Statistical Foundations of Data Science

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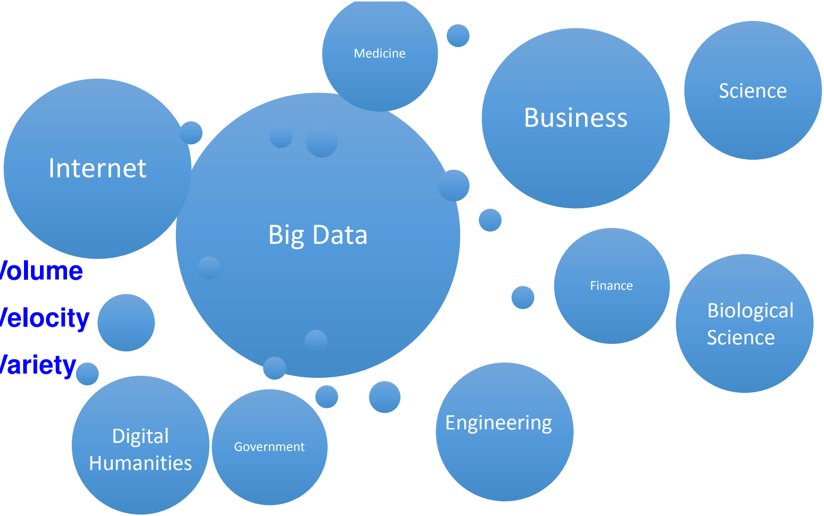
Big Data are ubiquitous



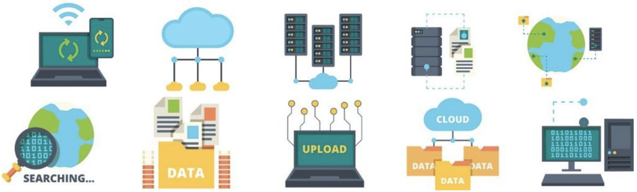
★**Volume**

★**Velocity**

★**Variety**

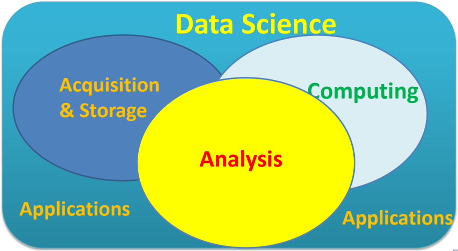
Impact of Data Tsunami Gives Rise to Data Science

System: storage, communication, security, computation architectures



Analysis: statistics, computation, optimization, privacy

Big Data $\Longrightarrow$



$\Longrightarrow$ **Smart Data**

What can big data do?

Hold great promises for understanding

- ★ **Heterogeneity**: personalized medicine or services
- ★ **Commonality**: in presence of large variations (noises)

from large pools of variables, factors, genes, environments and their interactions as well as **latent factors**.

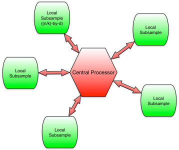
Aims of Data Science:

- **Prediction**: To construct as effective a method as possible to predict future observations.(**correlation**)
- **Inference and Prediction**: To gain insight into relationship between features and response for scientific purposes and to construct an improved prediction method. (**causation**)

Common Features and Techniques

Common Features of Big Data:

- ★ Dependence, heavy tails, endogeneity, spurious corr, heterogeneity,
- ♠ Missing data, measurement errors, survivor, sampling biases
- ♣ Computation, communication, privacy, ownership



Common Techniques for Data Science:

- ★ Statistical Techniques: Least-Squares, MLE, M-estimation
- ♠ Regression: Parametric, Nonparametric, Sparse, Factor(PCR)
- ♣ Principal Component Analysis: Supervised, unsupervised.

1. Multiple and Nonparametric Regression

1.1. Multiple Regression

■ Read materials and R-implementations here

https://fan.princeton.edu/fan/classes/245/chap11.pdf

Purpose of Multiple regression

- ★ Study assocations between dependent & independent variables
- ★ Screen irrelevant and select useful variables
- ★ Prediction

Example: Zillow is an online real estate database company founded in 2006. An important task for Zillow is to predict the house price. (Training data: 15129 cases, testing data: 6484 cases)

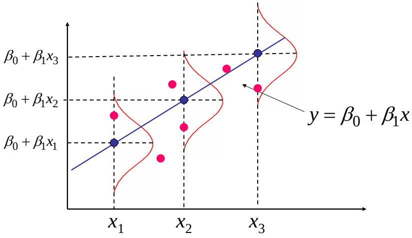
Interest: Associations between **housing** and its **attributes**.

