Least Squares Data Fitting

Stephen Boyd

EE103
Stanford University

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Outline

Setup

- we believe a scalar y and an n-vector x are related by *model*

$$y \approx f(x)$$

- x is called the *independent variable*
- y is called the *outcome* or *response variable*
- $f : \mathbf{R}^n \to \mathbf{R}$ gives the relation between x and y
- often x is a feature vector, and y is something we want to predict
- we don't know f, which gives the 'true' relationship between x and y

Data

- we are given some *data*

$$x^{(1)}, \ldots, x^{(N)}, \qquad y^{(1)}, \ldots, y^{(N)}$$

  also called *observations*, *examples*, *samples*, or *measurements*
- $x^{(i)}, y^{(i)}$ is ith *data pair*
- $x_j^{(i)}$ is the jth component of ith data point $x^{(i)}$

Model

- choose *model* $\hat{f} : \mathbf{R}^n \to \mathbf{R}$, a *guess* or *approximation* of f
- *linear in the parameters* model form:

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

- $f_i : \mathbf{R}^n \to \mathbf{R}$ are *basis functions* that we choose
- θ_i are *model parameters* that we choose
- $\hat{y}^{(i)} = \hat{f}(x^{(i)})$ is (the model's) *prediction* of $y^{(i)}$
- we'd like $\hat{y}^{(i)} \approx y^{(i)}$, *i.e.*, model is consistent with observed data

Least squares data fitting

- *prediction error* or *residual* is $r_i = y^{(i)} - \hat{y}^{(i)}$
- *least squares data fitting*: choose model parameters θ_i to minimize RMS prediction error on data set

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

- this can be formulated (and solved) as a least squares problem

Least squares data fitting

- express $y^{(i)}$, $\hat{y}^{(i)}$, and $r^{(i)}$ as N-vectors
  - $y^{\mathrm{d}} = (y^{(1)}, \ldots, y^{(N)})$ is vector of outcomes
  - $\hat{y}^{\mathrm{d}} = (\hat{y}^{(1)}, \ldots, \hat{y}^{(N)})$ is vector of predictions
  - $r^{\mathrm{d}} = (r^{(1)}, \ldots, r^{(N)})$ is vector of residuals
- $\mathbf{rms}(r^{\mathrm{d}})$ is *RMS prediction error*

- define $N \times p$ matrix A, $A_{ij} = f_j(x^{(i)})$, so $\hat{y}^{\mathrm{d}} = A\theta$
- least squares data fitting: choose θ to minimize

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

- $\hat{\theta} = (A^T A)^{-1} A^T y$ (if columns of A are independent)
- $\|A\hat{\theta} - y\|^2/N$ is *minimum mean-square (fitting) error*

Fitting a constant model

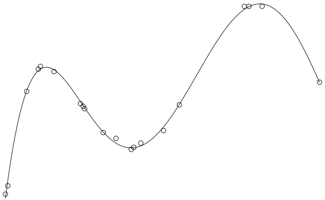
- simplest possible model: $p = 1$, $f_1(x) = 1$, so model $\hat{f}(x) = \theta_1$ is a constant function
- $A = \mathbf{1}$, so

$$\hat{\theta}_1 = (\mathbf{1}^T\mathbf{1})^{-1}\mathbf{1}^T y^{\mathrm{d}} = (1/N)\mathbf{1}^T y^{\mathrm{d}} = \mathbf{avg}(y^{\mathrm{d}})$$

- the mean of $y^{(1)}, \ldots, y^{(N)}$ is the least squares fit by a constant
- MMSE is $\mathbf{std}(y^{\mathrm{d}})^2$; RMS error is $\mathbf{std}(y^{\mathrm{d}})$
- more sophisticated models are judged against the constant model

Fitting univariate functions

- when $n = 1$, we seek to approximate a function $f : \mathbf{R} \to \mathbf{R}$
- we can plot the data (x_i, y_i) and the model function $\hat{y} = \hat{f}(x)$



Straight-line fit

- $p = 2$, with $f_1(x) = 1$, $f_2(x) = x$
- model has form $\hat{f}(x) = \theta_1 + \theta_2 x$
- matrix A has form

