Fundamentels of Machine Learning

Ullrich Köthe

WS 2017, Heidelberg

Skript zur Vorlesung an der Universität Heidelberg

Inhaltsverzeichnis

Rational of Machine Learning

- Interest in attributes/quantities Y ("response"), but they are not easily measurable.
- Choose attributes/quantities X ("features"), that are easy to measure.
- find a mapping $Y = f(X)$ to determine Y indirectly
- many problems don't have an explicit analytical $f(X)$
- $\Rightarrow$ use "generic mapping": $Y = f(X, \theta)$, θ : adjustable parameters (ideally a universal approximate) and adjust θ by learning from a training set:

$$TS = \{(X_i, Y_i)\}_{i=1}^{N}$$

- usually the relation between X and Y is not deterministic
- posterior probability:

$$p(Y|X;\theta)$$

$$f(X) = \begin{cases} Y_1 & \text{with probability } p(Y = Y_1|X;\theta) \\ Y_2 & \text{with probability } p(Y = Y_2|X;\theta) \end{cases}$$

Kinds of Variables

- numeric: $X \in \mathbb{R}^D, Y \in \mathbb{R}^M$ (usually M=1)
- discrete: $X \in \{A, B, C, ...\}$
- ordinal: categories are ordered $A < B < C$
- categorical: $X \in \{"red", "green", "blue"\}, Y \in \{"pea", "pear", "peach"\}$

if response is discrete $\Rightarrow$ classification
if response is numeric $\Rightarrow$ regression

Notation

- instances in training set subscript $i \in \{1, ..., N\}$
- X_i : features of training instance (row vector)
- Y_i : response
- features we measure: subscript $j \in \{1, ..., M\}$
- X_j : j-th feature of all instances (column vector)
- X_{ij} : j-th feature of instance i (a scalar)

Kinds of training data

- supervised learning: Y_i is known for all training instances
  - possible if we can obtain Y_i in a research setting
  - measuring, asking expert
  - measuring Y_i is destructive (crash test)
  - Y_i is only known in hind sight
  - we know the mapping $Y_i = f(Y_i)$ for $TS\{(X_i, Y_i)\}$
  - training strategies:
    - watch training: TS is given beforehand
    - online training
    - active training
- unsupervised learning: X_i are known, Y_i not ("data mining")
  - group data by similarity
  - determine useful categories
  - find interesting features
  - estimate probability distribution $p(X)$
  - novely detection - find unusual X

1 Classification

1.1 Rules

- instances are i.i.d. (independent identically distributed)
- Y is discrete with C categories $Y \in \{1, 2, ..., C\}$
  $C = 2 : Y \in \{0, 1\}, \{-1, 1\}$
- X is numeric or discrete
- if the outcome is certain: estimate posterior probability $p(Y|X; \theta)$
- but in many situations a hard decision is needed:

Example: hiring X, credentials: $p(Y =$ will design good bike$|X)$ needs a hard decision function:

$$f(x) = \begin{cases} \text{hire if X is convincing} \\ \text{not hire else} \end{cases}$$

1.2 How badly does a bad decision function perform?

Suppose we know the prior probability of each category (prior - before, without measuring X)

$$p(Y = K) = \pi_k \quad k = 1, ..., C$$

$$\Rightarrow \text{most sensible decision function:} \quad f(k) = \arg\max_k \pi_k = \hat{k}$$

$$\text{success rate} = \pi_{\hat{k}}$$

$$\text{error rate} = 1 - \pi_{\hat{k}} = 1 - \arg\max_k \pi_k$$

1.3 How good can a decision function perform in an uncertain environment?

Sources of uncertainty:

- intrinsic uncertainty:
  - fundamental(Q.M.)
  - noise (can measure X and Y only to certain accuracy)
- insufficient knowledge:
  - X may not have enough information to determine Y exactly
  - missing data
- modelling uncertainty:
  - $Y = f(X, \theta)$ may not be powered enough to express the true relationship $Y = f^*(X)$
  - θ may not be set to the optimal values

Assume that there is no modelling error and no noise in Y, no missing data

$$\Rightarrow \text{our posterior:} \quad \hat{p}(Y|X) = p^*(Y|X)$$

so we know the probability distribution.
What decision funtion $\hat{f}$ minimizes the error fo C = 2?

$$p^*(Y = 1|X) \quad p^*(Y = -1|X)$$

$$\text{Two decision functions:} \begin{cases} f_1(X) = f(X; \theta_1) = 1 \\ f_{-1}(X) = f(X; \theta_{-1}) = -1 \end{cases}$$

choose f_1:

- a) true positive $Y^*(X) = 1$
- b) false positive $Y^*(X) = -1$

choose f_{-1}:

- c) true negative $Y^*(X) = -1$

- d) false negative $Y^*(X) = 1$

Probabilities: a) = d): $p^*(Y = -1|X) = 1 - p^*(Y = 1|X)$
Success is maximized if we always decide fo most probable outcome, given X:

$$\hat{Y} = \hat{f}(X) = \arg\max_k p^*(Y = K|X) \quad \text{Bayes classifier rule}$$

$$\begin{aligned} p(error_{Bayes}) &= \mathbb{E}_x[p(error(x))] \\ &= \int (1 - \max_k(y = k|x))p^*(x)dx \quad x \in \mathbb{R}^D \text{ with } p^*(x) \end{aligned}$$

Definition: Decision regions are connected regions in $\mathbb{R}^D$ where $\hat{f}(x) = const$.

1.4 Discriminative vs. Generative models

$$\text{Bayes Rule:} \quad p(Y|X) = \frac{p(X|Y) * p(Y)}{p(X)}$$

$$\text{posterior} : p(Y|X) \quad \text{likelihood} : p(X|Y) \quad \text{prior} : p(Y) \quad \text{data density/evidence} : p(X)$$

discriminative model: learn LHS of Bayes: p(Y|X)
generative model: learn RHS of Bayes: p(Y), p(X|Y), p(X)

$$p(X) = \sum_{K=1}^{N} p(X|Y = K)p(Y = K)$$

⇒ can be used to create more data by simulation, disadvantage: usually needs more training data for the same success rate

$$C = \text{Bayes decision function} \quad f(x) = \begin{cases} +1 & \text{if} \quad p(y = 1|x) \geq p(y = -1|x) \\ -1 & else \end{cases}$$

$$\begin{aligned} \frac{p(x|y = 1)p(y = 1)}{p(x)} &> \frac{p(x|y = -1)p(y = -1)}{p(x)} \\ \iff \quad \frac{p(x|y = 1)p(y = 1)}{p(x|y = -1)p(y = -1)} &\geq 1 \\ \iff \quad \log(p(x|y = 1)p(y = 1)) - \log(p(x|y = -1)p(y = -1)) &\geq 0 \\ \iff \quad \log(\frac{p(x|y = 1)}{p(x|y = -1)}) + log(\frac{\pi_1}{\pi_{-1}}) &\geq 0 \end{aligned}$$

$$\pi_k = \frac{1}{C} = const \quad \pi_1 = \pi_{-1} = \frac{1}{C}$$

$$\Rightarrow \quad \text{max. likelihood decision rule} \quad f(x) = \begin{cases} 1 & if \frac{p(x|y=1)}{p(x|y=-1)} \geq 1 \\ -1 & else \end{cases}$$

