ORF307 – Optimization

4. Least squares data fitting

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Ed Forum

- Why is a Gram matrix symmetric?
- A_ij is the number of views for group i and dollars spent on channel j." Does this mean that each entry in the matrix has two values associated with it? Or are the entries some sort of ratio between the two (i.e. views for group i per dollar spent on channel j)?

Recap

Calculus derivation in vector form

$$f(x) = \|Ax - b\|^2 = (Ax - b)^T(Ax - b) = x^T A^T A x - 2(A^T b)^T x + b^T b$$

$$\nabla f(x^\star) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(x^\star) \\ \vdots \\ \frac{\partial f}{\partial x_n}(x^\star) \end{bmatrix} = 2A^T A x^\star - 2A^T b = 2A^T(Ax^\star - b) = 0$$

$n \times n$
square
linear system → **normal equations**

$$(A^T A)x^\star = A^T b$$

Solving normal equations

$$(A^T A)x^\star = A^T b$$

Inversion

$$x^\star = (A^T A)^{-1} A^T b$$

→

Pseudo-inverse

$$A^\dagger = (A^T A)^{-1} A^T$$

Factor-solve method

A has linearly independent columns

↓

$A^T A$ is **symmetric positive-definite**

→

Cholesky factorization

$$A^T A = LL^T$$

Optimal advertising

m demographic groups we want to advertise to → v^{des} is the m-vector of desired views/impressions

n advertising channels (web publishers, radio, print, etc.) → s is the n-vector of purchases

$m \times n$ matrix A gives demographic reach of channels → A_{ij} is the number of views for group i and dollar spent on channel j $(1000/\$)$

Views across demographic groups

$$v = As$$

Goal

$$\text{minimize} \quad \|As - v^{\text{des}}\|^2$$

Optimal advertising

Reusing factorization on large example

$m = 100,000$ groups, $n = 5,000$ channels

minimize $\quad \|As - v^{\text{des}}\|^2$

Pseudoinverse

Time: 263 sec

First solve

desired views $v^{\text{des},1} = (10^3)\mathbf{1}$

1. Form linear system $Mx = q$ where $M = A^T A, q = A^T b$
2. Factor $M = LL^T$
3. Solve $LL^T x = q$

Complexity

$2mn^2$

Time: 9 sec

Second solve

desired views $v^{\text{des},2} = 500\mathbf{1}$

1. Form $q = A^T b$
2. Solve $LL^T x = q$

Complexity

$2mn$

Time: 0.37 sec

Today’s lecture

Least squares data fitting

- Least squares model fitting
- Univariate regression
- Multivariate regression
- Validation
- Example

Least squares model fitting

Setup

We believe a scalar y and a n-vector are related by a model

$$y \approx f(x)$$

- x is the *independent variable* or *feature vector*
- y is the *outcome* or *response variable*
- $f : \mathbf{R}^n \to \mathbf{R}$ maps x to y

We don't know f and we want to estimate it from data

Data

All we have is data

n-vectors $x^{(1)}, \ldots, x^{(N)}$, and scalars $y^{(1)}, \ldots, y^{(N)}$

also called *observations, examples, samples* or *measurements*.

$(x^{(i)}, y^{(i)})$ is the ith data pair

$x_j^{(i)}$ is the jth component of ith data point $x^{(i)}$

Model

Guess a model $\hat{f} : \mathbf{R}^n \to \mathbf{R}$ to approximate f

$$\hat{f}(x) = \theta_1 f_1(x) + \cdots + \theta_p f_p(x)$$

- $f_i : \mathbf{R}^n \to \mathbf{R}$ are *feature mappings* or *basis functions*
- θ_i are *model parameters* to choose
- $\hat{y}^{(i)} = \hat{f}(x^{(i)})$ is the model's *prediction* for $y^{(i)}$
- Goal: $\hat{y}^{(i)} \approx y^{(i)}$ (consistent with observed data)

Least squares data fitting

Prediction error (residual) $r^{(i)} = y^{(i)} - \hat{y}^{(i)}$

Goal: choose model parameters θ_i to minimize mean squared error (MSE)

$$\frac{(r^{(1)})^2 + \cdots + (r^{(N)})^2}{N}$$

↓

This can be formulated as a least squares problem

Note. we sometimes compute the root mean squared error RMS = $\sqrt{\text{MSE}}$ because it has the same units as $y^{(i)}$

Least squares data fitting

Vector form

Express problems with N-vectors

- $y^{\rm d} = (y^{(1)}, \dots, y^{(N)})$, vector of outcomes
- $\hat{y}^{\rm d} = (\hat{y}^{(1)}, \dots, \hat{y}^{(N)})$, vector of predictions
- $r^{\rm d} = (r^{(1)}, \dots, r^{(N)})$, vector of residuals

$\longrightarrow$

Goal

minimize $\quad \|r^{\rm d}\|^2$

We can write $\hat{y}^{(i)} = \hat{f}(x^{(i)})$ in terms of parameters θ_i

$$\hat{y}^{(i)} = A_{i1}\theta_1 + \cdots + A_{ip}\theta_p, \qquad A_{ij} = f_j(x^{(i)}) \qquad \longrightarrow \qquad \hat{y}^{\rm d} = A\theta$$

Least squares problem

minimize $\quad \|r^{\rm d}\|^2 = \|y^{\rm d} - \hat{y}^{\rm d}\|^2 = \|y^{\rm d} - A\theta\|^2 = \|A\theta - y^{\rm d}\|^2$