- **Response** Y = Housing prices
- **Covariates**
  - No. of bathrooms X_1; No. of bedrooms X_2
  - sqft-living room X_3; sqft-lot X_4
  - zipcode X_5 (70 zipcodes); view X_6 (5 categories)
  - $\dots$

Multiple linear regression model

$$Y = \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p + \varepsilon$$

- Y: response / dependent variable
- X_j's: explanatory / independent variables or covariates
- ε: random error not explained / predicted by covariates
- include intercept by setting $X_1 = 1$

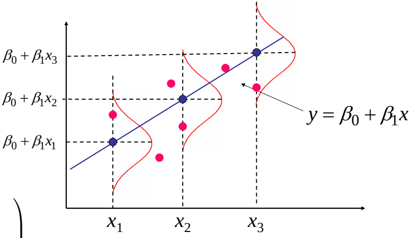


Method of Least-squares

Data: $\left\{\left(x_{i1}, x_{i2}, \cdots x_{ip}, y_i\right)\right\}_{1\le i\le n}$

Model: $y_i = \sum_{j=1}^{p} \beta_j x_{ij} + \varepsilon_i$

Matrix form: $\mathbf{y} = \mathbf{X}\beta + \varepsilon$



$$\mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}, \mathbf{X} = \begin{pmatrix} x_{11} & \cdots & x_{1p} \\ \vdots & \ldots & \vdots \\ x_{n1} & \cdots & x_{np} \end{pmatrix}, \beta = \begin{pmatrix} \beta_1 \\ \vdots \\ \beta_p \end{pmatrix}, \varepsilon = \begin{pmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_n \end{pmatrix}$$

Method of Least-Squares:

$$\min_{\beta\in\mathbb{R}^p} \quad \mathrm{RSS}\left(\beta\right) \triangleq \sum_{i=1}^{n}\left(y_i - \sum_{j=1}^{p} x_{ij}\beta_j\right)^2 = \|\mathbf{y}-\mathbf{X}\beta\|^2$$

- RSS stands for **residual sum-of-squares**

Closed-form solution

Least-squares: Minimize wrt $\beta \in \mathbb{R}^p$

$$\|\mathbf{y} - \mathbf{X}\beta\|^2 = (\mathbf{y} - \mathbf{X}\beta)^T(\mathbf{y} - \mathbf{X}\beta)$$

Setting gradients to zero yields **normal equations**:

$$\mathbf{X}^T\mathbf{y} = \mathbf{X}^T\mathbf{X}\beta$$

Least-squares estimator: (assume $\mathbf{X}$ has full column rank)

$$\widehat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

Multiple R^2: $R^2 = 1 - \frac{\mathrm{RSS}(\widehat{\beta})}{\mathrm{var}(\mathbf{y})}$, proportion of variance of y explained by regression. It measures the **goodness-of-fit**.

♦$\mathrm{var}(\mathbf{y}) = \mathrm{RSS}(1)$

Geometric interpretation of least-squares

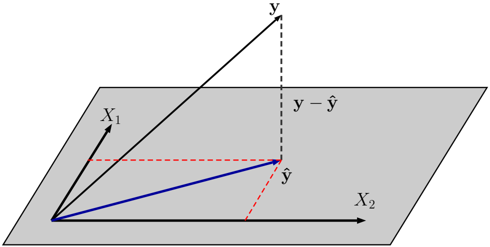
Fitted value: $$\widehat{\mathbf{y}} = \mathbf{X}\widehat{\beta} = \underbrace{\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T}_{\triangleq \mathbf{P} \in \mathbb{R}^{n \times n}}\mathbf{y}$$

Theorem 2.1 [Property of projection matrix]

★ $\mathbf{P}\mathbf{x}_j = \mathbf{x}_j, \quad j = 1, 2, \cdots, p$

★ $\mathbf{P}^2 = \mathbf{P} \quad \text{or} \quad \mathbf{P}(\mathbf{I}_n - \mathbf{P}) = \mathbf{0}$

★ Eigenvalues of $\mathbf{P}$ are 0 or 1, with number of 1's = rank($\mathbf{P}$)



■ project response vector **y** onto linear space spanned by **X**

Statistical properties of least-squares estimator

Assumption:

- **Exogeneity**: $\mathbb{E}(\varepsilon|\mathbf{X}) = 0$;
- **Homoscedasticity**: $\text{var}(\varepsilon|\mathbf{X}) = \sigma^2$.

Statistical Properties:

★ **bias**: $\mathbb{E}(\widehat{\beta}|\mathbf{X}) = \beta$

★ **variance**: $\text{var}(\widehat{\beta}|\mathbf{X}) = \sigma^2(\mathbf{X}^T\mathbf{X})^{-1}$

often dropped

■ Recall $\text{cov}(\mathbf{U},\mathbf{V}) = E(\mathbf{U}-\mu_u)(\mathbf{V}-\mu_v)^T$ and $\text{var}(\mathbf{U}) = \text{cov}(\mathbf{U},\mathbf{U})$

$$\text{cov}(\mathbf{AU},\mathbf{BV}) = \mathbf{A}\,\text{cov}(\mathbf{U},\mathbf{V})\mathbf{B}^T, \qquad \text{var}(\mathbf{a}^T\mathbf{U}) = \mathbf{a}^T\,\text{var}(\mathbf{U})\mathbf{a};$$

Gauss-Markov Theorem

How large is variance? Compared with other estimators?

