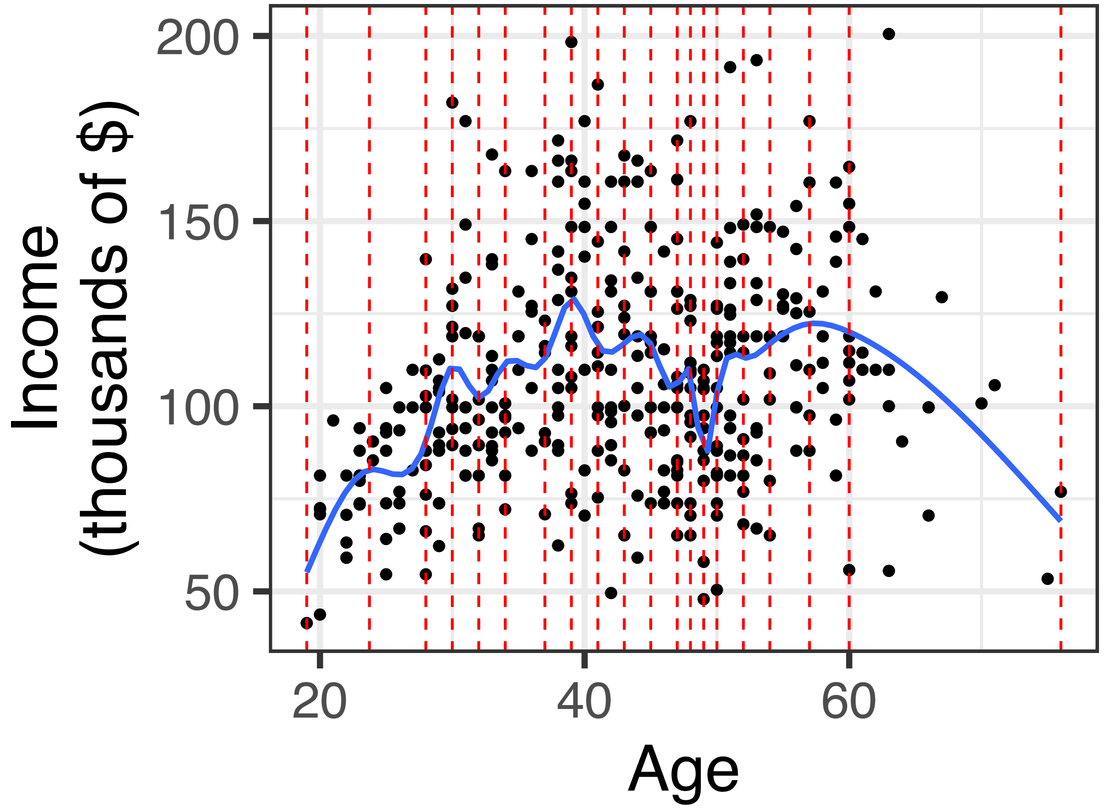

Fitting linear regression models via least squares

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Given training data $(x_1, y_1), \ldots, (x_n, y_n)$, they are fit using least squares:

$$(\widehat{\beta}_0, \ldots, \widehat{\beta}_{p-1}) \equiv \underset{\beta_0, \ldots, \beta_{p-1}}{\arg\min} \sum_{i=1}^{n} (y_i - (\beta_0 + \beta_1 \cdot g_1(x_i) + \cdots + \beta_{p-1} \cdot g_{p-1}(x_i)))^2,$$

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i.e. $(\widehat{\beta}_0, \ldots, \widehat{\beta}_{p-1})$ is the coefficient vector minimizing the the squared distance between the training responses y_i and their predictions.

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For example, the model above has p degrees of freedom.