Solution

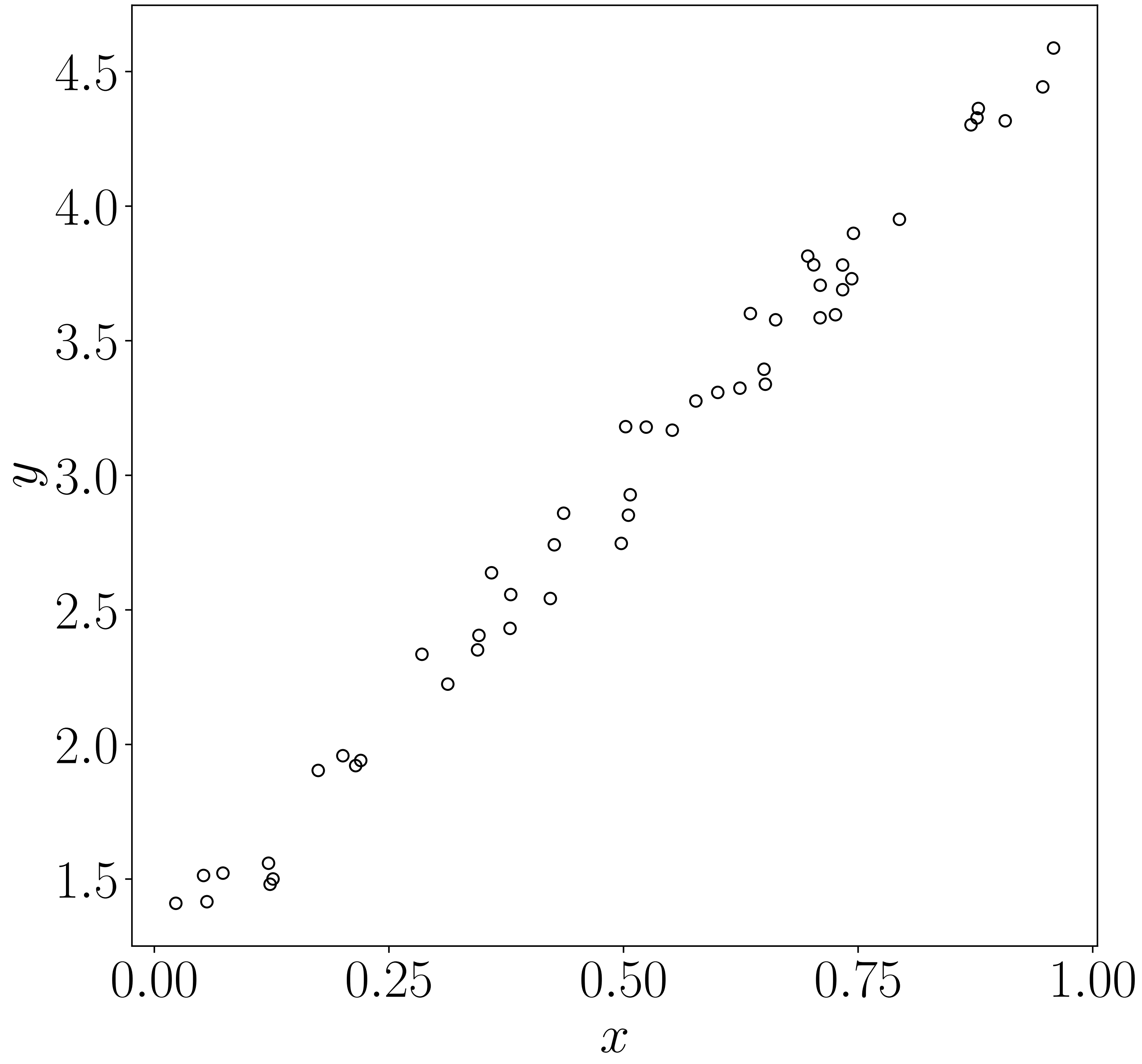
$$(A^T A)\theta^\star = A^T y^{\rm d}$$

Univariate fitting

Fitting univariate functions

We seek to approximate a function $f : \mathbf{R} \to \mathbf{R}$ $\qquad (n = 1)$

Data points $(x^{(i)}, y^{(i)})$



Straight line fit

Model

$$\hat{f}(x) = \theta_1 + \theta_2 x$$

- Parameters: $\theta = (\theta_1, \theta_2) \qquad (p = 2)$
- Features: $f_1(x) = 1,\ f_2(x) = x$

Least squares data

$$A = \begin{bmatrix} 1 & x^{(1)} \\ 1 & x^{(2)} \\ \vdots & \vdots \\ 1 & x^N \end{bmatrix} = \begin{bmatrix} \mathbf{1} & x^{\mathrm{d}} \end{bmatrix}$$

Goal

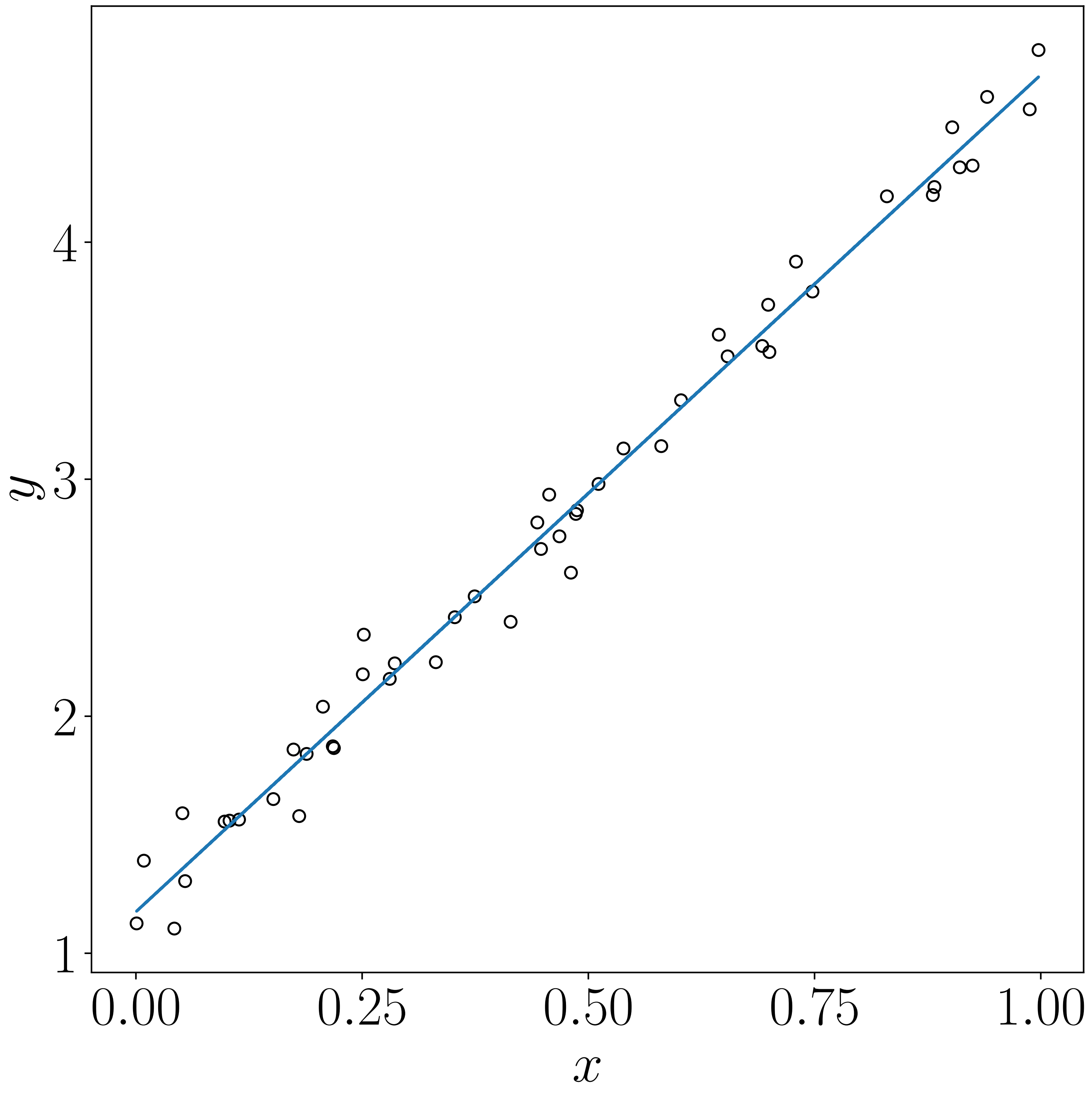
$$\text{minimize} \quad \|r^{\mathrm{d}}\|^2 = \|A\theta - y^{\mathrm{d}}\|^2$$