Theorem 2.2 [Gauss-Markov Theorem]

LSE $\widehat{\beta}$ is best linear unbiased estimator (BLUE):

- $\mathbf{a}^T\widehat{\beta}$ is a linear unbiased estimator of parameter $\theta = \mathbf{a}^T\beta$
- for any linear unbiased estimator $\mathbf{b}^T\mathbf{y}$ of θ,

$$\operatorname{var}(\mathbf{b}^T\mathbf{y}|\mathbf{X}) \geq \operatorname{var}(\mathbf{a}^T\widehat{\beta}|\mathbf{X})$$

Estimation of σ^2: $\widehat{\sigma}^2 = \frac{\text{RSS}}{\mathbf{n-p}} = \frac{\|\mathbf{y}-\mathbf{X}\widehat{\beta}\|^2}{n-p}$

$\widehat{\sigma}^2$ is is an unbiased estimator of σ^2

Statistical inference

Additional assumption: $\varepsilon \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I}_n)$

Under fixed design or conditioning on $\mathbf{X}$,

$$\widehat{\beta} = \beta + (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\varepsilon \quad \Longrightarrow \quad \widehat{\beta} \sim \mathcal{N}(\beta, (\mathbf{X}^T\mathbf{X})^{-1}\sigma^2)$$

★ $\widehat{\beta}_j \sim \mathcal{N}(\beta_j, v_j\sigma^2)$ where v_j is jth diag of $(\mathbf{X}^T\mathbf{X})^{-1}$

★ $(n-p)\widehat{\sigma}^2 \sim \sigma^2\chi^2_{n-p}$ and $\widehat{\sigma}^2$ is indep. of $\widehat{\beta}$.

★ **$1-\alpha$ CI for β_j**: $\widehat{\beta}_j \pm t_{n-p}(1-\alpha/2)\sqrt{v_j}\widehat{\sigma}$ (homework)

★ $H_0 : \beta_j = 0$: test statistics $t_j = \frac{\widehat{\beta}_j}{\sqrt{v_j}\widehat{\sigma}} \sim_{H_0} t_{n-p}$.

Proof of the classical result

1. RSS = $\mathbf{y}^T(\mathbf{I}_n - \mathbf{P})\mathbf{y} = \varepsilon^T(\mathbf{I}_n - \mathbf{P})\varepsilon$

2. By eigendecomposition, $\mathbf{P} = \mathbf{\Gamma}\,\mathrm{diag}(\overbrace{1,\cdots,1}^{p},0,\cdots,0)\mathbf{\Gamma}^T$.

3. $\mathrm{RSS} = \mathbf{Z}^T\,\mathrm{diag}(\overbrace{0,\cdots,0}^{p},1,\cdots,1)\mathbf{Z} \sim \sigma^2\chi^2_{n-p}$, where $\mathbf{Z} = \mathbf{\Gamma}\varepsilon \sim N(0,\sigma^2\mathbf{I}_n)$

4. RSS depends only on $(\mathbf{I}_n - \mathbf{P})\varepsilon$ and $\widehat{\beta}$ depends on $(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\varepsilon$. They are joint normal and uncorrelated $\Longrightarrow$ indep.

5. $\frac{\widehat{\beta}_j - \beta_j}{\sqrt{v_j}\widehat{\sigma}} = \frac{\widehat{\beta}_j - \beta_j}{\sqrt{v_j}\sigma} \Big/ \sqrt{\frac{\mathrm{RSS}}{\sigma^2(n-p)}} \sim t_{n-p}$, by definition.

Zillow Data Analysis: Regression outputs

$$\text{Out-of-sample } R^2 = 1 - \frac{\text{PE of a model}}{\text{PE of naive}} = 1 - \underbrace{\frac{\sum_{i \in \text{TEST}} (y_i - \widehat{y}_i)^2}{\sum_{i \in \text{TEST}} (y_i - \bar{y})^2}}_{\bar{y} = \text{ in-sample ave}} = \text{Normalized test error}$$

$$R^2 = 1 - \frac{\sum_{i \in \text{TRAIN}} (y_i - \widehat{y}_i)^2}{\sum_{i \in \text{TRAIN}} (y_i - \bar{y})^2}, \qquad \text{Adjusted } R^2 = 1 - \frac{\frac{1}{n-p} \sum_{i \in \text{TRAIN}} (y_i - \widehat{y}_i)^2}{\frac{1}{n-1} \sum_{i \in \text{TRAIN}} (y_i - \bar{y})^2)},$$

Model 1: lm(price $\sim$ bathrooms + bedrooms + sqft_living + sqft_lot)

R^2-values: In sample = 0.5101, adjusted = 0.5100, Out-sample = 0.5051

```
fit.lm1 = lm(price~bathrooms + bedrooms + sqft_living + sqft_lot, data = train_data)
#fit linear model
summary(fit.lm1)             #summarize the fit

Call:
lm(formula = price ~ bathrooms + bedrooms + sqft_living
+ sqft_lot, data = train_data)

Residuals:
Min        1Q   Median       3Q      Max
-1571803  -143678   -22595   103133  4141210

Coefficients:
Estimate Std. Error t value Pr(>|t|)
(Intercept)  8.083e+04  8.208e+03   9.848  < 2e-16 ***
bathrooms    3.682e+03  4.178e+03   0.881    0.378
```

```
bedrooms    -5.930e+04  2.753e+03 -21.537  < 2e-16 ***
sqft_living  3.167e+02  3.750e+00  84.442  < 2e-16 ***
sqft_lot    -4.267e-01  5.504e-02  -7.753 9.52e-15 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 257200 on 15124 degrees of freedom
Multiple R-squared:  0.5101,Adjusted R-squared:   0.51
F-statistic:  3937 on 4 and 15124 DF,  p-value: < 2.2e-16
```