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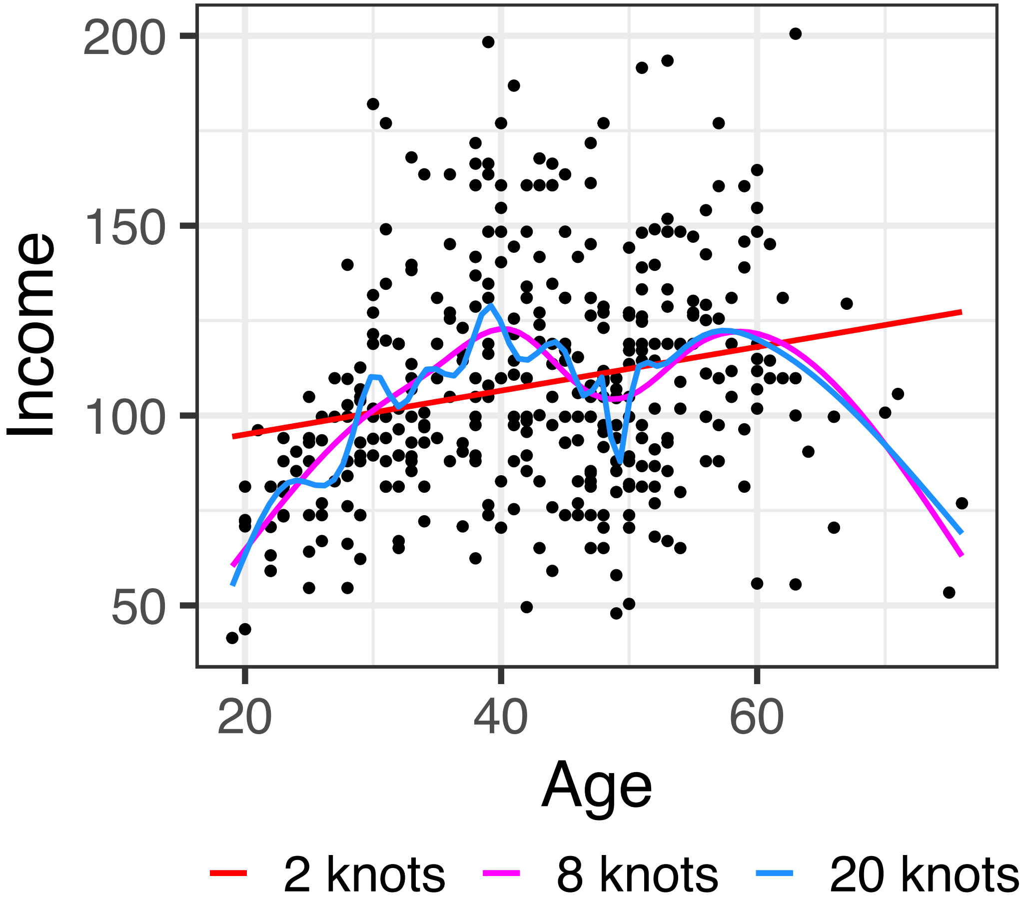

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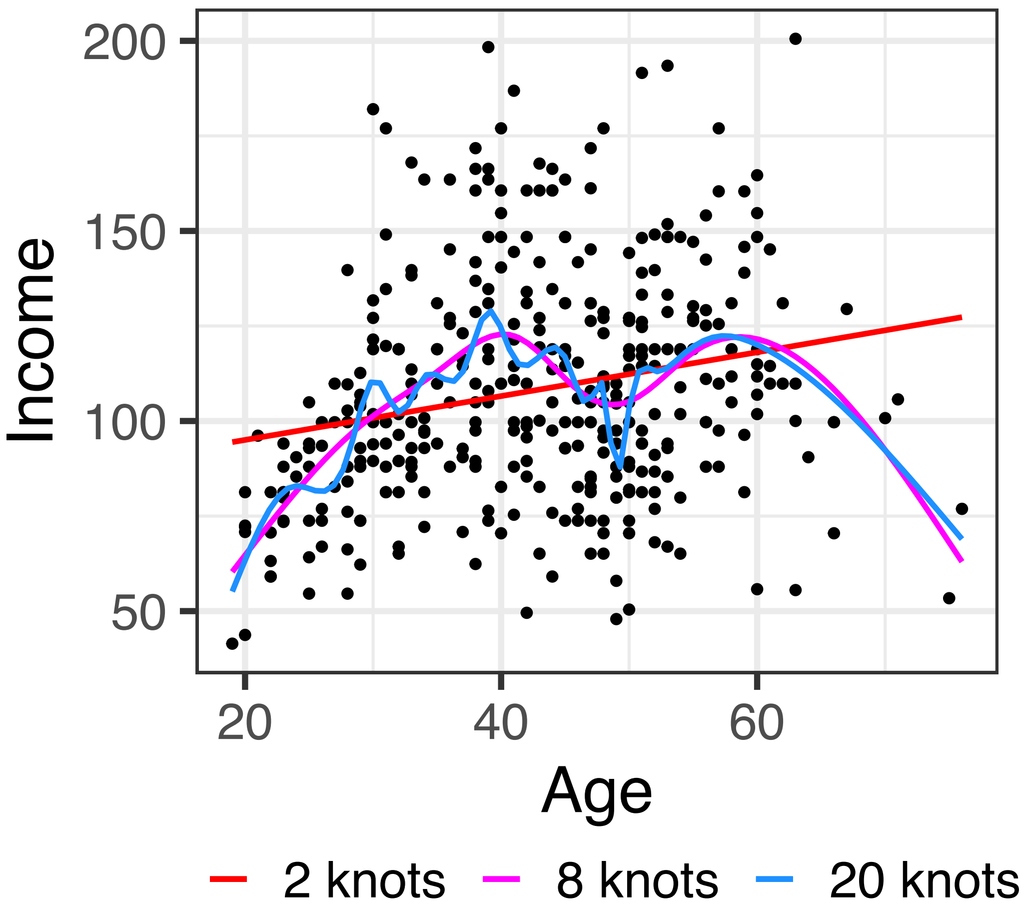