Straight line fit

Example

$$\theta^\star = (1.75, 3.53)$$

$$\hat{f}(x) = \theta_1 + \theta_2 x$$



Asset α and β in finance

whole market returns

$$x^{\mathrm{d}} = (r_1^{\mathrm{mkt}}, \ldots, r_T^{\mathrm{mkt}})$$

r_t^{mkt} is the return of the *whole market* at time t

individual asset returns

$$y^{\mathrm{d}} = (r_1^{\mathrm{ind}}, \ldots, r_T^{\mathrm{ind}})$$

r_t^{ind} is the return of an *individual asset* at time t

→ **Goal**
predict individual asset return from whole market return

Linear model

$$\hat{y} = (r^{\mathrm{rf}} + \alpha) + \beta(x - \mu^{\mathrm{mkt}})$$

asset α
average asset return above r^{rf}

asset β
relates market return fluctuations to asset return

- μ^{mkt} is the average market return over period
- r^{rf} is the risk-free interest rate over the period

Time series trend

$y^{(i)}$ is the value of quantity at time $x^{(i)} = i$

$y^{\mathrm{d}} = (y^{(1)}, \ldots, y^{(N)})$ is the *time series*

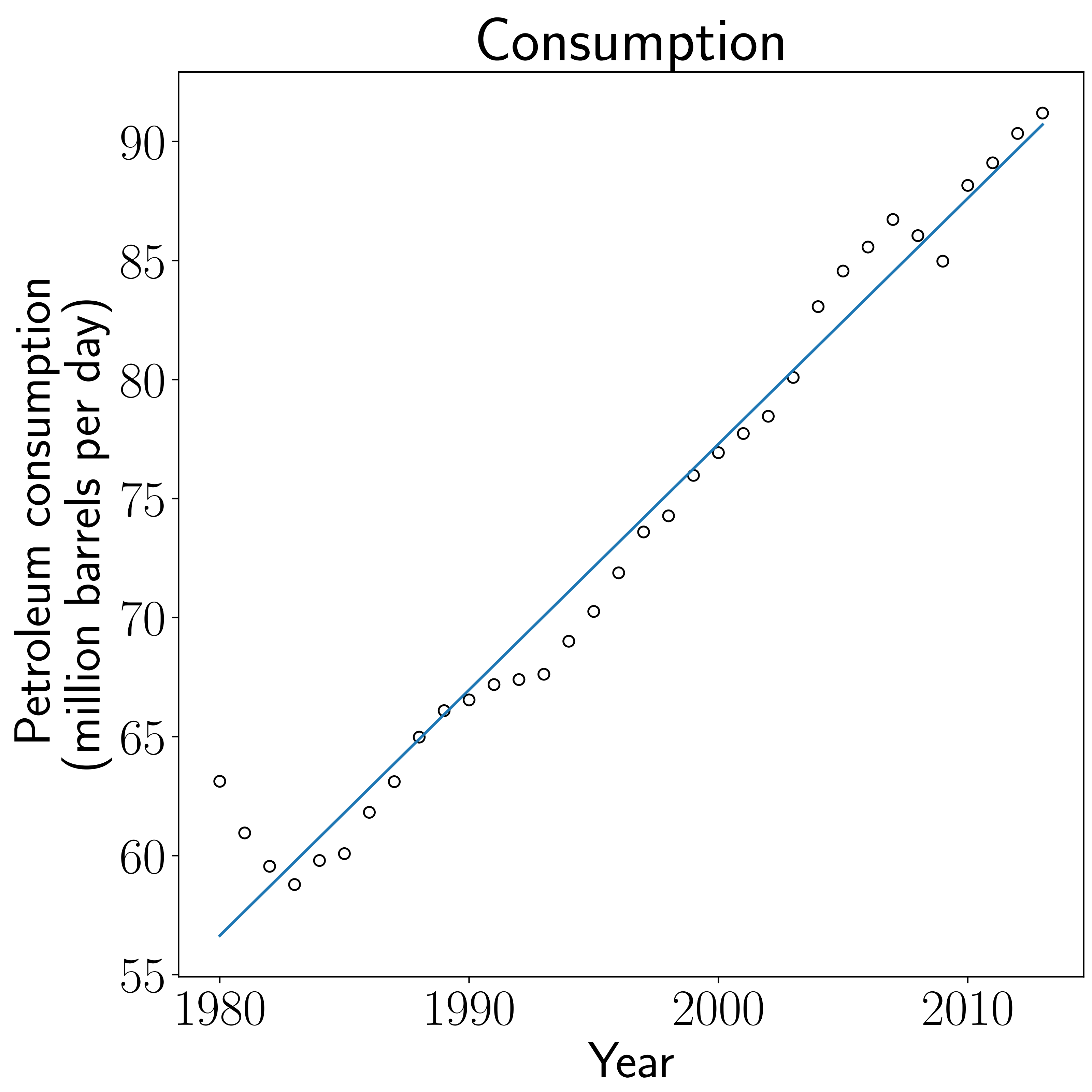
Model (trend line)