Example: Y ∈ red, blue, X ∈ ball pen, marker

$$\pi_{red} = \pi_{blue} = 0.5$$

$$p(marker|red) = \frac{5}{7} \quad p(marker|blue) = \frac{2}{7} \quad p(ball|red) = \frac{2}{7} \quad p(ball|blue) = \frac{5}{7}$$

$$\begin{aligned} p(ball) &= p(ball|y = red) * p(red) + p(ball|y = blue) * p(blue) \\ &= \frac{2}{7} * \frac{1}{2} + \frac{5}{7} * \frac{1}{2} = \frac{1}{2} \end{aligned}$$

$$p(red|ball) = \frac{p(ball|red)}{p(ball)} = \frac{\frac{2}{7} * \frac{1}{2}}{\frac{1}{2}}$$

$$p(blue|ball) = \frac{5}{7} \quad p(red|marker) = \frac{5}{7} \quad p(blue|marker) = \frac{2}{7}$$

⇒ Bayes decision:

$$f(x = marker) = \arg\max_k p(y = k|marker) \quad = \text{red}$$

$$f(x = ball) = \arg\max_k p(y = k)|ball) \quad = \text{blue}$$

1.5 Nearest Neighbor Classification

Intuition: in an unknown situation, act as you did in the most similar situation in the past

- 'past': training set
- 'act as you did': copy the training label to the new instance

For 'most similar' we need a distance function between features $d(x, x')$

$$\text{decision rule} : f_{NN}(x) = y_i, \quad i = \underset{n \in Trainingset}{\arg\min} \quad d(x_i, x_{i'})$$

effect: split feature space according to the distanc to training examples

$$neighbors(x_i) = \{x|d(x, x_i) \leq d(x, x_{i'})\} \quad \forall i \neq i'$$

'Voroni tessellation' with centers $\{x_i\}_{i=1}^N$

each region is a voroni cell of x_i
decision boundaries: bisectors between centers

1.5.1 Performance Analysis of NN classifier

- derive analytic formulas for error for finite training set, this ist the best, but usually very difficult
- derive analytic error formulas in the limit for infinitly many training data 'asymptotic analysis', this is usually easier, but often unrealistic (when error decreases slowly with N)
- measure error empirically on independent test data('ground truth'): most ralistic, but must be repeated for every model and application, beware of the multiple testing bias if test data is reused

finite sample analysis example:

$$C = 2 \quad y \in \{0, 1\}, \quad p(y = 0) = p(y = 1) = \frac{1}{2}$$

$$p(x|y = 0) = 2 - 2x \quad p(x|y = 1) = 2x$$

$$\begin{aligned} \int_0^1 P(x|y = 0)dx &= \int_0^1 (2 - 2x)dx \\ &= 2x - x^2\Big|_0^1 = 1 \end{aligned}$$

$$\begin{aligned} p(x) &= p(x|y = 0)p(y = 0) + p(x|y = 1)p(y = 1) \\ &= (2 - 2x)\frac{1}{2} + 2x\frac{1}{2} \\ &= 1 - x + x = 1 \end{aligned}$$

$$\begin{aligned} \text{postkrias} \quad p(y = 0|x) &= \frac{p(x|y = 0)p(y = 0)}{p(x)} \\ &= \frac{(2 - 2x)\frac{1}{2}}{1} \\ &= 1 - x \end{aligned}$$

$$p(y = 1|x) = \frac{2x\frac{1}{2}}{1} = x$$

define two decision rules with 'threshold' t:

$$A: \quad f_A(x;t) = \begin{cases} 0 & \text{if } x \leq t \\ 1 & \text{if } x > t \end{cases}$$

$$B: \quad f_B(x;t) = \begin{cases} 1 & \text{if } x \leq t \\ 0 & \text{if } x > t \end{cases}$$

$$\mathbb{1}[condition] = \begin{cases} 1 & \text{if condition = true} \\ 0 & \text{if condition = false} \end{cases} \quad \text{'Indicator function'}$$

$$\begin{aligned} p(A;t|error) &= \mathbb{E}_x[p(f_A(x;t) \neq Y^*|t)] \\ &= \mathbb{E}_x[p(y=1|x)\mathbb{1}[x \leq t]] + \mathbb{E}_x[p(y=0|x)\mathbb{1}[x;t]] \\ &= \int_0^1 p(y=1|x)\mathbb{1}[x]p(x)dx + \int_0^1 p(y=0|x)\mathbb{1}[x>t]p(x)dx \\ &= \int_0^1 p(y=1|x)p(x)dx + \int_t^1 p(y=0|x)p(x)dx \\ &= \int_0^t x dx + \int_t^1 (1-x)dx \\ &= \frac{x^2}{2}\Big|_0^t + (x - \frac{x^2}{2})\Big|_t^1 \\ &= \frac{t^2}{2} - 0 + 1 - \frac{1}{2} - t + t^2 \\ &= t^2 - t + \frac{1}{2} = (t - \frac{1}{2})^2 + \frac{1}{4} \\ &= p(error|A,t) \end{aligned}$$

$$p(error|B,t) = \frac{3}{4} - (t - \frac{1}{2})^2 = 1 - p(error|A,t)$$

Bayes classifier(minimizes error): rate A with $t = \frac{1}{2}$

$$p(error|A, t = \frac{1}{2}) = \frac{1}{4}$$

Error of NN classifier, simplest possible TS with N = 2:

- sample z = (x, y)
- repeat: sample z' = (x', y') until $y' \neq y$, 'rejection sampling'