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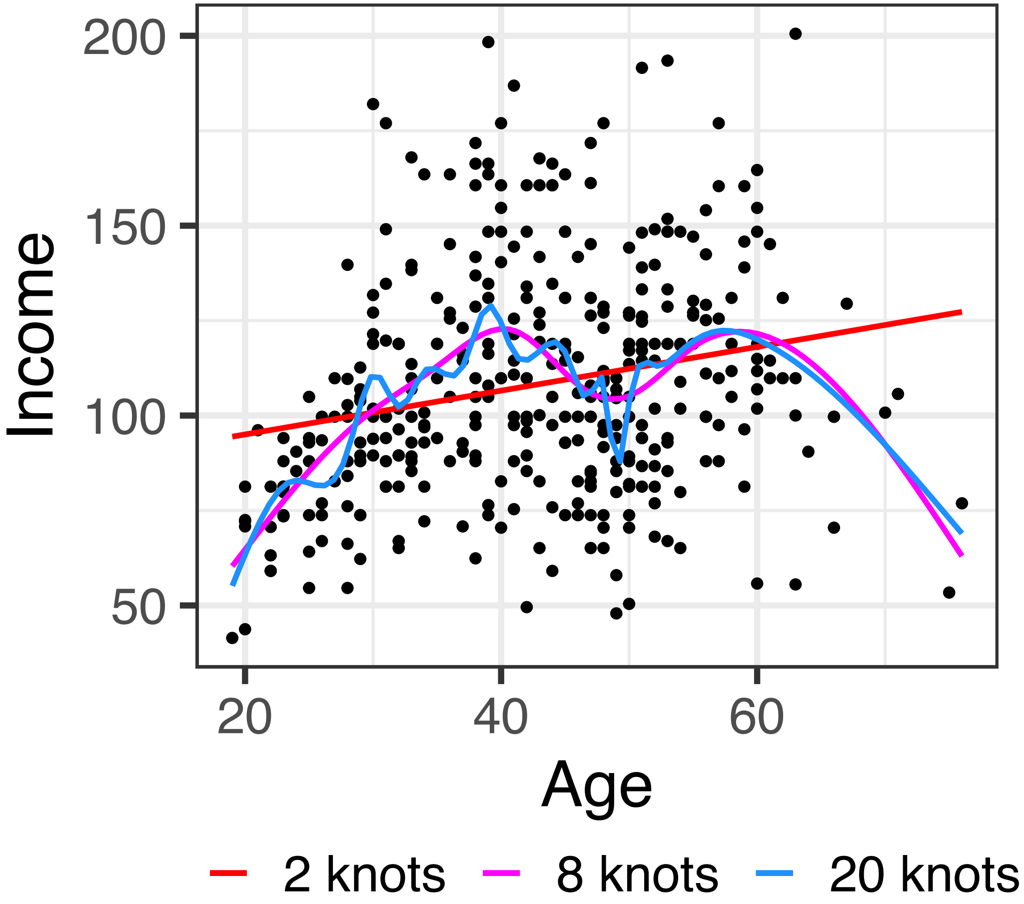

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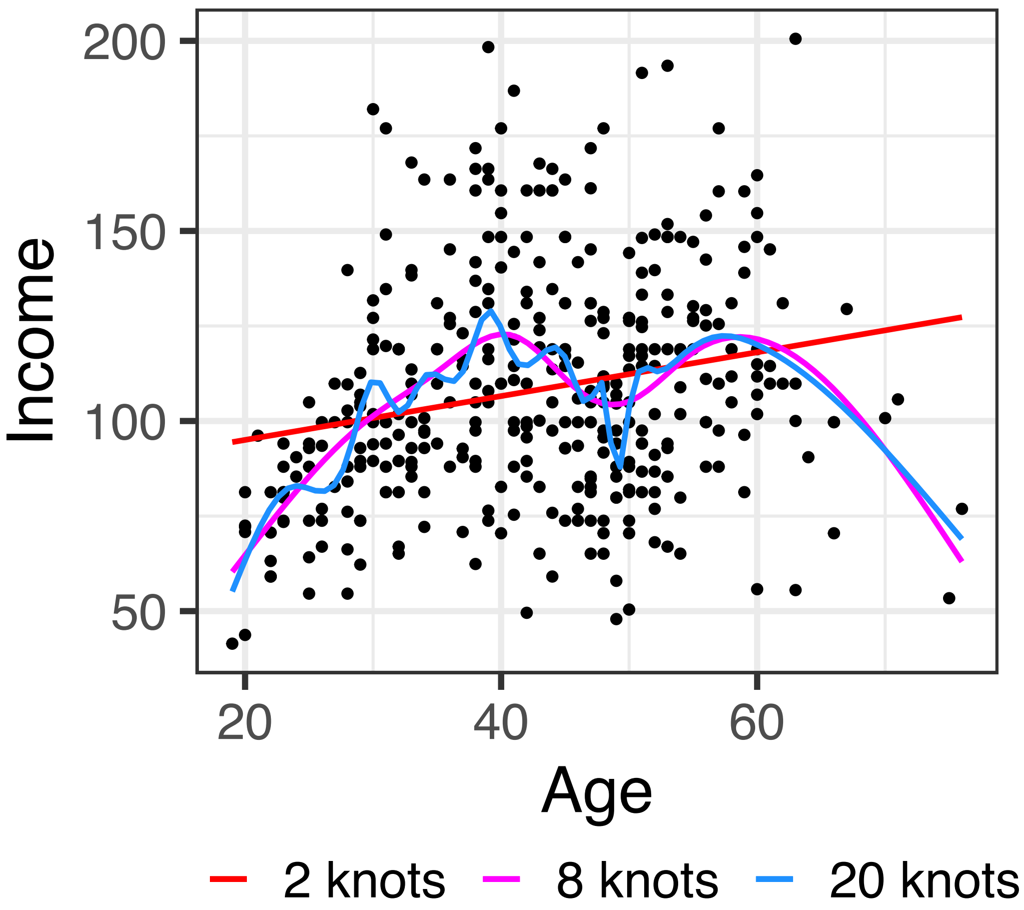