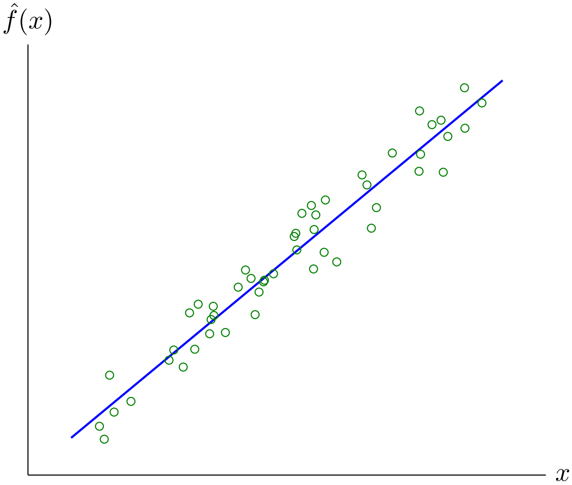
$$A = \begin{bmatrix} 1 & x^{(1)} \\ 1 & x^{(2)} \\ \vdots & \vdots \\ 1 & x^{(N)} \end{bmatrix}$$

- can work out $\hat{\theta}_1$ and $\hat{\theta}_2$ explicitly:

$$\hat{f}(x) = \mathbf{avg}(y^{\mathrm{d}}) + \rho \frac{\mathbf{std}(y^{\mathrm{d}})}{\mathbf{std}(x^{\mathrm{d}})}(x - \mathbf{avg}(x^{\mathrm{d}}))$$

where $x^{\mathrm{d}} = (x^{(1)}, \ldots, x^{(N)})$

Example



Asset α and β

- x is return of whole market, y is return of a particular asset
- write straight-line model as

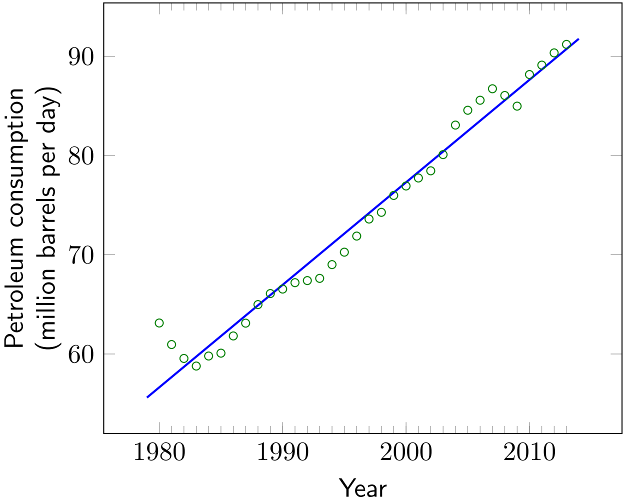
$$\hat{y} = (r^{\mathrm{rf}} + \alpha) + \beta(x - \mu^{\mathrm{mkt}})$$

  - μ^{mkt} is the average market return
  - r^{rf} is the risk-free interest rate
  - several other slightly different definitions are used
- called asset 'α' and 'β', widely used

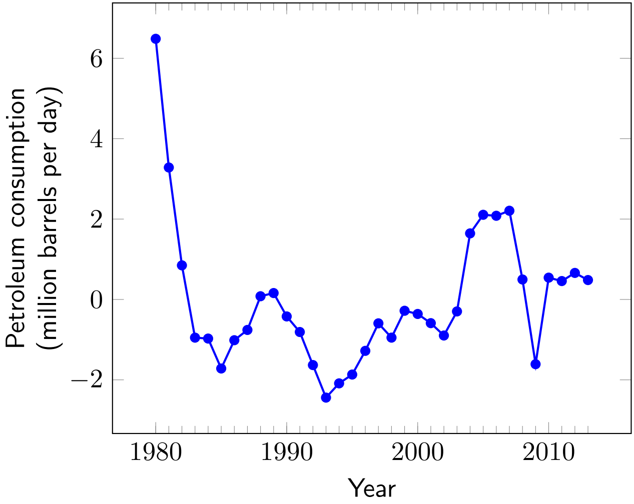
Time series trend

- $y^{(i)}$ is value of quantity at time $x^{(i)} = i$
- $\hat{y}^{(i)} = \hat{\theta}_1 + \hat{\theta}_2 i, \quad i = 1, \ldots, N$, is called *trend line*
- $y^{\mathrm{d}} - \hat{y}^{\mathrm{d}}$ is called *de-trended time series*
- $\hat{\theta}_2$ is *trend coefficient*