Two possible outputs:

$$\left.\begin{array}{l} A : x_0(y_0 = 0) \leq x_1(y_1 = 1) : ruleA \\ B : x_0(y_0 = 0) > x_1(y_1 = 1) : ruleB \end{array}\right\} t = \frac{x_0 + x_1}{2}$$

$$p(error) = \mathbb{E}_{TS}[p(error|TS)] = \mathbb{E}_{TS(A)}[p(error(A,t))] + \mathbb{E}_{TS(B)}[p(error|B,t)]$$

$$\begin{aligned} \mathbb{E}_A &= \int_0^1 \int_0^1 \int_0^1 \underbrace{p(error|A,t)}_{=(t-\frac{1}{2})^2+\frac{1}{4}} \underbrace{p(A,t|x_0,x_1)}_{=\mathbb{1}[x_0\leq x_1]\delta(t-\frac{x_0+x_1}{2})} \underbrace{p(x_0,x_1)}_{=p(x|y=0)p(x|y=1)} dt dx_1 dx_0 \\ &= \int_0^1 p(x|y=0) \int_{x_0}^1 p(x|y=1) p(error|A, t = \frac{x_0 + x_1}{2}) dx_1 dx_0 \\ &= \int_0^1 (2 - 2x) \int_{x_0}^1 2x_1((\frac{x_0 + x_1}{2} - \frac{1}{2})^2) + \frac{1}{4}) dx_1 dx_0 \\ &= \frac{83}{360} \end{aligned}$$

$$p(error|B) = \frac{43}{360} \Rightarrow p(error) = \frac{7}{20}$$

Cross Validation We need: generalization error (on unseen, new data) p(error)
We have: training error/fit error

$$h_{TS} = \frac{1}{N} \sum_{i=1}^{N} \mathbb{1}[f(x_i) \neq y_i']$$

$$p_{error} = h_{TS} + w_{modeloptimism} \quad w \geq 0$$

if $p_{error} - h_{TS} = w$ is big, the model overfits the training set. Many models tend to overfit quite badly.
$\Rightarrow$ solutions:

- use more training data (expensive)
- use better models
- use regularization

e.q. nearest neighbor classifier $h_{TS} = 0$
how to estimate the error?

- split the training set at random in two subsets for training and test
- train on the training subset
- calculate the error on the test subset

$\Rightarrow$ since the choice of training and testset was arbitrary, reverse their roles and repeat and take the average of the two error (2-fold cross validation)
results are improved (error more reliable) by using more subsets 'K-fold cross validation'

- bring data into a random order (random-shuffle)
- put the first $\frac{N}{K}$ instances into fold 1
- put the second $\frac{N}{k}$ instances into fold 2
- repeat for $l = 1, ..., K$
- use all folds except fold l for training
- use fold l for testing
- compute means and variance of the K errors
- popular $K = 2, 5, 10$ K = N: 'leave-one-out-cross-validations' for theoretical analysis

Asymptotic Analysis

- find analytic formulas for how the method performs with infinite training data
- $N \to \infty$ (training data)
- Definition: A learning algorithm is called consistent if it converges to the optimal Bayes classifier as $N \to \infty$
- prove now: NN classifier is <u>not</u> consistent, but not too far of (a factor of 2): $p_{00}^{NN} \leq 2p*$
- let $p(error|x, x')$ be the expected error for test point x, when x' is its nearest training point
- let p(x|x') be the probabilty that x' is n.n. of test point

$$\begin{aligned} p(error|y) &= \int p(error|x, x')p(x'|x)dx' \quad \text{(marginalize over unknown point x')} \\ &= \mathbb{E}_{x'}[p(error|x, x')] \end{aligned}$$

1) If density p(x) is continous and positive:

$$\lim_{N\to\infty} p(x'|x) = \delta(x - x')$$

Let $p_\varepsilon(x)$ be the probability that an ε-ball around x:

$$B_\varepsilon(x) = \{x' | \|x - x'\| \leq \varepsilon\}$$

contains at least one training point. Then $(1 - p_\varepsilon)^N$ is the probabilty, that none of N training points is in $B_\varepsilon(x)$

$$\text{By assumption} \quad \forall\varepsilon > 0 \quad p_\varepsilon(x) = \int_{B_\varepsilon(x)} p(x')dx' > 0$$

$$\lim_{N\to\infty}(1-p_\varepsilon(x))^N = 0 \Rightarrow \forall\varepsilon > 0 \quad \text{there is a point in } B_\varepsilon(x)$$

2)

$$\begin{aligned} p(error|x,x') &= 1 - p(correct|x,x') \\ &= 1 - \sum_{k=1}^{c} p(y=k, y'=k|x,x') \\ &= 1 - \sum_{k=1}^{c} p(y=k|x)p(y'=k|x') \quad \text{due to i.i.d.} \end{aligned}$$

3)

$$\text{Insert:} \quad p_\infty(error|x) = \int \underbrace{p(error|x,x')}_{1-\sum_i^c} \underbrace{p(x'|x)}_{\delta(x-x')} dx'$$

$$= 1 - \sum_{k=1}^{c} p(y=k|x)^2 \quad \text{Gini impurity at point x}$$

- if data at point x are pure, i.e. only one class occurs, say $y = k^* \Rightarrow p(y=k^*|x) = 1$ and $p(y=k|x) = 0$ for $k \neq k^* \Rightarrow p_\infty(error|x) = 0$
- worst: data are impure, i.e. all classes gave same probability $p(y=k|x) = \frac{1}{c} \Rightarrow$

$$p_\infty(error|x) = 1 - \sum_{k}^{c} \frac{1}{c^2} = 1 - \frac{1}{c} = \frac{c-1}{c} \geq \frac{1}{2}$$

4) Derive worst case behavior aver all x as a function of Bayes error p^*

$$p_\infty(error) = \mathbb{E}_x[p_\infty(error|x)]$$

Let $p(y=\hat{k}|x)$ be the Bayes decision at x, $\hat{k} = \arg\max_k p(y=k|x)$
$\Rightarrow$ Bayes error at x:

$$p^*(error|x) = 1 - p(y=\hat{k}|x)$$

$$\sum_{k=1}^{c} p(y=k|x)^2 = (1-p^*(error|x))^2 + \sum_{k=\hat{k}} p(y=k|x)^2$$

worst case analysis: make the error big, i.e. make this sum small

$$\text{Probability:} \quad \sum_k p_k^2 \quad \text{is minimized under constrains} \quad p_k \geq 0 \quad \text{and} \quad \sum_k p_k = const$$

$$if \quad p_k = p'_k \forall k, k' \quad p_k = p^*(error|x)$$

$$\Rightarrow p_k = \frac{p^*(error|x)}{c}$$

worst case error:

$$\sum_{k=1}^{c} p(y=k|x) \geq (1-p^*(error|x))^2 + \sum_{k=k'} (\frac{p^*(error|x)}{c-\frac{1}{2}})^2$$
$$= 1 - 2p^*(error|x) + p^*(error|x) + \frac{p^*(error|x)^2}{c-1} \quad = 1 - 2p^*(error|x) + \frac{c}{c-1} p^*(error|x)^2$$

5) Inserting gives the relationship between error of NN classifier and Bayes classifier:

$$p_\infty(error|x) = 1 - \sum_{k}^{c} p(y=k|x) \leq 1 - (1 - 2p^*(error|x)) + \frac{c}{c-1} p^*(error|x)^2$$
$$= 2p^*(error|x) - \frac{c}{c-1} p^*(error|x)^2$$