- ★ The first part reminds us the models used;
- ★ the second part summarizes the residual statistics;
- ★ the third part depicts estimated coefficients $\widehat{\beta}_j$ (second column), its standard error $\sqrt{v_j}\widehat{\sigma}$ (third column), and t-statistic t_j,
- ★ the last part summarizes overall model fits: $\widehat{\sigma} = 257200$, $n - p = 15124$, $R^2 = 0.5101$, adj-R^2 = 0.51, F-statistic for testing $H_0 : \beta = 0$ is 3937 with degree of freedom $p - 1 = 4$ and $n - p = 15124$. Small P-value suggests that we reject H_0 that these four variables are not related to the house price.

Now, let us compute the out-of-sample R^2, showing roughly percentage of predicability.

```
##### out-of-sample R^2########
fit.lm1.pred.out <- predict(fit.lm1, newdata = test_data)

SS.total <- sum((test_data$price - mean(train_data$price))^2)
SS.residual <- sum( (test_data$price - fit.lm1.pred.out)^2)
1 - SS.residual / SS.total
```

[1] 0.5051489

Non-normal error

Appeal to asymptotic theory:

$$\sqrt{n}(\widehat{\beta}-\beta) = \underbrace{(n^{-1}\mathbf{X}^T\mathbf{X})^{-1}}_{n^{-1}\sum_{i=1}^n \mathbf{x}_i\mathbf{x}_i^T} \underbrace{n^{-1/2}\mathbf{X}^T\varepsilon}_{n^{-1/2}\sum_{i=1}^n \mathbf{x}_i\varepsilon_i}$$

LLN **CLT**

Using Slutsky's theorem, (homework)

$$\sqrt{n}(\widehat{\beta}-\beta) \xrightarrow{d} N(0, \mathbf{\Sigma}^{-1}) \quad \text{or} \quad \widehat{\beta} \xrightarrow{d} \mathcal{N}(\beta, (\mathbf{X}^T\mathbf{X})^{-1}\sigma^2) \text{ (informal)}$$

Holds approx. for large *n*

Correlated errors

$$\mathbf{y} = \mathbf{X}\beta + \varepsilon, \quad \text{where} \quad \mathrm{var}(\varepsilon|\mathbf{X}) = \sigma^2\mathbf{W}$$

Transform data: $\mathbf{y}^* = \mathbf{W}^{-1/2}\mathbf{y}$, $\mathbf{X}^* = \mathbf{W}^{-1/2}\mathbf{X}$, $\varepsilon^* = \mathbf{W}^{-1/2}\varepsilon$. Then

$$\mathbf{y}^* = \mathbf{X}^*\beta + \varepsilon^*, \quad \text{with} \quad \mathrm{var}(\varepsilon^*|\mathbf{X}) = \sigma^2\mathbf{I}.$$

General Least-Squares:

$$\min_{\beta \in \mathbb{R}^p} \quad ||\mathbf{y}^* - \mathbf{X}^*\beta||^2 = (\mathbf{y} - \mathbf{X}\beta)^T \mathbf{W}^{-1} (\mathbf{y} - \mathbf{X}\beta)$$

Heteroscedastic errors: $\mathbf{W}_i = \sigma^2 \,\mathrm{diag}(v_1, \cdots, v_n)$

Weighted Least-squares: $\min_\beta \sum_{i=1}^n (y_i - \mathbf{X}_i^T\beta)^2 / v_i$.

1.2. Arts of Model Building

Nonlinear and nonparametric regression

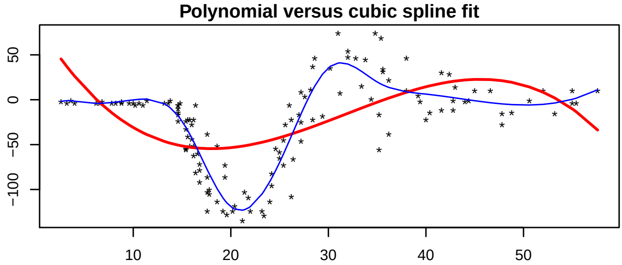
Nolinear regression

Polynomial regression: univariate

$$Y = \overbrace{\beta_0 + \beta_1 X + \cdots + \beta_d X^d}^{\approx f(X)} + \varepsilon$$

★multiple regression with $X_1 = X, \cdots, X_d = X^d$ (**basis function**)

Drawback: not suitable for functions with **varying** degrees of smoothness



motorcycle data: time vs. head acceleration (red: cubic **polynomial**; blue: cubic **splines**)