World petroleum consumption



World petroleum consumption, de-trended



Polynomial fit

- $f_i(x) = x^{i-1}, \quad i = 1, \ldots, p$
- model is a polynomial of degree less than p

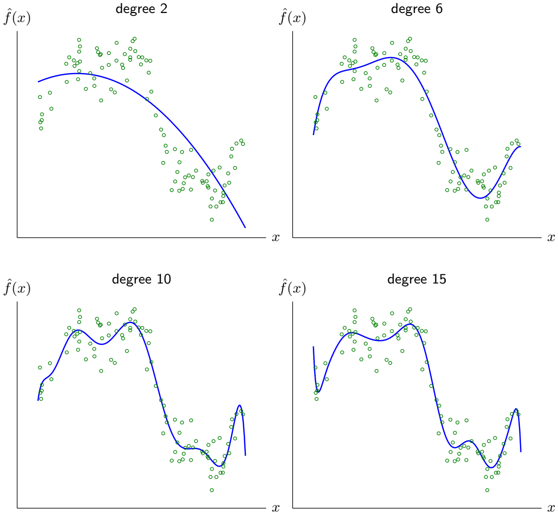
$$\hat{f}(x) = \theta_1 + \theta_2 x + \cdots + \theta_p x^{p-1}$$

  (here x^i means scalar x to ith power; $x^{(i)}$ is ith data point)
- A is Vandermonde matrix

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

Example

$N = 100$ data points



Regression as general data fitting

- regression model is affine function $\hat{y} = \hat{f}(x) = x^T\beta + v$
- fits general fitting form with basis functions

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

so model is

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

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

General data fitting as regression

- general fitting model $\hat{f}(x) = \theta_1 f_1(x) + \cdots + \theta_p f_p(x)$
- common assumption: $f_1(x) = 1$
- same as regression model $\hat{f}(\tilde{x}) = \tilde{x}^T \beta + v$, with
  - $\tilde{x} = (f_2(x), \ldots, f_p(x))$ are 'transformed features'
  - $v = \theta_1$, $\beta = \theta_{2:p}$

Auto-regressive time series model

- time zeries $z_1, z_2, \ldots$
- *auto-regressive* (AR) prediction model:

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

- M is *memory* of model
- $\hat{z}_{t+1}$ is prediction of next value, based on previous M values
- we'll choose β to minimize sum of squares of prediction errors,

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

- put in general form with

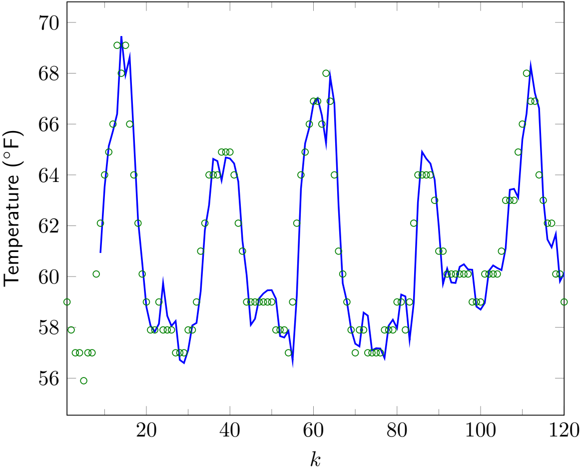
$$y^{(i)} = z_{M+i}, \quad x^{(i)} = (z_{M+i-1}, \ldots, z_i), \quad i = 1, \ldots, T-M$$

Example

- hourly temperature at LAX in May 2016, length 744
- average is 61.76°F, standard deviation 3.05°F
- predictor $\hat{z}_{t+1} = z_t$ gives RMS error 1.16°F
- predictor $\hat{z}_{t+1} = z_{t-23}$ gives RMS error 1.73°F
- AR model with $M = 8$ gives RMS error 0.98°F

Example

solid line shows one-hour ahead predictions from AR model, first 5 days



Outline

Generalization

basic idea:

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

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

Validation

a simple and effective method to guess if a model will generalize

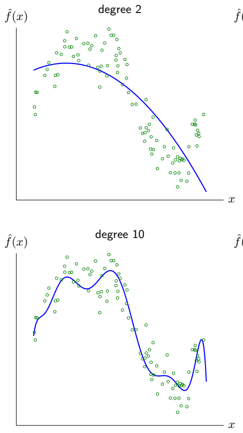
- split original data into a *training set* and a *test set*
- typical splits: 80%/20%, 90%/10%
- build ('train') model on training data set
- then *check the model's predictions on the test data set*
- (can also compare RMS prediction error on train and test data)
- if they are similar, we can *guess* the model will generalize