6) Total error = expectation over x

$$p_\infty(error) = \mathbb{E}_x[p_\infty(error|x)] = \int p_\infty(error|x)p(x)dx$$
$$\leq \int 2p^*(error|x)p(x)dx - \int \frac{c}{c-1} p^*(error|x)^2 p(x)dx$$
$$= 2\mathbb{E}_x[p^*(error|x)] - p^*(error)$$
$$\leq 2p^*(error) - \frac{c}{c-1} p^*(error)^2$$

simplified by non neg. of variance:

$$\int (p^*(error|x) - p^*(error))^2 p(x)dx \geq 0$$
$$\leftrightarrow \int p^*(error|x)^2 p(x)dx \geq p^*(error)^2$$

$$\text{Result:} \quad p^*(error) \leq p_\infty^N N(error) \leq p^*(error)(2 - \frac{c}{c-1} p^*(error))$$

Special Cases:

- best case: $p^* = 0 \Rightarrow p^\infty \leq 0 \quad 0(2 - \frac{c}{c-1}0) = 0 \quad$ NN is perfect

- worst case: $p^* = \frac{c-1}{c}$ (pure guessing) $\Rightarrow$

$$\begin{aligned} p_\infty &< \frac{c-1}{c}(2 - \frac{c}{c-1}\frac{c-1}{c}) \\ &= \frac{c-1}{c} \end{aligned}$$

- normal case: Bayes classifier performs well, but not perfect:

$$\begin{aligned} p^* = \varepsilon \ll 1 \forall c \geq 2 : \frac{c}{c-1} \leq 2 \\ p_\infty \leq \varepsilon(2 - \underbrace{\frac{c}{c-1}}_{\ll 1}\varepsilon) \leq 2\varepsilon = 2p^* \end{aligned}$$

  Advantages of NN-method:

  - simple and intuitive
  - often easy to implement
  - performs elecently in practice

1.5.2 Limitations of Nearest Neighbor Classifier

1. NN is not consistent: $p_\infty(error) \leq 2p^*(error)$ (consistent: $p_\infty(error) = p^*(error)$)
solution: K-nearest neighbor algorithm:

- find the k nearest neighbors
- take majority vote
- is consistent if $k(N)$ such that

$$\lim_{N\to\infty} k(N) = \infty, \quad \lim_{N\to\infty} \frac{k(N)}{N} = 0$$

- e.g. k(N) $\log N$

2. nearest neighbor search is expensive: naive algorithm $\mathcal{O}(D * N)$ D: feature dimension, N: instances
solutions:

- reduce D:
  - dimension reduction(later, ch.'unsupervised learning')
  - relevant feature selection
- reduce N, relevant instance selection e.g.:
  - sort TS randomly
  - memorize the next instance only if the memorized set so far classifies incorrect

exactly:

- compute Voronoi tesselation
- drop all instances whose neighbors all have the same class
- clustering: find groups of similar instances ('clusters') which can be replaced by simple representative (later in chapter 'unsupervised learning')

use an efficient search algorithm: D-dimensional search trees('k-d tree, x tree, R^H tree')
use approximate n.n. search: find a near neighbor fast and with high probability of being correct ⇒ several ANN libraries in the internet

3. nearest neighbor selection depends on the distance function $d(x, x')$. How to define a 'good' $d()$?
Depending on units, different neighbor might minimize $d(x, x')$ solution. Therefor use dimensionless features, i.e. standardize data. Divide each feature by its TS standard deviation [actually, also substract means - 'centralization']
Better solution: learn the metric from the TS (or from additional TS with 'is similar'/'is not similar')-labels.
⇒ research area: 'metric learning'
Much of the success of neural networks is their ability to implicilly find a good set of intermediate features and metric.

1.6 Quadratic and Linear Discriminant Analysis

1.6.1 Motivation

In nearest neighbors, we can reduce search time by reducing N ⇒ extreme case: One representatice per label.
Obvious choice is the mean of each class:

$$\forall k \in 1, ..., c: \quad \mu_k = \frac{1}{N_k} \sum_{i:y_i=k} x_i \quad N_k = \text{instances in class k}$$

This works well, if clusters are roughly circular.
To find the desired decision bound, we neet to consider the actual shape of the class ⇒ correction for non-circularity
Simplest generalization: approximate cluster shape by an ellipse instead of circle (higher dimension: ellipsoid)
⇒ Natural choice: multi-dimensional Gaussian distribution

1.6.2 QDA

assumptions:

- each class prior $p(y = k)$ is well approximatet by the TS proportion $\hat{p}(y = k) = \frac{N_k}{N} = \pi_k$
- the data likelihood for each class p(x|y=k) is well approximated by a Gaussian distribution

⇒ generative model:

$$p(y = k|x) = \frac{p(x|y = k)p(y = k)}{p(x)}$$

$$p(x) = \sum_{k=1}^{c} p(x|y=k)p(y=k)$$

Gaussian distribution

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{\frac{x-\mu}{2\sigma^2}}$$

generalization of σ^2: Σ covariance matrix D x D, symmetric, positive definite

$$\Sigma = \frac{1}{N} \sum_i (x_i - \mu)(x_i - \mu)^T$$

$$\text{for example:} \quad \Sigma = R^{-1} \begin{pmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{pmatrix} R$$

principle axes of ellipse: directin of largest and smallest width $\leftrightarrow$ eigenvectors of covariance matrix Σ

$$\text{multivariable Gaussian} \quad p(x; \vec{\mu}, \Sigma) = \frac{1}{\sqrt{det(2\pi\Sigma)}} e^{-\frac{1}{2}(x-\vec{\mu})^T \Sigma^{-1} (x-\vec{\mu})}$$

To find $p(x|y=k)$, we must define $\underbrace{\vec{\mu_k}}_{\text{cluster pos.}}$, $\underbrace{\Sigma_k}_{clustershape}$ for each k:

How to fit a multi-dim. Gaussian Let $\{x_i\}_{i=1}^N$ be the instance of just a single class (drop index k for clarity).

$$p(x) = \text{multi-dim. Gaussian}$$

Fit according to maximum likelihood principle assumed that TS is typical for true (unknown) distribution.
$\Rightarrow$ we want the TS to be typical for our model as well, when simulating our model, the TS should occur with high (maximum) probability.

$$\begin{aligned} p(TS) &= p(x_1, ..., x_N) \Rightarrow \text{maximized under our model} \\ &\overset{i.i.d.}{=} p(x_1; \mu, \Sigma) p(x_2; \mu, \Sigma) ... p(x_N, \mu, \Sigma) \end{aligned}$$

$$\log(p(x_1, ..., x_N)) = \sum_{i=1}^{N} \log(p(x_i; \mu, \Sigma))$$

To maximize, take derivatives with respect to parameter set to 0
$\Rightarrow$ system of equations, solve to find $\hat{\mu}, \hat{\Sigma}$

$$\frac{d\sum_i \log(x_i;\mu,\Sigma)}{d\mu} \stackrel{!}{=} 0 \quad \frac{d\sum_i \log(x_i;\mu,\Sigma)}{d\Sigma} \stackrel{!}{=} 0$$