Spline regression

- ★ piecewise polynomials with degree d and continuous $(d-1)^{th}$ derivative.
- ★ **Knots**: $\{\tau_j\}_{j=1}^{K}$ where discontinuity occurs. ★data quantiles

$$Y = \text{Spline}_K(X) + \varepsilon = \sum_{j=0}^{D+K} B_j(X) + \varepsilon$$

Basis functions: $\{1, x, \cdots, x^d, (x-\tau_j)_+^d, \quad j = 1, \cdots, K\} = \{B_j(x)\}_{j=0}^{d+K}$

- ★ cubic spline: $d = 3$, widely used;
- ★ multiple regression with $X_j = B_j(x)$. (feature)

Nonparametric: When K is large, $K_n \to \infty$

Extension to multiple covariates

- Bivariate quadratic regression model:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1^2 + \beta_4 \underbrace{X_1 X_2}_{\text{interaction}} + \beta_5 X_2^2 + \varepsilon$$

- Multivariate quadratic regression: (linear in parameters)

$$Y = \sum_{j=1}^{p} \beta_j X_j + \sum_{\mathbf{j \le k}} \beta_{jk} X_j X_k + \varepsilon$$

- Multivariate quadratic regression with main effect and interactions

$$Y = \sum_{j=1}^{p} \beta_j X_j + \sum_{\mathbf{j < k}} \beta_{jk} X_j X_k + \varepsilon$$

Model 2: (heterogeneity + interaction) Consider four variables and **their interaction** with zipcode. This amounts to fit a multiple regression with the four variables for each zip code. There are 70 different zip codes, representing different intercepts. The estimated coefficients are typically presented as the difference (contrast) to the baseline factor (zipcode: 98001).

```
train_data$zipcode = as.factor(train_data$zipcode)  #treat zipcode as factor
test_data$zipcode = as.factor(test_data$zipcode)

fit.lm4 = lm(price ~ bathrooms + bedrooms + sqft_living + sqft_lot+ zipcode
+ zipcode*bathrooms + zipcode*bedrooms+zipcode*sqft_lot
+ zipcode*sqft_living, data = train_data)
summary(fit.lm4)
```

```
Residual standard error: 156900 on 14779 degrees of freedom
Multiple R-squared:  0.822, Adjusted R-squared:  0.8178
F-statistic: 195.5 on 349 and 14779 DF,  p-value: < 2.2e-16
```

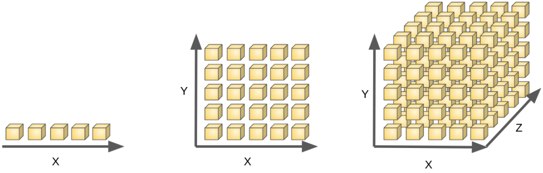
```
fit.lm4.pred.out <- predict(fit.lm4, newdata = test_data)
SS.residual <- sum( (test_data$price - fit.lm4.pred.out)^2)
1 - SS.residual / SS.total
[1] 0.7950443
```

Multivariate spline regression

Idea: Tensor products of univariate basis functions

$$\{B_{i_1}(x_1)B_{i_2}(x_2)\cdots B_{i_p}(x_p)\}_{i_1=1}^{b_1}\cdots{}_{i_p=1}^{b_p}$$

Drawbacks: **curse of dimensionality**, namely, number of basis functions scales exponentially with p



d	n^d	accuracy $n^{-\frac{2}{d+4}}$
1	**100**	**100**
2	10^4	250
5	10^{10}	4000
10	10^{20}	40000
100	10^{200}	$4 * 10^{41}$

Structured multivariate regressions

Remedy: Add additional structure to $f(\cdot)$

Example: Additive model

$$Y = f_1(X_1) + \cdots + f_p(X_p) + \varepsilon$$

- Number of basis functions scales **linearly** with p

Example: Bivariate interaction models:

$$Y = \sum_{1 \le i \le j \le p} f_{ij}(X_i, X_j) + \varepsilon$$

- Number of basis functions scales **quadratically** with p
- Implementation: Bivariate tensors

Best predictor and nonparametric regression

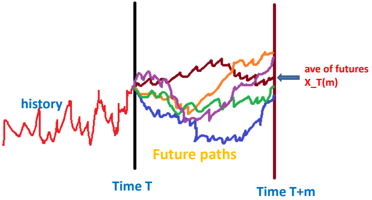
Double Expectation: $EZ = E\{E(Z|\mathbf{X})\}$, for any $\mathbf{X}$

Bias-var in prediction: Letting $f^*(\mathbf{X}) = E(Y|\mathbf{X})$, then

$$E(Y - f(\mathbf{X}))^2 = \underbrace{E(Y - f^*(\mathbf{X}))^2}_{\text{var}=E\sigma^2(\mathbf{X})} + E(\underbrace{f^*(\mathbf{X}) - f(\mathbf{X})}_{\text{bias}})^2.$$

Best prediction: $E(Y|\mathbf{X}) = \operatorname{argmin}_f E(Y - f(\mathbf{X}))^2$

Nonparametric reg.: Estimating $f^*(\cdot)$ directly



Bias variance decomposition

Bias-var in estimation: letting $\bar{f}(\mathbf{x}) = E\widehat{f}_n(\mathbf{x})$, then

$$E(\widehat{f}_n(\mathbf{X}) - f^*(\mathbf{X}))^2 = \underbrace{E(\widehat{f}_n(\mathbf{X}) - \bar{f}(\mathbf{X}))^2}_{\text{var}} + E(\underbrace{\bar{f}(\mathbf{X}) - f^*(\mathbf{X})}_{\text{bias}})^2.$$