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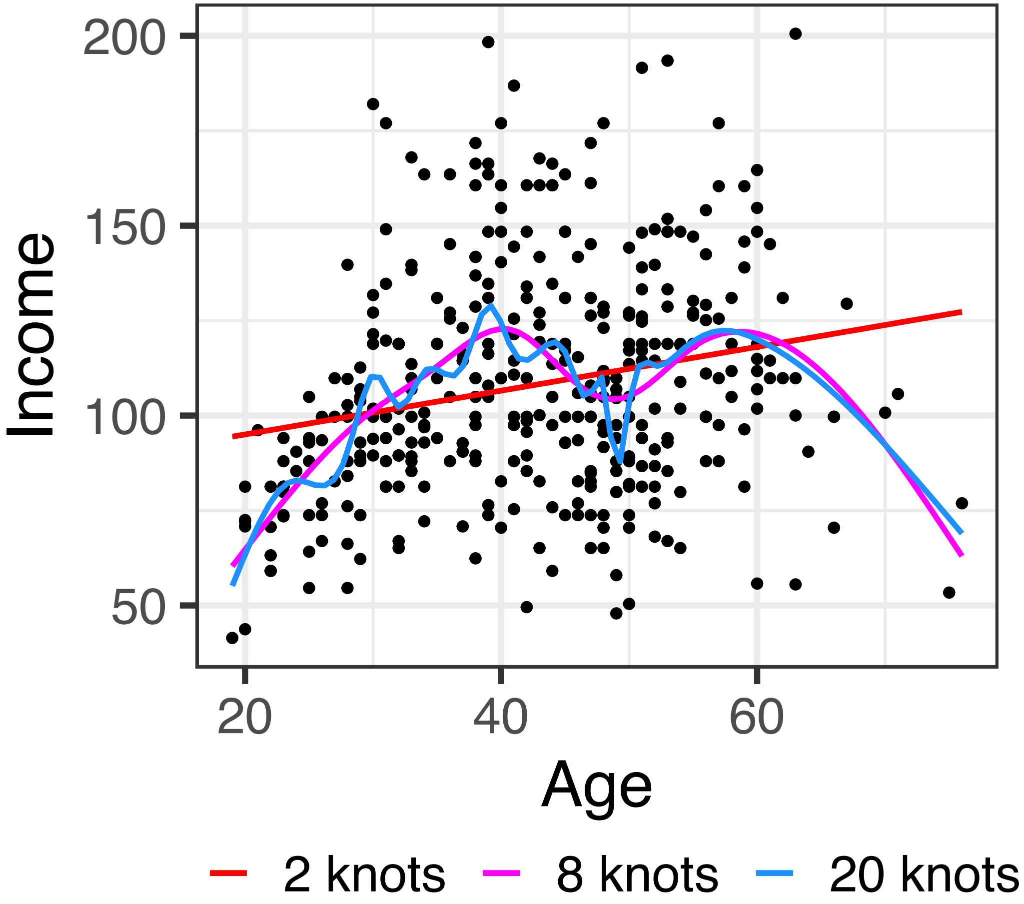
    - Not flexible enough → can't capture the underlying trend