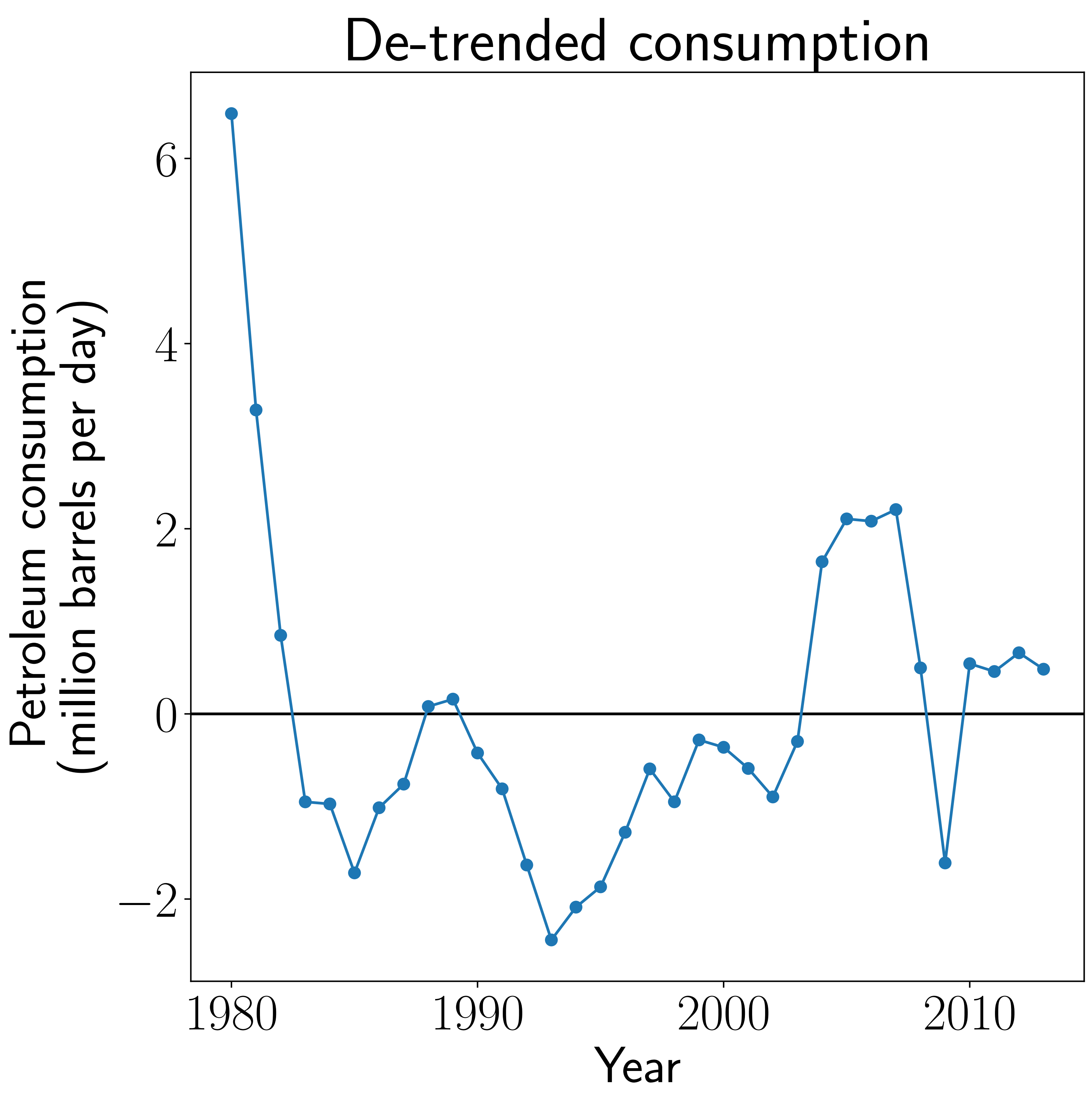
$$\hat{y}^{(i)} = \theta_1 + \theta_2 i, \qquad i = 1, \ldots, N$$

trend coefficient

$y^{\mathrm{d}} - \hat{y}^{\mathrm{d}}$ is the *de-trended time series*

Time series trend
Petroleum consumption





Polynomial fit

Features

$$f_i(x) = x^{i-1}, \quad i = 1, \dots, p$$

Model

$$\hat{f}(x) = \theta_1 + \theta_2 x + \dots \theta_p x^{p-1}$$

degree at most $p-1$

Notation remark

x^i means scalar to ith power

$x^{(i)}$ means ith data point

Least squares data

Vandermonde matrix

$$A = \begin{bmatrix} 1 & x^{(1)} & \dots & (x^{(1)})^{p-1} \\ 1 & x^{(2)} & \dots & (x^{(2)})^{p-1} \\ \vdots & \vdots & & \vdots \\ 1 & x^{(N)} & \dots & (x^{(N)})^{p-1} \end{bmatrix}$$

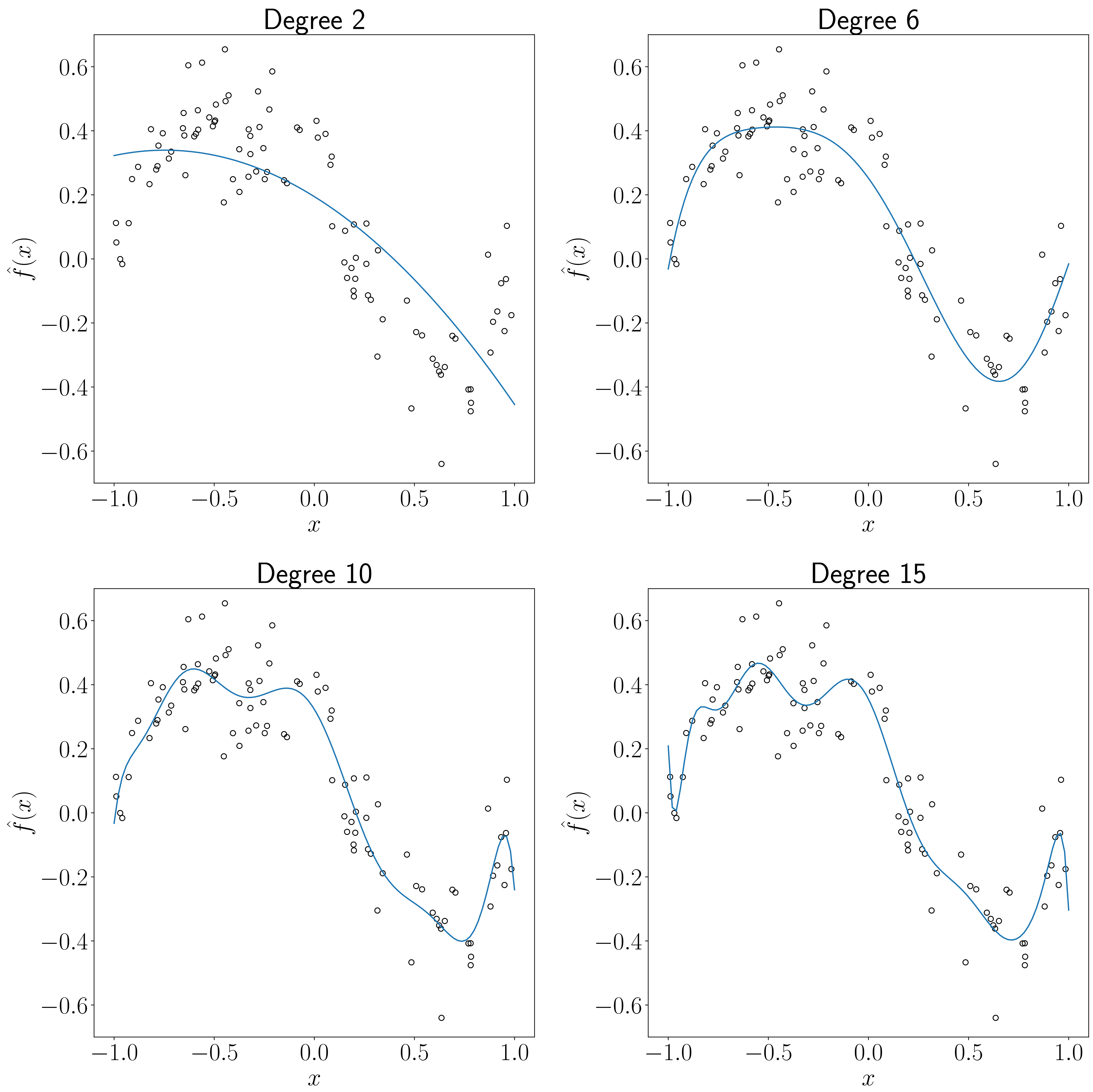
Goal

minimize $\quad \|r^{\mathrm{d}}\|^2 = \|A\theta - y^{\mathrm{d}}\|^2$

Polynomial fit

$N = 100$ data points

Which model is better?