How to fit a Gaussian? maximize likelihood of TS:

$$\begin{aligned}\hat{\Theta} &= \arg\max \log p(x_1, ...x_n|\Theta) \\ &\stackrel{i.i.d.}{=} \arg\max \sum_{i=1}^{N} \log p(x_1, ...x_n|\Theta)\end{aligned}$$

$$p(x_i;\Theta) = \frac{1}{\sqrt{\det(2\pi\Sigma)}} e^{-\frac{1}{2}(x_i-\mu)^T\Sigma^{-1}(x_i-\mu)}$$

Define: $K = \Sigma^{-1}$ 'precession matrix'

Lin. Algebra: $\det(a * A) = a^D \det A \quad \det(A^{-1}) = \frac{1}{\det(A)}$ a: Scalar, A: D*D Matrix

$$\Rightarrow \frac{1}{\sqrt{\det(2\pi\Sigma)}} = (2\pi)^{-\frac{D}{2}} \frac{1}{\sqrt{\det(K^{-1})}} = (2\pi)^{-\frac{D}{2}} \det(K)^{\frac{1}{2}}$$

$$\log p(x_i;\mu,K) = \sum_{i=1}^{N} -\frac{D}{2}\log 2\pi + \frac{1}{2}\log\det(K) - \frac{1}{2}(x_i-\mu)^T K(x_i-\mu)$$

$$\begin{aligned}\text{find } \mu \text{ by } \quad & \frac{\partial}{\partial\mu}\log p(x_i, ...x_n) \stackrel{!}{=} 0 \\ \iff & \sum_{i=1}^{N} -K(x_i-\mu) = 0 \\ \iff & \sum_{i=1}^{N} (x_i-\mu) = 0 \\ \iff & \sum_{i=1}^{N} x_i = \sum_{i=1}^{N} \mu = N\mu \\ \implies & \mu = \frac{1}{N}\sum_{i=1}^{N} x_i \quad \text{empirical mean of TS}\end{aligned}$$

Lin. Algebra: $\frac{\partial}{\partial v} v^T A v = 2Av$

$$\text{find K:} \quad \frac{\partial}{\partial K} \log p(x_1, ..., x_N) \stackrel{!}{=} 0$$
$$\iff \sum_{i=1}^{N} (\frac{1}{2} K^{-1} - \frac{1}{2} z_i z_i^T) = 0 \quad \text{centered coordinate } z_i = x_i - \mu$$

$$\text{Matrix calculus:} \quad \frac{\partial}{\partial K} \log \det (K^T)^{-1} = (K^T)^{-1} = K^{-1} = \Sigma$$

$$\frac{\partial}{\partial A} v^T A v = v v^T$$

$$N\Sigma = \sum_{i=1}^{N} \Sigma = \sum_{i=1}^{N} \underbrace{(x_i - \mu)(x_i - \mu)^T}_{scatter matrix}$$

$$\Sigma = \frac{1}{N} \sum_{i=1}^{N} (x_i - \hat{\mu})(x_i - \hat{\mu})^T \quad \text{sample/empirical covariance matrix}$$

Training of QDA Repeat this for every class to get $\mu_1, \Sigma_1, ..., \mu_c, \Sigma_c$
QDA prediction: -generative model:

$$\begin{aligned}
\hat{k} &= \arg\max_k p(y = k] x) \\
&= \arg\max_k \frac{p(x|y=k)p(y=k)}{p(x)} \\
&= \arg\max_k \underbrace{p(x|y=k)}_{Gauss(x, \mu_k, \Sigma_k)} \underbrace{p(y=k)}_{\pi_k = \frac{N_k}{N}} \\
&= \arg\min_k - \log p(y=k|x) \\
&= \arg\min_k \frac{D}{2} \log 2\pi + \frac{1}{2} \log \det \Sigma_k + \frac{1}{2} (x - \mu_k)^T \Sigma_k^{-1} (x - \mu_k) - \log \pi_k \\
&= \arg\min_k \cancel{\frac{1}{2}} \underbrace{\log \det \Sigma_k - 2 \log \pi_k}_{= b_k} + \cancel{\frac{1}{2}} (x - \mu_k)^T \Sigma_k^{-1} (x - \mu_k) \\
&= \arg\min_k \underbrace{(x - \mu_k)^T \Sigma_k^{-1} (x - \mu_k)}_{\text{squared Mambalanbis distance btw. } x \text{ and } \mu_k} + b_k
\end{aligned}$$

Euclidean: $\Sigma = \mathbb{1} \quad \sigma \neq \mathbb{1}$ adjust for elliptic cluster sphere.

Define square root of matrix $A^{\frac{1}{2}} \iff A = (A^{\frac{1}{2}})^T (A^{\frac{1}{2}})$

Find Σ^{-1} by decomposition $z_k = \Sigma_k^{-\frac{1}{2}} (x - \mu_k)$

$$\Rightarrow z_k^T z_k = (x-\mu_k)^T \frac{\Sigma_k^{-\frac{1}{2}T}\Sigma_k^{-\frac{1}{2}}}{\Sigma_k^{-\frac{1}{2}}}(x-\mu_k)$$

$\Rightarrow$ can use standard nordmed of z_k

1.6.3 LDA Linear Discriminant Analysis

simplifications: assume that clusters have the same size elliptic shape

$$\forall k, k' \quad \Sigma_k = \Sigma_{k'} = \Sigma$$

$$QDA: \quad \hat{k} = \arg\min_k (x-\mu_k)^T \Sigma_k^{-1}(x-\mu_k) + b_k$$

$$\begin{aligned} LDA: \quad \hat{k} &= \arg\min_k (x-\mu_k)^T \Sigma^{-1}(x-\mu_k) \\ &= \arg\min_k x^T\Sigma^{-1}x - \Sigma\mu_k^T\Sigma^{-1}x + \mu_k^T\Sigma^{-1}\mu_k \\ &= \arg\min_k -\Sigma\mu_k^T\Sigma^{-1}x + \mu_k^T\Sigma^{-1}\mu_k + b_k \\ &= \arg\min_k w_k^T x + b_k' \end{aligned}$$

New variables: $w_k^T = \Sigma\mu_k^T\Sigma^{-1} \quad b_k' = -\mu_k^T\Sigma^{-1}\mu_k - b_k$
LDA is a particular way to define w_k and b_k'. There are many other possible ways, e.g. logistic regression.