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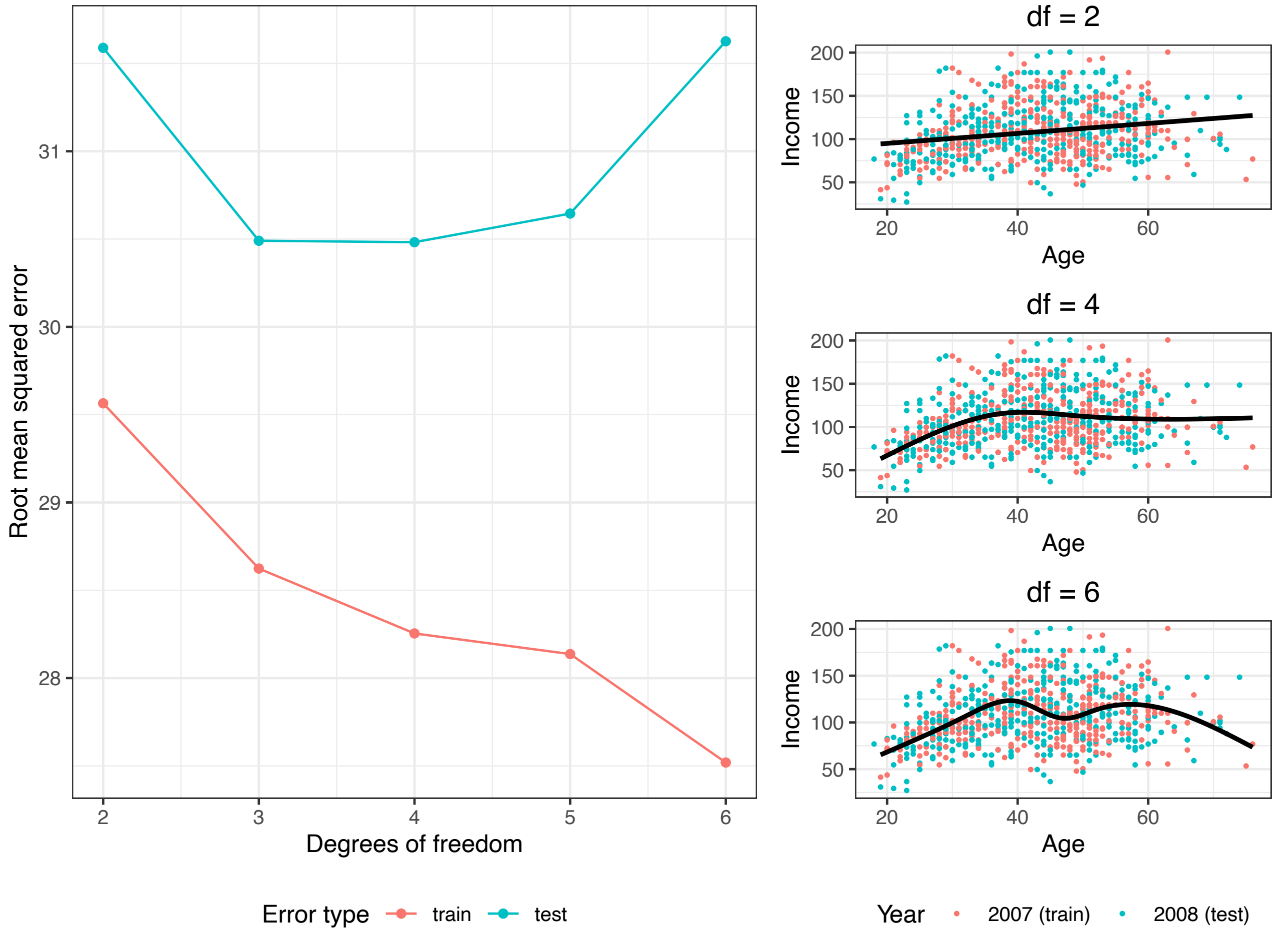
Prediction quality is quantified by test error: extent to which $Y_i^{\text{test}} \approx \hat{Y}_i^{\text{test}}$, e.g.