Auto-regressive time series model

$z_1, z_2, \ldots$ is a **time series**

auto-regressive (AR) prediction model

$$\hat{z}_{t+1} = \theta_1 z_t + \cdots + \theta_M z_{t-M+1}, \quad t = M, M+1, \ldots$$

(predict $\hat{z}_{t+1}$ based on previous M values, where M is the memory)

Goal: Chose θ to minimize sum of squares of prediction errors

$$(\hat{z}_{M+1} - z_{M+1})^2 + \cdots + (\hat{z}_T - z_T)^2$$

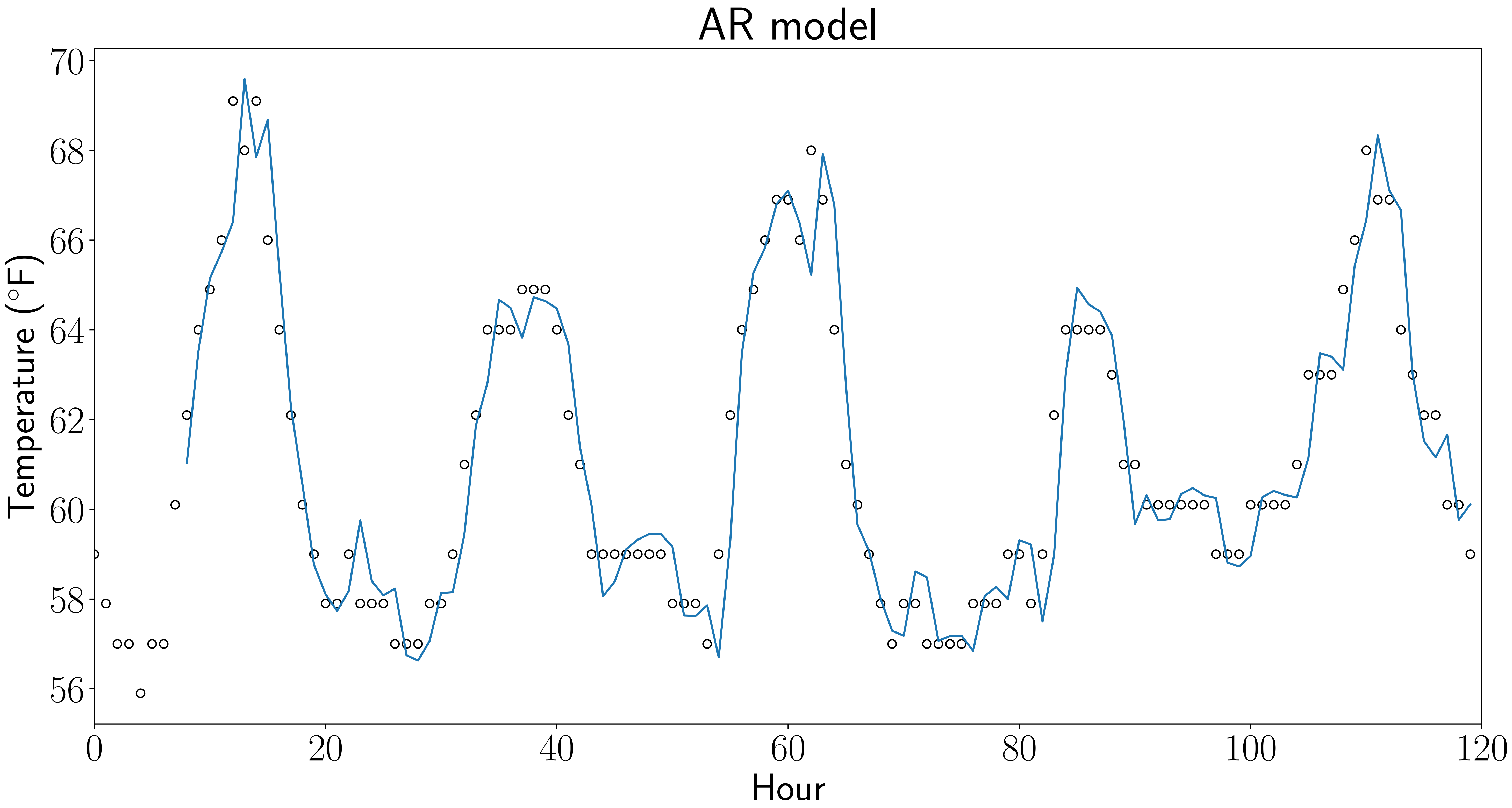
General data fitting form

$$y^{(i)} = z_{M+i}, \qquad x^{(i)} = (z_{M+i-1}, \ldots, z_i), \quad i = 1, \ldots, T-M$$

Auto-regressive time series model

5 days hourly temperature at Los Angeles International Airport (LAX)

- Previous hour: $\hat{z}_{t+1} = z_t$, MSE 1.35
- 24 hours before: $\hat{z}_{t+1} = z_{t-23}$, MSE = 3.00
- AR model with $M = 8$, MSE = 1.02



Multivariate regression

Linear regression as general data fitting

Standard linear regression model

$$\hat{y} = \hat{f}(x) = x^T\beta + v$$

Equivalent general data fitting model

$$\hat{f}(x) = \theta_1 f_1(x) + \cdots + \theta_p f_p(x)$$

with basis functions

$$f_1(x) = 1, \quad f_i(x) = x_{i-1}, \qquad i = 2, \ldots, n-1$$

Therefore, we can write the linear regression model as

$$\hat{y} = \hat{f}(x) = \theta_1 + \theta_2 x_1 + \cdots + \theta_{n+1} x_n = x^T\theta_{2:n} + \theta_1$$

with $\beta = \theta_{2:n+1},\ v = \theta_1$

General data fitting as linear regression

General data fitting model

$$\hat{f}(x) = \theta_1 f_1(x) + \cdots + \theta_p f_p(x)$$

Equivalent linear regression model

$$\hat{y} = \hat{f}(x) = \tilde{x}^T \beta + v$$

- $f_1(x) = 1$ (common assumption)
- $\tilde{x} = (f_2(x), \ldots, f_p(x))$ (transformed features)
- $v = \theta_1$ and $\beta = \theta_{2:p}$ (linear regression parameters)

Our general data fitting framework is nothing more than
linear regression on transformed data

Validation

Generalization

Main goal

- The goal of model is not to predict outcome for *given data*
- Instead, it is to predict the outcome on *new, unseen data*

↓

Seen/Unseen data

- A model that makes reasonable predictions on new, unseen data has **generalization ability** or it **generalizes**
- A model that makes poor predictions on new, unseen data is said to suffer from **over-fitting**