Special case: C=2

$$\begin{aligned} \hat{k} &= \begin{cases} 0 & \text{if} \quad w_0^T x + b_0' > w_1^T x + b_1' \\ 1 & \text{if} \quad w_0^T x + b_0' < w_1^T x + b_1' \end{cases} \\ &= \begin{cases} 0 & \text{if} \quad (w_0^T - w_1^T)x + b_0' - b_1' > 0 \\ 1 & \text{otherwise} \end{cases} \\ &= \begin{cases} 0 & \text{if} \quad w^T x + b' > 0 \\ 1 & \text{if} \quad w^T x + b' < 0 \end{cases} \end{aligned}$$

Define: $w = w_1 - w_0 \quad b' = b_1' - b_0'$
$a = w^T x$ is a 1D projection of x onto the vector w
$\Rightarrow$ apply the mean classifier to the a value

1.6.4 LDA

Two classes C = 2

$$\hat{y} = \begin{cases} 1 & \text{if } w^T x + b \geq 0 \\ 0 & else \end{cases}$$

Three different derivations of how to choose the best w and b:

1. our derivation: LDA is the same as QDA with all classes having the same cluster shape ⇒ we just fit a Gaussian distribution to within - class covariance

$$\hat{\Sigma} = \frac{1}{N} \Sigma_{i=1}^{N} (x_i - \mu_{k=y_i})(x_i - \mu_{y_i})^T$$

$$w^T = 2(\mu_1 - \mu_0)\hat{\Sigma}^{-1}$$

2. R. Fishers original derivation: we seek the optimal 1-dimensional projection of D-dimensional data

- compute μ_0, μ_1, Σ
- define 1-D projection $z_1 = w^T x_i$ ⇒ projected means $m_k = w^T \mu_k$, 1-D variance $\sigma^2 = w^T \Sigma$
- determine w such that the z_i are seperated as good as possible

$$m_0 - m_1 = w^T(\mu_1 - \mu_0)$$

- Fisher criterion: Choose w that maximizes $\frac{(m_1 - m_0)^2}{\sigma^2}$

3. derivation via least-squares regression
define class labels $Y \in \{-1, 1\}$
LSQ: find w, b that minimzes:

$$\sum_{i=1}^{N} (w^T x_i + b_i - y_i)^2$$

if classes are balanced: $N_{-1} = N_{+1}$
⇒ optimal solution is again the same ⇒ proof: home-work

1.7 Logistic Regression LR

- Not really regression, because it's a classifier, term is partially justified because LR predicts class probabilities. It actually computs the posterior $p(Y|X)$
- generative model (LDA) vs. discriminative model (LR)
- LDA:

  - define RHS of Bayes theorem (likelihood and prior)
  - learn the parameters of RHS (fit a Gaussian for every class)
  - apply Bayes to compute the posterior
- LR
  - define RHS of Bayes
  - apply Bayes to compute posterior (LHS)
  - learn parameters of the LHS
  - or: merge first two steps and define LHS model directly (e.g. NN)

derive LR from LDA: 2 classes C=2, equal priors $p(y=0) = p(y=1) = \frac{1}{2}$, cluster shape (e.g. covariance Σ of both classes equal)

$$\begin{aligned} p(y=1|x) &= \frac{p(x|y=1)\cancel{p(y=1)}}{p(x|y=0)\cancel{p(y=0)} + p(y|y=1)\cancel{p(y=1)}} \\ &= \frac{p(x|y=1)}{p(x]y=0) + p(x|y=1)} \\ &= \frac{p(x|y=1)}{p(x|y=1)} * \frac{1}{\frac{p(x|y=0)}{p(x|y=1)} + 1} \end{aligned}$$

Gaussian likelihoods:

$$p(x|y=0) = \frac{1}{\sqrt{det(2\pi\Sigma)}} e^{-\frac{1}{2}(x-\mu_0)^T\Sigma^{-1}(x-\mu_0)}$$

$$p(x|y=1) = \frac{1}{\sqrt{det(2\pi\Sigma)}} e^{-\frac{1}{2}(x-\mu_1)^T\Sigma^{-1}(x-\mu_1)}$$

$$\mu = p(y=0)\mu_0 + p(y=1)\mu_1 = \frac{\mu_0 + \mu_1}{2} = 0$$

assume that dara are centered $\Rightarrow \mu = 0$

$$\begin{aligned} p(y=1|x) &= \frac{1}{1 + \frac{p(x|y=0)}{p(x|y=1)}} \\ &= \frac{1}{1 + \exp(-0.5[(x_{\mu 1})^T\Sigma^{-1}(x+\mu_1) - (x-\mu_1)^T\Sigma^{-1}(x-\mu_1)])} \\ &= \frac{1}{1 + exp(-0.5[4\mu_1^T\Sigma^{-1}x])} \\ &= \frac{1}{1 + exp(-2\mu_1^T\Sigma^{-1}x)} \\ &= \frac{1}{1 + exp(-w^Tx)} \end{aligned}$$

$$w^T = 2\mu_1^T \Sigma^{-1}$$

$$p(y=0|x) = 1 - p(y=1|x)$$

$$\underline{Decisionrule}: \quad \hat{y} \begin{cases} 1 & if \quad p(y=1|x) \geq p(y=0|x) = 1 - p(y=1|x) \\ 0 & otherwise \end{cases}$$

$$\text{logistic sigmoid function}: \quad \sigma(t) = \frac{1}{1+exp(-t)}$$

Properties:

$$\sigma(-t) = 1 - \sigma(t)$$

$$\sigma(-t) = \frac{1}{1+exp(t)} = 1 - \frac{1}{1+exp(-t)} = \frac{exp(-t)}{1+exp(-t)} = \frac{1}{exp(t)+1}$$

Derivative:

$$\frac{d}{dt}\sigma(t) = \frac{d}{dt}(1+exp(-t))^{-1} = (1+exp(-t))^{-2}exp(-t) = \sigma(t)\sigma(-t) = \sigma(t)(1-\sigma(t))$$

1.7.1 Learning LR

- maximum likelihood principle: choose the model such that the training data are a typical realization means:

$$\begin{aligned}
\hat{w} &= \arg\max_w p((x_1,y_1),...,(x_n,y_n)|w) \\
&= \arg\min_w -\log p((x_i,y_i)|w) \\
&\overset{i.i.d.}{=} \arg\min_w -\Sigma_{i=1}^N \log p(y=y_i|x_i,w) \\
&= \arg\min_w -[\Sigma_{i,y_i=1} \log p(y=1|x_i,w) + \Sigma_{i,y_i=0} \log(1-p(y=1|x_i,w))] \\
&= \arg\min_w = -\Sigma_{i=1}^N [y_i \log p(y=1|x_i,w) + (1-y_i)\log(1-p(y=1|x_i,w))]
\end{aligned}$$

Find w

$$\begin{aligned}\frac{\partial}{\partial w} - \sum_{i=1}^{N} ... &= -\sum_{i=1}^{N}[y_i \frac{1}{\sigma(w^T x_i)}\sigma(w^t x_i)\sigma(-w^T x_i)x_i + (1-y_i)\frac{1}{1-\sigma(w^T x_i)}(-1)\sigma(w^T x_i)\sigma(-w^T x_i)x_i] \\ &= -\sum_{i=1}^{N}(y_i \underbrace{\sigma(-w^T x_i)}_{1-\sigma(w^T x_i)} x_i - (1-y_i)\sigma(w^T x_i)x_i) \\ &= -\sum_{i=1}^{N} y_i x_i - y_i\sigma(w^T x_i)x_i - \sigma(w^T x_i)x_i + y_i\sigma(w^T x_i)x_i \\ &= \sum_{i=1}(y_i - \sigma(w^T x_i))x_i \stackrel{!}{=} 0\end{aligned}$$

no analytical solution ⇒ need to solve numerically
Numerical algorithms:

- classical: few training data $N \leq 1000$ ⇒ use Newton-Raphson algorithm ⇒ Iterative Reweighted Least Squares (RLS ⇒ later)
  - advantage: needs few iterations
  - drawback: each iteration is expensive when N gets bigger $\mathcal{O}(N^3)$ or $\mathcal{O}(N^2)$ with tricks
- modern: lots of training data: stochastic gradient descent
  - choose initial guess for $w^{(0)}$ e.g. $w^{(0)} = 0 \Rightarrow \sigma(w^T x) = \frac{1}{2} \quad \forall x \Rightarrow p(y=1|x) = p(y=0|x)$
  - for t = 1, ..., T (or until convergence)
    - bring TS into random order (e.g. random shuffle) of indices
    - for i = 1,..., N: $w' = w - \tau(y_i - \sigma(w^T x_i)x_i), \quad \tau$: learning rate
    - reduce learning rate $\tau \leftarrow \frac{t}{t-1}\tau$

1.8 Histogramms and Density Trees

1.8.1 Introduction

- we had: generative models vs. discriminative models (learn LHS or RHS of Bayes)
- new distinction:
  - parametric models: choose probabilities from a family with analytic formula (Gaussian) and we learn its parameters (Gaussian: μ, Σ)
  - non-parametric models: don't restrict the probability - 'universal model' (neural net) and learn many more parameters (network weights)

	generative	discriminative
parametric	LDA and QDA	LR
non-parametric	histogramm, density tree	nearest neighbors

- histogramm: count the frequency of random events:

$$\frac{\sum_{i=1} \mathbb{1}[x_i = z]}{N}$$

  z: events considered and create table for all events

- x is discrete, throwing dice: $z \in \{1, ..., 6\}$

$$\text{hist}(z) = \frac{[x = z]}{N}$$

- x is continous $x \in R \Rightarrow$ discretize into bins

$$b_l = \{x | \underbrace{x_{min} + l\Delta x}_{x_l} \leq x \leq \underbrace{x_{min} + (l+1)\Delta x}_{x_{l+1}}\}$$

- find bin index of x:

$$l = \left\lfloor \frac{x - x_{min}}{\Delta x} \right\rfloor \quad \Delta x: \text{ bin width} \quad \lfloor\rfloor: \text{ floor function}$$

$$\mathbb{1}[a] = \begin{cases} 1 & \text{if a is true} \\ 0 & \text{else} \end{cases}$$

  p_l= prob for X in bin l

- approx likelihood:

$$p(x|y) \approx \sum_l p(l) \mathbb{1} \lfloor x \in b_l \rfloor$$

- meaning: piecewise constant approximation $\Rightarrow$ can make error arbitrarily small by choosing more bins, but not more than the TS allows

- optimal approx, given TS and Δx

$$\hat{p} = \arg\min_p Error = \int \underbrace{(p^*(x) - p(x))^2 dx}_{\cancel{p^*(x)^2} - 2p^*(x)p(x) + p(x)^2} \quad p^*: \text{ truth} \quad \hat{p}: \text{ best approx.}$$

$$
\begin{aligned}
-2^*(x)p(x)dx &= -2\int p^*(x)\sum_l p(l)\mathbb{1}[x\in b_l]dx \\
&= -2\sum_l p(l)\int p^*(x)\mathbb{1}[x\in b_l]dx \\
&= -2\sum_l p(l)\int_{x_l}^{x_{l+1}} p^*(x)dx \\
&= -2\sum_l p(l)\mathbb{E}_{p^*(x)}[\mathbb{1}[x\in b_l]]
\end{aligned}
$$

$$
\mathbb{E}_{p^*(x)}[\mathbb{1}(x\in b_l)] \approx \frac{N_l}{N} \quad {}_l = (x \text{ is in } l)
$$

$$
\mathbb{1}[x\in b_l]^2 = \mathbb{1}[x\in b_l] \quad l\neq l': \quad \mathbb{1}[x\in b_l]\mathbb{1}[x\in b_{l'}] = 0
$$

$$
\begin{aligned}
\int p(x)^2dx &= \int (\sum_l p_l \mathbb{1}[x\in b_l])^2 \\
&= \int \sum_l p_l^2 \mathbb{1}[x\in b_l]dx \\
&= \sum_l p_l^2 \int \mathbb{1}[x\in b_l]dx \\
&= \sum_l p_l^2 \int_{x_l}^{x_{l+1}} 1dx \\
&= \sum_l p_l^2 \Delta x
\end{aligned}
$$

$$
Error =^* (x)^2dx - 2\sum_l p_l\frac{N_l}{N} + \sum_l p_l^2\Delta x
$$

$$
\hat{p_l} = \arg\min \text{Error} = \arg\max_{p_l} \sum_l p_l^2\Delta x - 2\sum_l p_l\frac{N_l}{N}
$$

$$
\frac{\partial}{\partial p_l}... = 2p_l\Delta x - 2\frac{N_l}{N} \stackrel{!}{=} 0
$$

$$
p_l = \frac{N_l}{N\Delta x} \quad \text{probability density estimate}
$$

insert into error:

$$\begin{aligned} Error &= \int p^*(x)^2 dx - 2\sum_l \frac{N_l}{N\Delta x}\frac{N_l}{N} + \sum_l (\frac{N_l}{N\Delta x})^2 \Delta x \\ &= \int p^*(x)^2 dx - \sum_l (\frac{N_l}{N})^2 \frac{1}{\Delta x} \\ &= \int p^*(x)^2 dx - \sum_l \hat{p_l}^2 \Delta x \end{aligned}$$

- how to choose Δx: Difficult, rules of thumb:
  - Scotts's rule:

$$\Delta x = \frac{3.5\sigma}{\sqrt[3]{N}} \quad \text{exactly optimal if } p^* \text{ is Gaussian)}$$

  - Freedman-Diaconis rule:

$$\Delta x = \frac{2\text{IQR}(x)}{\sqrt[3]{N}}$$

    IQR: inter-quartile range: place data in sorted order: $x_{[1]}, x_{[2]}, ..., x_{[N]}$

$$IQR = x_{[\frac{3}{4}N]} - x_{[\frac{1}{4}N]}$$

  - Shimazaki/Shinomoto rule:

$$\hat{\Delta x} = \arg\max_{\Delta x} \frac{2m - v}{(\Delta x)^2} \quad m\text{: mean bin count, } v\text{: variance}$$

  - cross-validation: split into training sets of size N and test sets of size M
    for each candidate δx compute error

$$\sum_l \frac{1}{\Delta x}(\frac{N_l}{N} - \frac{M_l}{M})^2$$

    and choose Δx that minimizes error
    in general: if φ is a hyperparameter (here: Δx): use Cross Validation and grid search