Role of Modeling:

★variance is small when n large, big when no. of parameters is big

★biases are small when model is complex (no. of parameters is big)

1.3. Ridge Regression

Ridge Regression

Drawbacks of OLS: ★$n > p$

★large variance when collinearity: $\text{Var}(\widehat{\beta}) = \sigma^2(\mathbf{X}^T\mathbf{X})^{-1}$

Remedy: Ridge regression (Hoerl and Kennard, 1970)

$$\widehat{\beta}_\lambda = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$$

★$\lambda > 0$ is a regularization parameter.

Tikhonov (1943) regularization

Interpretation: Penalized LS $\|\mathbf{y} - \mathbf{X}\beta\|^2 + \lambda\|\beta\|^2$.

—Setting the gradient to zero, we get $\mathbf{X}^T(\mathbf{X}\beta - \mathbf{y}) + \lambda\beta = \mathbf{0}$.

Bias-Variance Tradeoff

Smaller variances:

$$\mathrm{Var}(\widehat{\beta}_\lambda) = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{X}(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\sigma^2 \prec \mathrm{Var}(\widehat{\beta}).$$

Larger biases:

$$E(\widehat{\beta}_\lambda) - \beta = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{X}\beta - \beta = -\lambda(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\beta.$$

Overall error:

$$\mathrm{MSE}(\widehat{\beta}_\lambda) = E\,\|\widehat{\beta}_\lambda - \beta\|^2 = \mathrm{tr}\{(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-2}[\lambda^2\beta\beta^T + \sigma^2\mathbf{X}^T\mathbf{X}]\}.$$

Generalization: ℓ_q Penalized Least Squares

ℓ_q penalized least-squares estimate:

$$\min_{\beta} = \|\mathbf{y} - \mathbf{X}\beta\|^2 + \lambda \|\beta\|_q^q, \quad q \geq 0.$$

- λ tuning parameter, $\|\beta\|_q^q = |\beta_1|^q + \cdots + |\beta_p|^q$
- $q = 0$ is the best subset selection $\quad \|\beta\|_0 = \#\{j : \beta_j \neq 0\}$
- Only $q = 2$ admits a closed-form solution.
- Known as Bridge estimator (Frank and Friedman, 1993);
- When $q = 1$, called Lasso estimator (Tibshirani, 1996);
- Folded concave when $0 < q < 1$ and convex when $q > 1$;

Prediction by similarity

Theorem 2.4. Alternative expression $\widehat{\beta}_\lambda = \mathbf{X}^T(\mathbf{X}\mathbf{X}^T + \lambda \mathbf{I})^{-1}\mathbf{y}$

Prediction at $\mathbf{x}$ is $\widehat{y} = \mathbf{x}^T\widehat{\beta}_\lambda = \mathbf{x}^T\mathbf{X}^T(\mathbf{X}\mathbf{X}^T + \lambda\mathbf{I})^{-1}\mathbf{y}$.

Note that $(\mathbf{X}\mathbf{X}^T)_{ij} = \langle \mathbf{x}_i, \mathbf{x}_j \rangle$ and $\mathbf{x}^T\mathbf{X}^T = (\langle \mathbf{x}, \mathbf{x}_1 \rangle, \cdots, \langle \mathbf{x}, \mathbf{x}_n \rangle)$.

- Prediction depends only **pairwise inner products**; **similarity**
- Generalize to other **similarity measures** $K(\cdot, \cdot)$, called **kernel** trick.

$K\Big($ ,  $\Big) = +10$ $\quad \mathcal{K}\Big($ ,  $\Big) = -10$

Kernel regression

Kernel: $\mathbf{K} = (K(\mathbf{x}_i, \mathbf{x}_j))_{n\times n}$ is PSD, for any $\{\mathbf{x}_i\}_{i=1}^n$.

Commonly used kernels: $K(\mathbf{u}, \mathbf{v})$

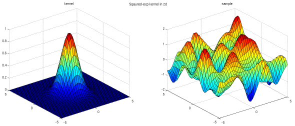
★linear $\langle \mathbf{u}, \mathbf{v} \rangle$ ★polynomial $(1 + \langle \mathbf{u}, \mathbf{v} \rangle)^{\mathbf{d}}$, $d = 2, 3, \cdots$;

★Gaussian $e^{-\gamma\|\mathbf{u}-\mathbf{v}\|^2}$ ★Laplacian $e^{-\gamma\|\mathbf{u}-\mathbf{v}\|}$

Basis: $\{K(\cdot, \mathbf{x}_j)\}_{j=1}^n$ and express $f(\mathbf{x}) = \sum_{j=1}^n \alpha_j K(\mathbf{x}, \mathbf{x}_j)$. Fit

$$\min_{\alpha \in \mathbb{R}^n} \left\{ \|\mathbf{y} - \mathbf{K}\alpha\|^2 + \lambda \alpha^T \mathbf{K} \alpha \right\}, \quad \mathbf{K} = (K(\mathbf{x}_i, \mathbf{x}_j))$$

■No curse-of-dim in implementation!