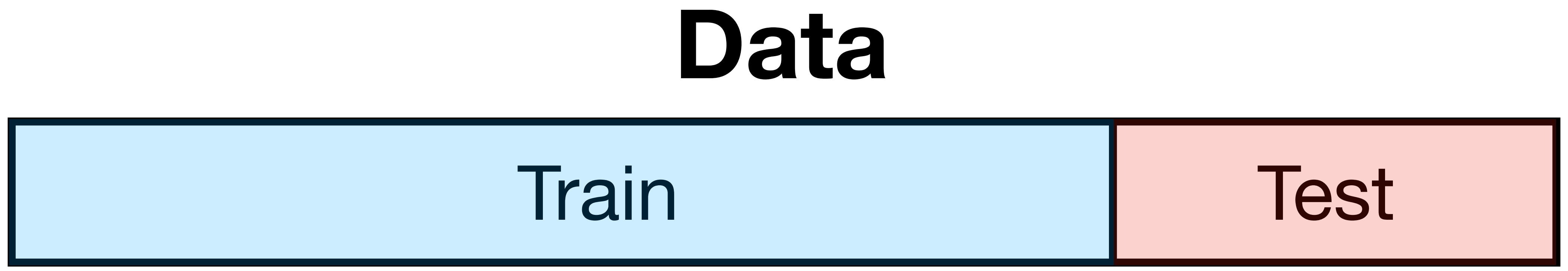
(Almost) always true in decision making

The objective function (here, the training error) is just a “surrogate” of the true goal

Overfitting example

Validation

Simple and effective method to guess if a model generalize

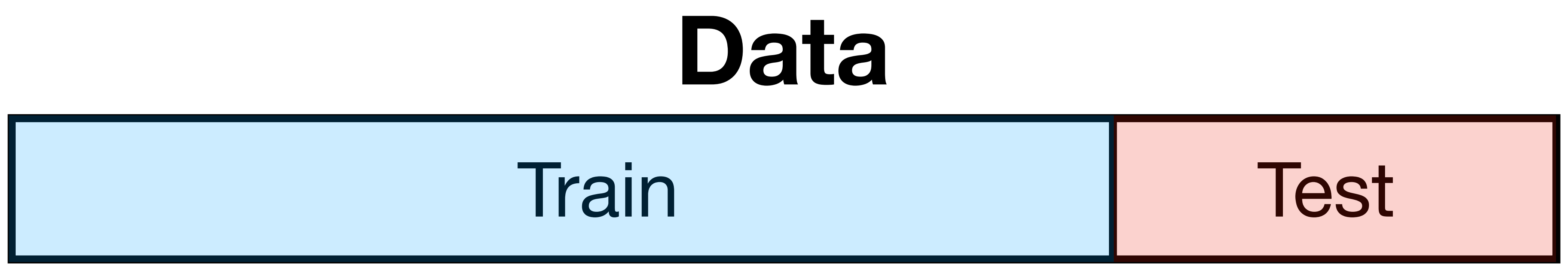


1. Split data in *training* and *test set* (typical 80%/20% or 90%/10%)
2. Build (train) model on training data set (i.e., compute $\theta^\star$)
3. Check model's prediction on test data set

Compare the MSE prediction error on test vs train data set

If similar, we can *guess* that the model will generalize

Validation



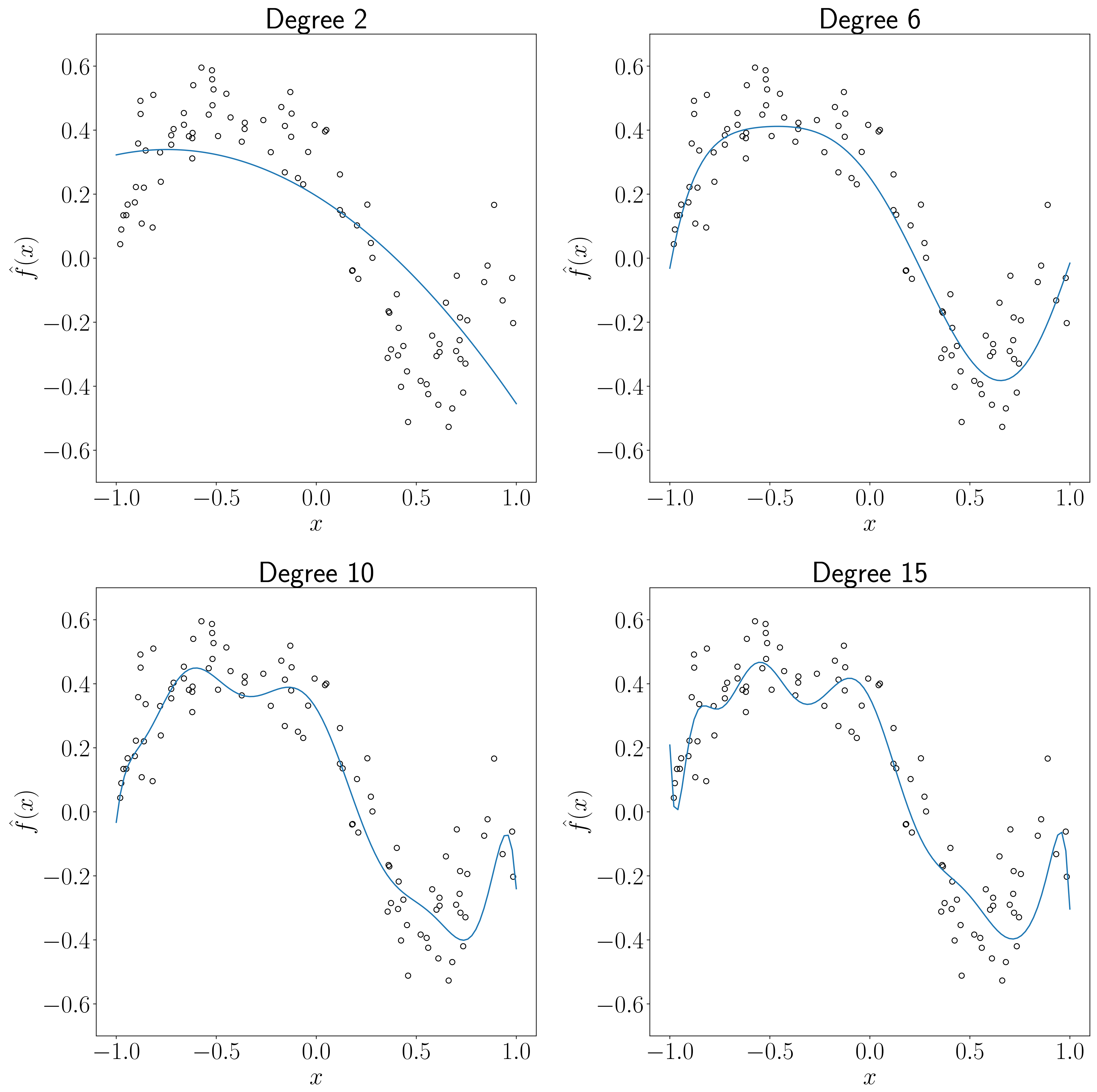
Useful to choose among different candidate models