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

Model complexity impacts prediction performance



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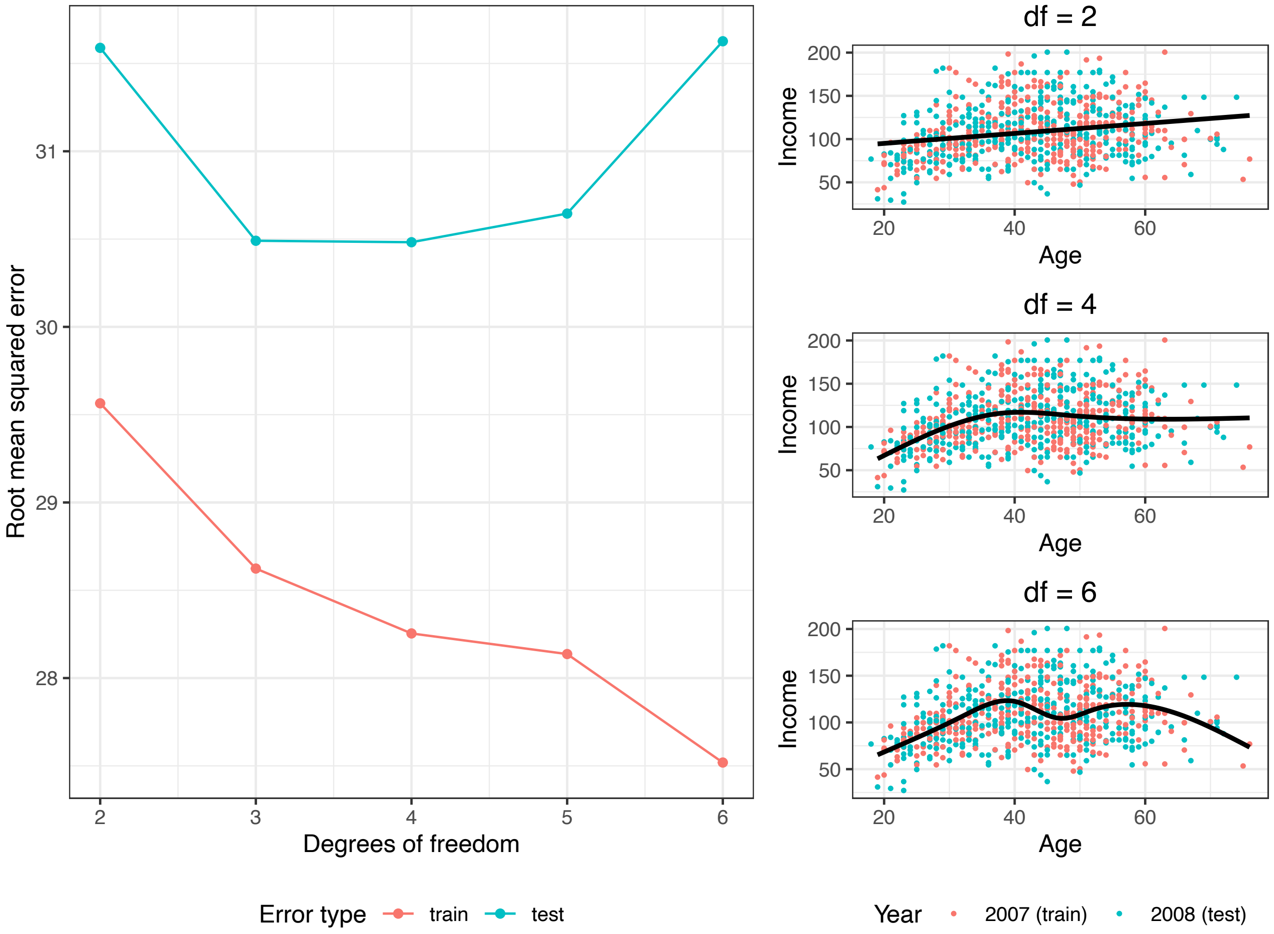

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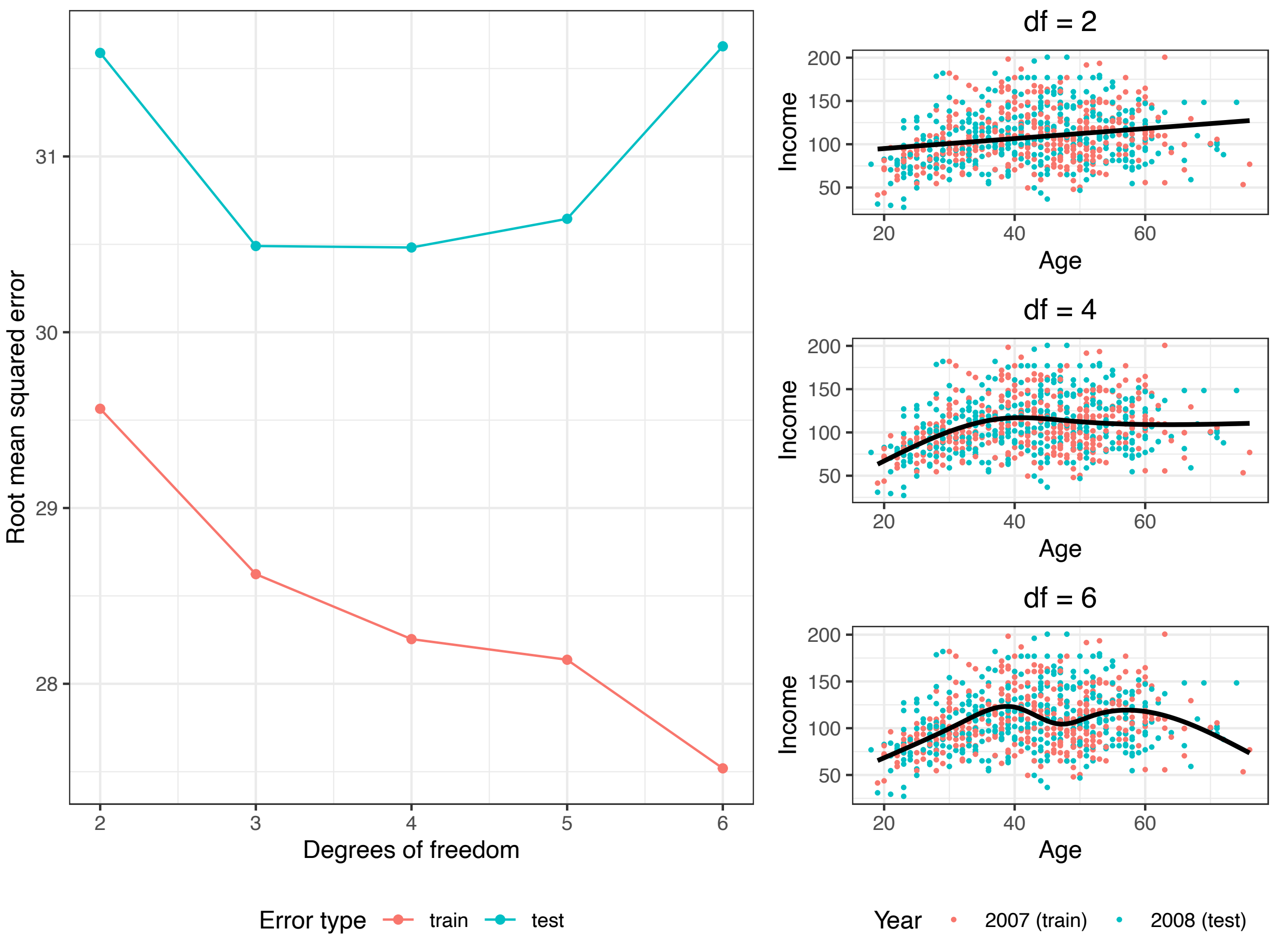