Validation

- can be used to choose among different candidate models, *e.g.*
  - polynomials of different degrees
  - regression models with different sets of regressors
- we'd use one with low, or lowest, test error

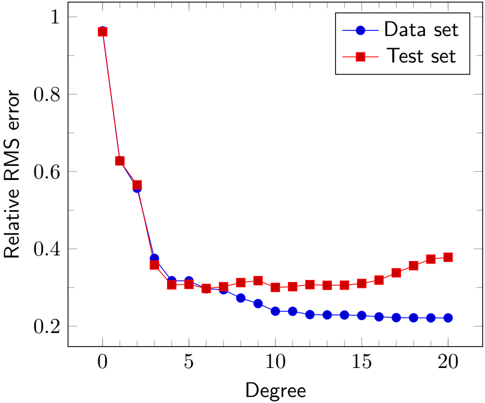
Example

- polynomials fit using *training set* of 100 points
- plots below show performance with *test set* of 100 points



Example

- suggests degree 4, 5, or 6 are reasonable choices



Cross validation

to carry out cross validation:

- divide data into 10 *folds*
- for $i = 1, \ldots, 10$, build (train) model using all folds except i
- test model on data in fold i

interpreting cross validation results:

- if test RMS errors are much larger than train RMS errors, model is over-fit
- if test and train RMS errors are similar and consistent, we can *guess* the model will have a similar RMS error on future data

Example

- house price, regression fit with $x = (\text{area}/1000 \text{ ft.}^2, \text{ bedrooms})$
- 774 sales, divided into 5 folds of 155 sales each
- fit 5 regression models, removing each fold

	Model parameters			RMS error	
Fold	v	β_1	β_2	Train	Test
1	60.65	143.36	-18.00	74.00	78.44
2	54.00	151.11	-20.30	75.11	73.89
3	49.06	157.75	-21.10	76.22	69.93
4	47.96	142.65	-14.35	71.16	88.35
5	60.24	150.13	-21.11	77.28	64.20

Outline

Feature engineering

- start with original or base feature n-vector x
- choose basis functions $f_1, \ldots, f_p$ to create 'mapped' feature p-vector

$$(f_1(x), \ldots, f_p(x))$$

- now fit linear in parameters model with mapped features

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

- *check the model using validation*

Transforming features

- *standardizing features*: replace x_i with $(x_i - b_i)/a_i$
  - $b_i \approx$ mean value of the feature across the data
  - $a_i \approx$ standard deviation of the feature across the data

  new features are called *z-scores*
- *log transform*: if x_i is nonnegative and spans a wide range, replace it with $\log(1 + x_i)$
- *hi and lo features*: create new features given by

$$\max\{x_1 - b, 0\}, \qquad \min\{x_1 - a, 0\}$$

  (called hi and lo versions of original feature x_i)

Example

- house price prediction
- start with base features
  - x_1 is area of house (in 1000ft.^{2})
  - x_2 is number of bedrooms
  - x_3 is 1 for condo, 0 for house
  - x_4 is zip code of address (62 values)
- we'll use $p = 8$ basis functions:
  - $f_1(x) = 1$, $f_2(x) = x_1$, $f_3(x) = \max\{x_1 - 1.5, 0\}$
  - $f_4(x) = x_2$, $f_5(x) = x_3$
  - $f_6(x)$, $f_7(x)$, $f_8(x)$ are Boolean functions of x_4 which encode 4 groups of nearby zipcodes (*i.e.*, neighborhood)
- five fold model validation

Example

	Model parameters								RMS error	
Fold	θ_1	θ_2	θ_3	θ_4	θ_5	θ_6	θ_7	θ_8	Train	Test
1	122.35	166.87	-39.27	-16.31	-23.97	-100.42	-106.66	-25.98	67.29	72.78
2	100.95	186.65	-55.80	-18.66	-14.81	-99.10	-109.62	-17.94	67.83	70.81
3	133.61	167.15	-23.62	-18.66	-14.71	-109.32	-114.41	-28.46	69.70	63.80
4	108.43	171.21	-41.25	-15.42	-17.68	-94.17	-103.63	-29.83	65.58	78.91
5	114.45	185.69	-52.71	-20.87	-23.26	-102.84	-110.46	-23.43	70.69	58.27