- Polynomials of different degrees
- Models with different transformed features

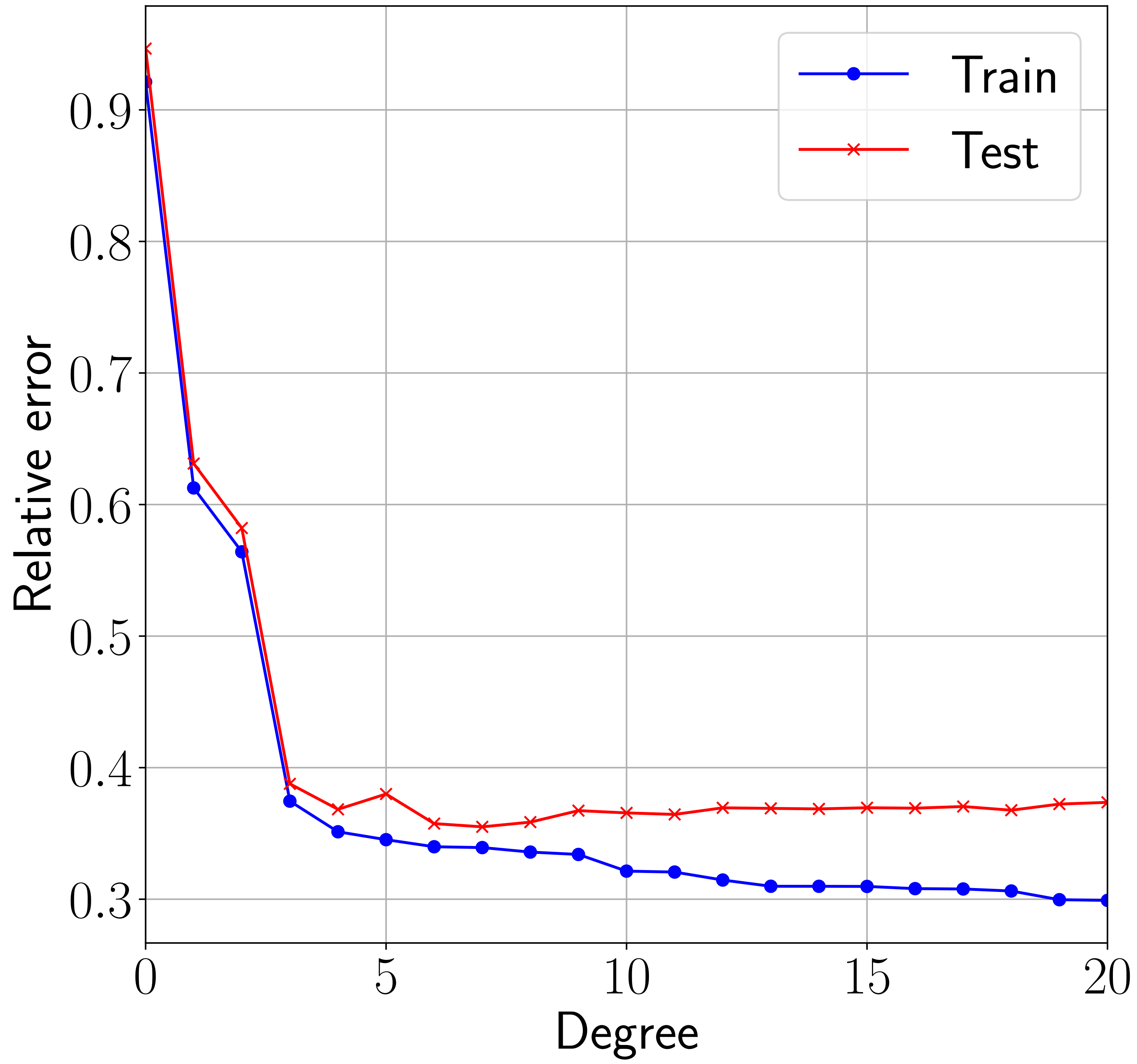
We choose the one with ***lowest test error***

Example

Polynomial fit



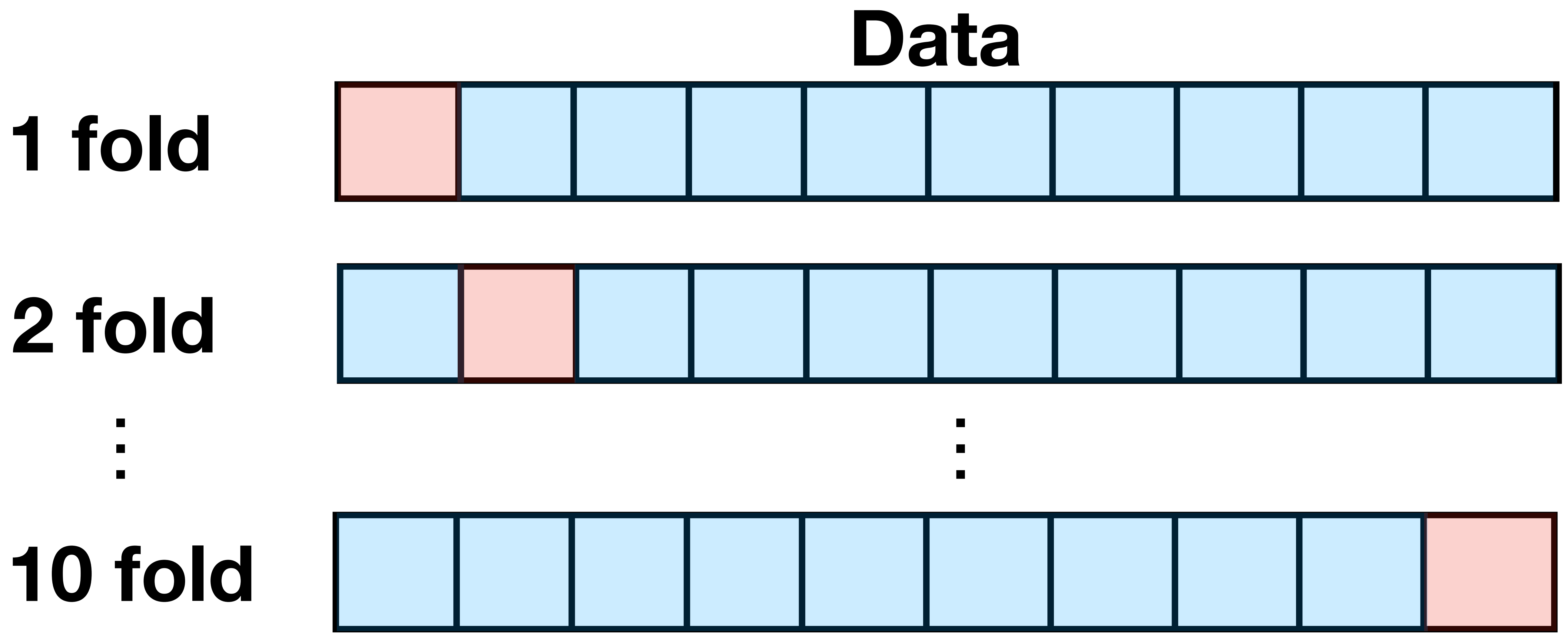
100 points *training set*,
100 points *test set*



It suggests degrees 6/7/8 are reasonable choices

Cross validation

Check **which method** provides the better models
(e.g., choice of features, basis functions, etc.)