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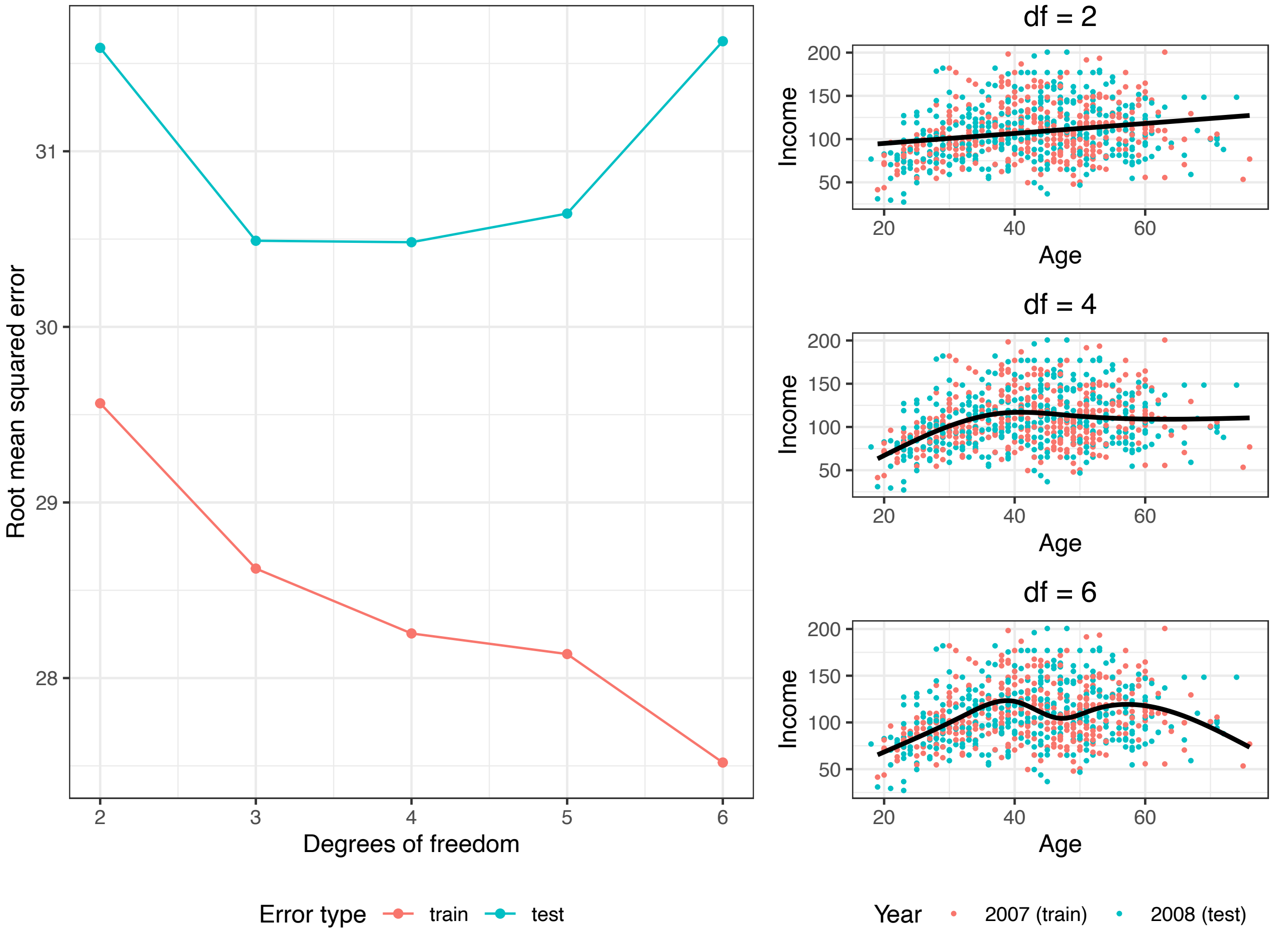