Kernel ridge regression

Kernel ridge regression

With $\mathbf{K} = (K(\mathbf{x}_i, \mathbf{x}_j)) \in \mathbb{R}^{n\times n}$, prediction at $\mathbf{x}$ is

$$\widehat{y} = (K(\mathbf{x}, \mathbf{x}_1), \cdots, K(\mathbf{x}, \mathbf{x}_n))(\mathbf{K} + \lambda \mathbf{I})^{-1}\mathbf{y},$$

★ $\widehat{y} = \overbrace{\widehat{f}(\mathbf{x})}^{\text{pred}} = \sum_{i=1}^{n} \overbrace{\alpha_i}^{\text{weight}} K(\mathbf{x}, \mathbf{x}_i),$ $\quad\widehat{\alpha} = (\mathbf{K} + \lambda\mathbf{I})^{-1}\mathbf{y};$

testing testing training

★ tune the parameter λ to minimize prediction errors.

1.4 Reproducing Kernel Hilbert Spaces

Justification of Kernel Tricks by Representer Theorem

Hilbert Space

Hilbert space: a linear space of functions endowed with an inner product.

■ $\mathcal{X}$ = set, $\mathcal{H}$ = a space of functions on $\mathcal{X}$ with inner product $\langle \cdot, \cdot \rangle$.

Kernel function $K(\cdot, \cdot)$: Matrix $(K(\mathbf{x}_i, \mathbf{x}_j))_{n \times n}$ is PSD, for all $\{\mathbf{x}_i\}_{i=1}^n$,

Eigen-decomposition:

$$K(\mathbf{x}, \mathbf{x}') = \sum_{j=1}^{\infty} \gamma_j \psi_j(\mathbf{x}) \psi_j(\mathbf{x}'), \qquad \sum_{j=1}^{\infty} \gamma_j^2 < \infty$$

— $\{\gamma_j\}_{j=1}^{\infty}$ are **eigenvalues**, and $\{\psi_j\}_{j=1}^{\infty}$ are **eigen-functions**.

Reproducing Hilbert Space

Hilbert space associated with K: $\mathcal{H}_K = \{g = \sum_{j=1}^{\infty} \beta_j \psi_j\}$, endowed with inner product

$$\langle g, g' \rangle_{\mathcal{H}_K} = \sum_{j=1}^{\infty} \gamma_j^{-1} \beta_j \beta_j'; \qquad \|g\|_{\mathcal{H}_K} = \sqrt{\langle g, g \rangle_{\mathcal{H}_K}},$$

for any $g, g' \in \mathcal{H}_K$ with $g = \sum_{j=1}^{\infty} \beta_j \psi_j, g' = \sum_{j=1}^{\infty} \beta_j' \psi_j$.

Reproducibility: $\langle K(\cdot, x'), g \rangle_{\mathcal{H}_K} = \sum_j \gamma_j^{-1} \{\gamma_j \psi_j(\mathbf{x}')\} \beta_j = g(\mathbf{x}')$.

Representer Theorem

Theorem 2.6. For a loss L and increasing function $P_\lambda(\cdot)$, let

$$\widehat{f} = \text{argmin}_{f \in \mathcal{H}_K} \left\{ \sum_{i=1}^{n} L\big(y_i, f(\mathbf{x}_i)\big) + P_\lambda(\|f\|_{\mathcal{H}_K}) \right\}, \quad \lambda > 0,$$

Then (homework)

$$\widehat{f}(\cdot) = \sum_{j=1}^{n} \widehat{\alpha}_j K(\cdot, \mathbf{x}_j),$$

where $\widehat{\alpha} = (\widehat{\alpha}_1, \cdots, \widehat{\alpha}_n)^T$ solves

$$\min_{\alpha} \left\{ \sum_{i=1}^{n} L\Big(y_i, \sum_{j=1}^{n} \alpha_j K(\mathbf{x}_i, \mathbf{x}_j)\Big) + P_\lambda\left(\sqrt{\alpha^T \mathbf{K} \alpha}\right) \right\}.$$

★ **Infinite-dimensional** regression problem;

★ **Finite-dimensional** representation for the solution.

Outline of Proof

1. Any f can be written as $f = f_K + r$, where $f_K(\cdot) = \sum_{j=1}^n \alpha_j K(\cdot, \mathbf{x}_j)$ (projection) and r is in its orthogonal complement.

2. Orthogonality entails $0 = \langle K(\cdot, x_j), r \rangle_{\mathcal{H}_K} = r(x_j)$ by reproducibility. Hence, $f(x_i) = f_K(x_i)$ (the same loss).

3. But $\|f\|^2_{\mathcal{H}_K} = \|f_K\|^2_{\mathcal{H}_K} + \|r\|^2_{\mathcal{H}_K} \geq \|f_K\|^2_{\mathcal{H}_K}$.

4. Optimality reaches only if $r = 0$.

5. $\langle f, f \rangle_{\mathcal{H}_K} = \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j \langle K(\cdot, x_i), K(\cdot, x_j) \rangle_{\mathcal{H}_K} = \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j K(x_i, x_j)$.