1. Divide data in 10 folds
2. For $i = 1, \ldots, 10$ build (train) model using all folds except i
3. Test model on data in fold i

For each fold, compare the MSE prediction error on test vs train data

↓

If test vs train MSE are similar and consistent, we can *guess* the model will generalize

Remark

This returns many models,
to get a model, we have to afterwards train over the whole data set

Example

House price regression

774 house sales in Sacramento area

Model

$$\hat{f}(x) = \theta_1 f_1(x) + \cdots + \theta_8 f_8(x)$$

Base features

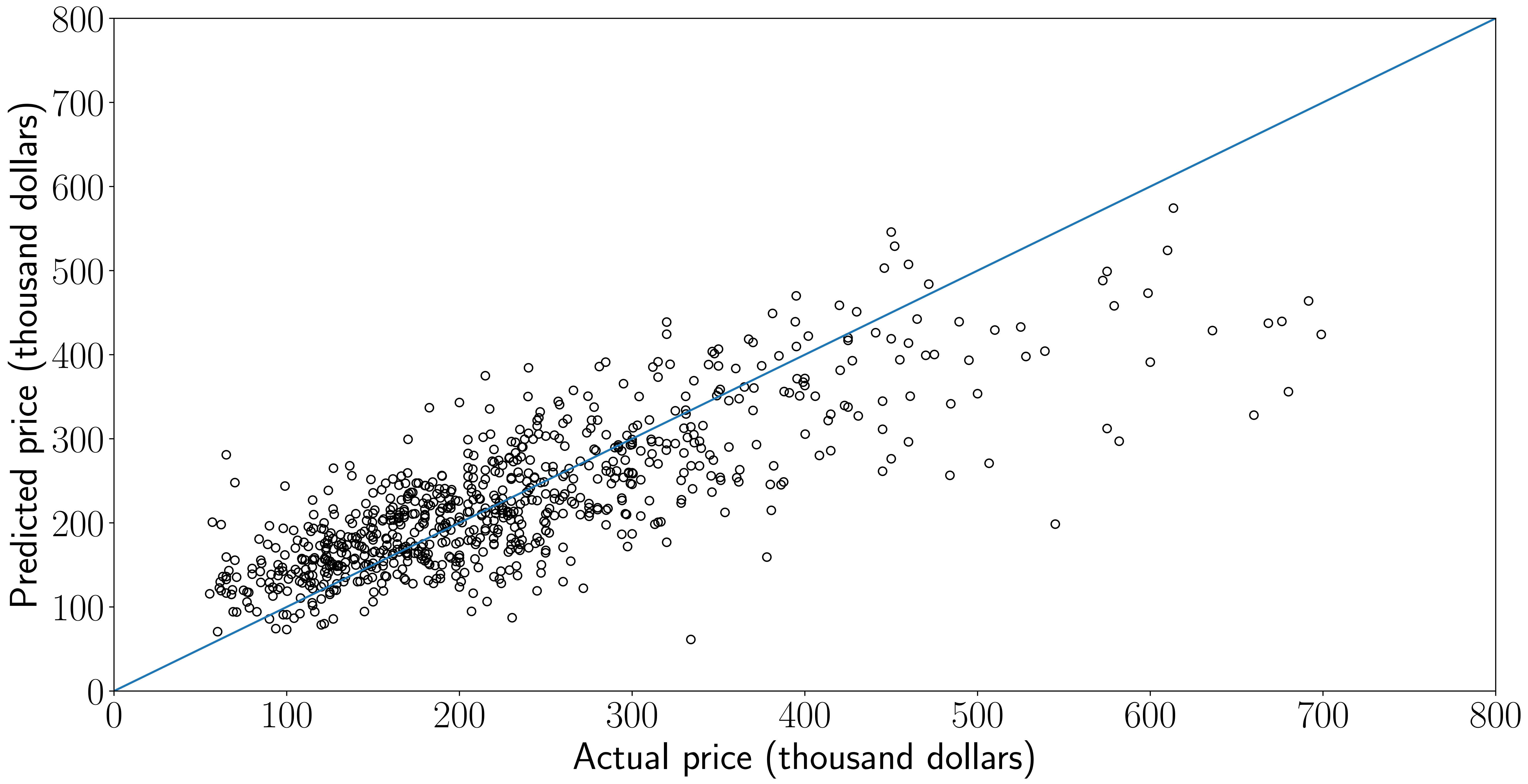
- x_1 is the area of the house (in 1000ft^2)
- x_2 is the number of bedrooms
- x_3 is 1 for condo and 0 for house (boolean)
- x_4 is the ZIP code (62 values)

Transformed features

- $f_1(x) = 1$ (offset)
- $f_2(x) = x_1$
- $f_3(x) = \max\{x_1 - 1.5, 0\}$ is the house area above 1500ft^2
- $f_4(x) = x_2$
- $f_5(x) = x_3$
- $f_6(x), f_7(x), f_8(x)$ are Boolean functions of x_4 to encode 4 groups of nearby zip codes (i.e., neighborhood)

House price prediction

Fitting over the whole dataset



How can we be sure it generalizes?

House price regression

Crossvalidation

5 folds of 155 sales each

Fold	Train error	Test error	θ_1	θ_2	θ_3	θ_4	θ_5	θ_6	θ_7	θ_8
1	0.26	0.30	115.60	177.53	-47.05	-14.64	-13.90	-112.00	-122.59	-36.51
2	0.26	0.29	121.59	165.48	-30.35	-17.74	-20.21	-95.22	-103.67	-7.94
3	0.27	0.25	117.83	181.18	-49.78	-19.30	-18.68	-106.50	-112.76	-32.37
4	0.27	0.25	104.00	174.54	-41.96	-18.81	-17.13	-85.68	-92.09	-6.99
5	0.27	0.27	119.40	178.57	-44.82	-19.50	-25.98	-103.95	-111.56	-36.89

Good feature choice

- Models (parameters) reasonably stable across folds
- Similar train and test errors

Least squares data fitting

Today, we learned to:

- **Formulate** many data fitting problems as least squares
- **Avoid** overfitting by keeping our models simple
- **Compare** our models using validation

References

- S. Boyd, L. Vandenberghe: Introduction to Applied Linear Algebra – Vectors, Matrices, and Least Squares
  - Chapter 13: least squares data fitting

Next lecture

- Multi-objective least squares