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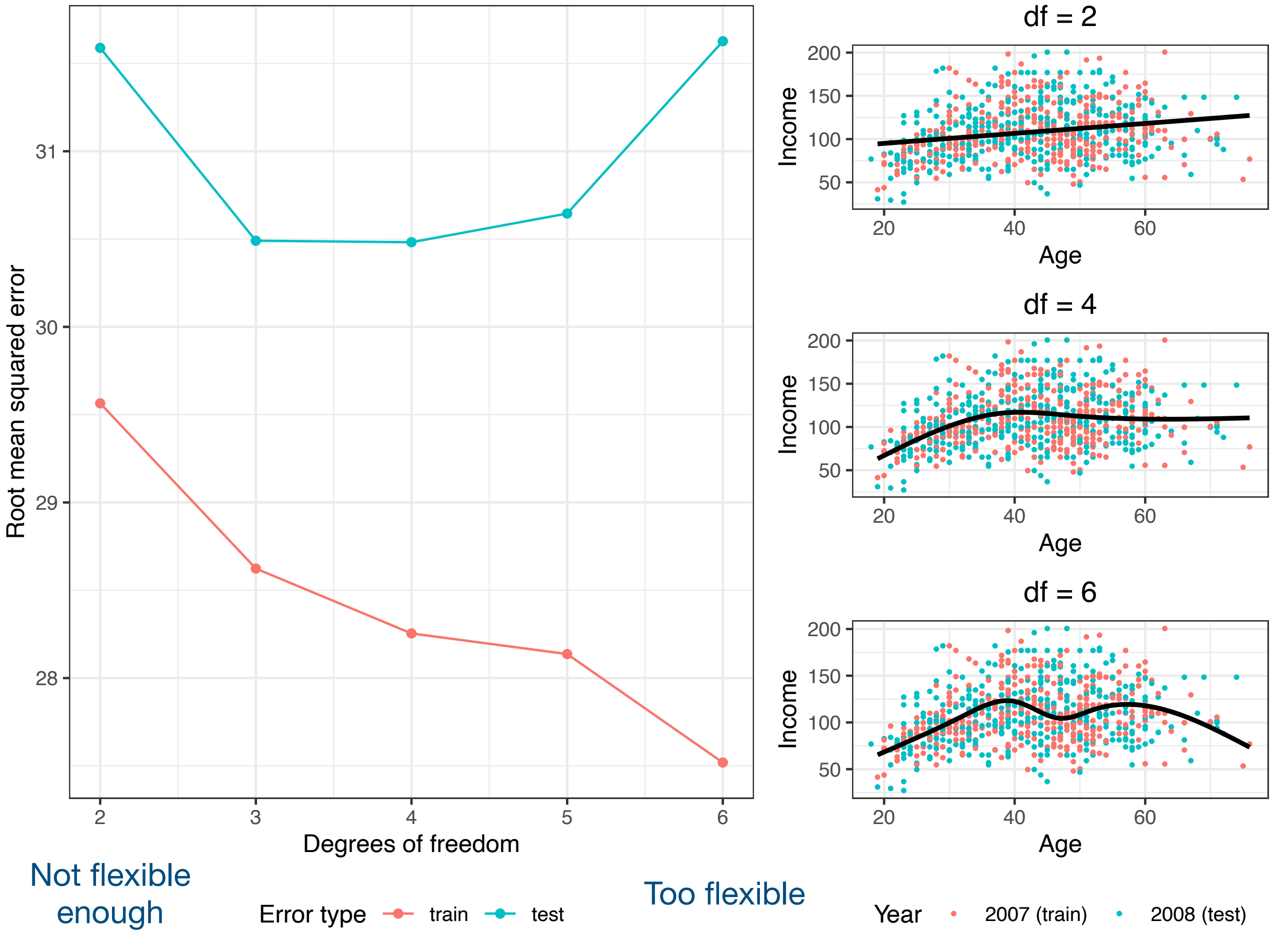

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Model complexity: how closely the model $\hat{f}$ fits the training data:

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

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).