Applications of Representer Theorem

Apply representer theorem to **kernel ridge regression**

$$\widehat{f} = \mathrm{argmin}_{f \in \mathcal{H}_K} \left\{ \sum_{i=1}^{n} \big(y_i - f(\mathbf{x}_i)\big)^2 + \lambda \|f\|^2_{\mathcal{H}_K} \right\}.$$

We must have $\widehat{f} = \sum_{i=1}^{n} \widehat{\alpha}_i K(\cdot, \mathbf{x}_i)$ with $\widehat{\alpha} \in \mathbb{R}^n$ solving

$$\min_{\alpha \in \mathbb{R}^n} \left\{ \|\mathbf{y} - \mathbf{K}\alpha\|^2 + \lambda \alpha^T \mathbf{K}\alpha \right\}.$$

It is easily seen that

$$\widehat{\alpha} = (\mathbf{K} + \lambda \mathbf{I})^{-1} \mathbf{y}.$$

1.5 Cross-Validation

Cross-Validation

Purpose: To estimate **Prediction Error** for a procedure; to select tuning parameters, and compare multiple methods

k-fold Cross-Validation (CV)

- ★ Divide data randomly and evenly into k subsets;
- ★ Use one fold as **testing set** and remaining as **training set** to compute testing errors;
- ★ Repeat for each of k subsets and average testing errors.

PE for training size: $(1 - 1/k)n$

Choice of k: $k = n$ (best, but expensive; leave-one out), 10 or 5 (5-fold).

Leave-one-out: $\mathrm{CV} = \frac{1}{n}\sum_{i=1}^{n}[y_i - \widehat{f}^{-i}(\mathbf{x}_i)]^2$, $\widehat{f}^{-i}(\mathbf{x}_i) =$ predicted value based on $\{(\mathbf{x}_j, y_j)\}_{j \neq i}$

Linear smoother

■ $\widehat{\mathbf{y}} = \mathbf{S}\mathbf{y}$ for data $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$, **S** depends only on **X**.

Self-stable if $\bar{f}(\mathbf{x}) = \widehat{f}(\mathbf{x})$, where $\bar{f}$ is estimated function based on data $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$ and $(\mathbf{x}, \widehat{f}(\mathbf{x}))$, and $\widehat{f}$ based on $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$

Theorem 2.7. For a self-stable linear smoother $\widehat{\mathbf{y}} = \mathbf{S}\mathbf{y}$,

$$y_i - \widehat{f}^{-i}(\mathbf{x}_i) = \frac{y_i - \widehat{y}_i}{1 - S_{ii}}, \quad \forall i \in [n], \qquad \mathrm{CV} = \frac{1}{n}\sum_{i=1}^n \left(\frac{y_i - \widehat{y}_i}{1 - S_{ii}}\right)^2.$$

Proof: By self-stability, $\{(\mathbf{x}_j, y_j), j \neq i\}$ and $\{(\mathbf{x}_j, y_j), j \neq i, (\mathbf{x}_i, \widehat{\mathbf{f}}^{(-i)}(\mathbf{x}_i))\}$ have the same fit: $\widehat{f}^{(-i)}(\mathbf{x}_i) = S_{ii}\widehat{f}^{(-i)}(x_i) + \sum_{j\neq i} S_{ij} y_j$ or $\widehat{f}^{(-i)}(\mathbf{x}_i) = \sum_{j\neq i} S_{ij} y_j/(1 - S_{ii})$. The proof follows from $\widehat{y}_i = S_{ii} y_i + \sum_{j\neq i} S_{ij} y_j$ and a simple algebra.

Generalized Cross-Validation

GCV (Golub et al., 1979): $\mathrm{GCV} = \frac{\frac{1}{n}\sum_{i=1}^{n}(y_i - \widehat{y}_i)^2}{[1-\mathrm{tr}(\mathbf{S})/n]^2}$.

■ $\mathrm{tr}(\mathbf{S})$ is called **effective degrees of freedom**.

GCV chooses λ by minimizing

$$\mathrm{GCV}(\lambda) = \frac{\frac{1}{n}\mathbf{y}^T(\mathbf{I}-\mathbf{S}_\lambda)\mathbf{y}}{[1-\mathrm{tr}(\mathbf{S}_\lambda)/n]^2}.$$

Self-stable Method	$\mathbf{S}$	$\mathrm{tr}(\mathbf{S})$
Multiple Linear Regression	$\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$	p
Ridge Regression	$\mathbf{X}(\mathbf{X}^T\mathbf{X}+\lambda\mathbf{I})^{-1}\mathbf{X}^T$	$\sum_{j=1}^{p}\frac{d_j^2}{d_j^2+\lambda}$
Kernel Ridge Regression in RKHS	$\mathbf{K}(\mathbf{K}+\lambda\mathbf{I})^{-1}$	$\sum_{j=1}^{n}\frac{\gamma_j}{\gamma_j+\lambda}$

★ $\{d_j\}$ and $\{\gamma_j\}$ are singular values of $\mathbf{X}$ and $\mathbf{K}$.