- typical bin counts (e.g. Freedman-Diaconis): scale x such that IQR $(x) = \frac{1}{2}$

$$\Rightarrow \Delta x = \frac{1}{\sqrt[3]{N}}$$

if data are uniformely distributed:

$$x_{max} - x_{min} = 2\text{IQR}x = 1$$

$$\text{bin count} \quad \frac{x_{max} - x_{min}}{\Delta x} = \frac{1}{\Delta x} = \sqrt[3]{N}$$

$$N = 1000 \Rightarrow 10 \text{ bins} \quad N = 10^6 \Rightarrow 100 \text{ bins}$$

- generalize to the multi-dimensional case $x \in \mathbb{R}^D$
  naive solution: split each dimension according to Freedman/Diaconis
  $\Rightarrow$ 10 bins per dimension $\Rightarrow 10^D$ bins in total
  $\Rightarrow$ no TS can ever fill 10^D bins $\Rightarrow$ most are empty $\Rightarrow$ no estimate
  $\Rightarrow$ doesn't work
- use a 1-dimensional histogram for each dimension (only 10*D bins)
- only use 1-D histogramms, one per feature per class
- probabalistic interpretation: if we know the class y, all fearture dimension are statistically independent

$$p(x|y) = p(\{x_j\}|y) = p(x_{j=1}|y)p(x_{j=2}|y)p(x_{j=D}|y)$$

- density trees: place bins adaptively: many bins in subregions with many data bins, few bins in subregions with few data points

1.8.2 Naive Bayes

Using one histogramm per dimension $\iff$ assumption that values of different features are independent, given the class $\iff$ if we know the class label y_i, then knowing the feature x_{i1} doesn't tell us anything about other feature values $x_{ij} \quad j \neq 1$
This assumption is often violated, e.g. in images. Consider an image region with class label 'sky'. Let one pixel in the sky have color 'blue'. Than it's likely that the neighbor pixels are probably also 'blue'. The same applies to other colors (e.g. grey for clouds or red for sunset).
If assumption is true, joint probability

$$p(x_i = [x_{i1}, ..., x_{iD}]|y_i) = \Pi_{j=1}^{D} p_j(x_{ij}|y_i)$$

$$\text{Bayes:} \quad p(y_i|x_i) = \frac{p(x_i|y_i)p(y_i)}{p(x_i)} \overset{\text{naive}}{=} \frac{\Pi_{j=1}^{D} p_j(x_{ij}|y_i)p(y_i)}{p(x_i)}$$

$$\text{simplify} \quad p(y_j) = p(y_{ji}) = \frac{1}{C} \quad \text{uniform priors}$$

$$\begin{aligned} \text{decision rule:} \quad \hat{y_i} &= \arg\max_k p(y_i = k|x_i) \\ &= \arg\max_k \Pi_{j=1}^{D} p_j(x_{ij}|y_i = k) \\ &= \arg\max_k \sum_{j=1}^{D} \log p_j(x_{ij}|y_i = k) \end{aligned}$$

training: for $k = 1, ...C$ for $j = 1, ..., D$: fit 1-D histogram $p_j(x_{ij}|y_i = k)$ using the j-th feature of all instances of class k

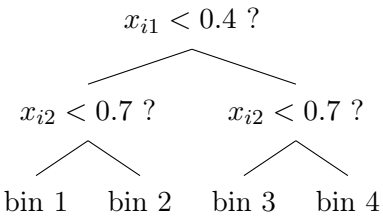
Variant: Instead of 1-D histogramms, fit 1-D Gaussian distributions $\Rightarrow$ naive BAyes becomes equivalent to QDA with constraint that covariance matrices Σ_k are all diagonal $\Longleftrightarrow$ axes of ellipses are parallel to coordinate axes.

1.8.3 Density trees

- idea: place bins adaptively, small bins where there are many datapoints, big bins where there are few
- how to find the bin for a data point efficently:

$$1 - D \quad l = \left\lfloor \frac{x - x_{min}}{\Delta x} \right\rfloor$$

- higher dimensions: represent binning by a binary tree



- bin index for L bins can be found with $\mathcal{O}(\log L)$ decisions (if tree balanced) - 'recursive subdivision'
- training
  - build the tree
  - define response ($\hat{p_l}$) of the leaves, e.g. as in 1-D histograms

$$\hat{p_l} = \frac{N_l}{NV_l} \quad N_l \text{ instances in bin l, } V_l \text{ volume of bin l}$$

or: fit Gaussian to each bin (adjust normalization for finite bin size)

Build tree by 'recursive best-first expansion'
Init:

- put all data into a single bin (root of tree), size: bounding rectangle of data points
- fix bins $L = \tau \sqrt[3]{N}$

- for $t = 1, ..., L-1$
  - compute 'score' of all current leave modes
  - split best leaf into two children (original leaf is now an interior node)

score of a leaf: maximal improvement of our objective funtion (e.g. error) if we would split this leaf)

- Criminisi et al.: try a number of random splits and remember the best (allow oblique splits)
- exhaustive search for best split (preferable when we split axis orthogonal)

exhaustive search: give leaf with boundaries $x_j \in [m_j, M_j]$, $N_l =$ instances in this leaf for each feature $j \in 1, ..., D$:

- define candidate split thresholds

$$s_j = \{s_{ja}, ..., s_{j(N_l+1)}\}: \quad \text{sort data according to feature j}$$

$$x_{[0]j} = m_j = x_{[1]j} \leq x_{[2]j} \leq ... \leq x_{[N_l]j} \leq M_j = X_{[N_l+1]j}$$

  place candidate threshold in the middle of each pair

- compute the score of every candidate split return dimension j and threshold s_{ja} and score g_{ja} of best candidate split (among $D(N_l + 1)$)

scores:

- minimize squared error of histogram:

$$\text{error} = \int p^*(x)^2 dx - \sum_l^{L_t} \hat{p_l}^2 V_l \quad \text{before split}$$
$$\text{error'} = \int p^*(x)^2 dx - \sum_{l=1}^{L_t+1} \hat{p_l'}^2 V_l$$

  suppose split leaf l into λ and ρ

$$\text{gain } g = \text{error} - \text{error'} = -\hat{p_l}^2 V_l + \hat{p_\lambda}^2 V_\lambda + \hat{p_\rho}^2 V_\rho$$

- split nodes where data distribution is far from uniform $\iff \frac{N_l}{N} \sim V_l$

$$\text{non-uniformity}: \left| \frac{N_\lambda}{N_l} - \frac{V_\lambda}{V_l} \right|$$

- split to minimize etropy (ex. fit Gaussian)

$$H = \frac{1}{2} \log(\det(2\pi e \Sigma))$$

$$g = H_l - \frac{N_\lambda}{N} H_\lambda - \frac{N_\rho}{N} H_\rho$$

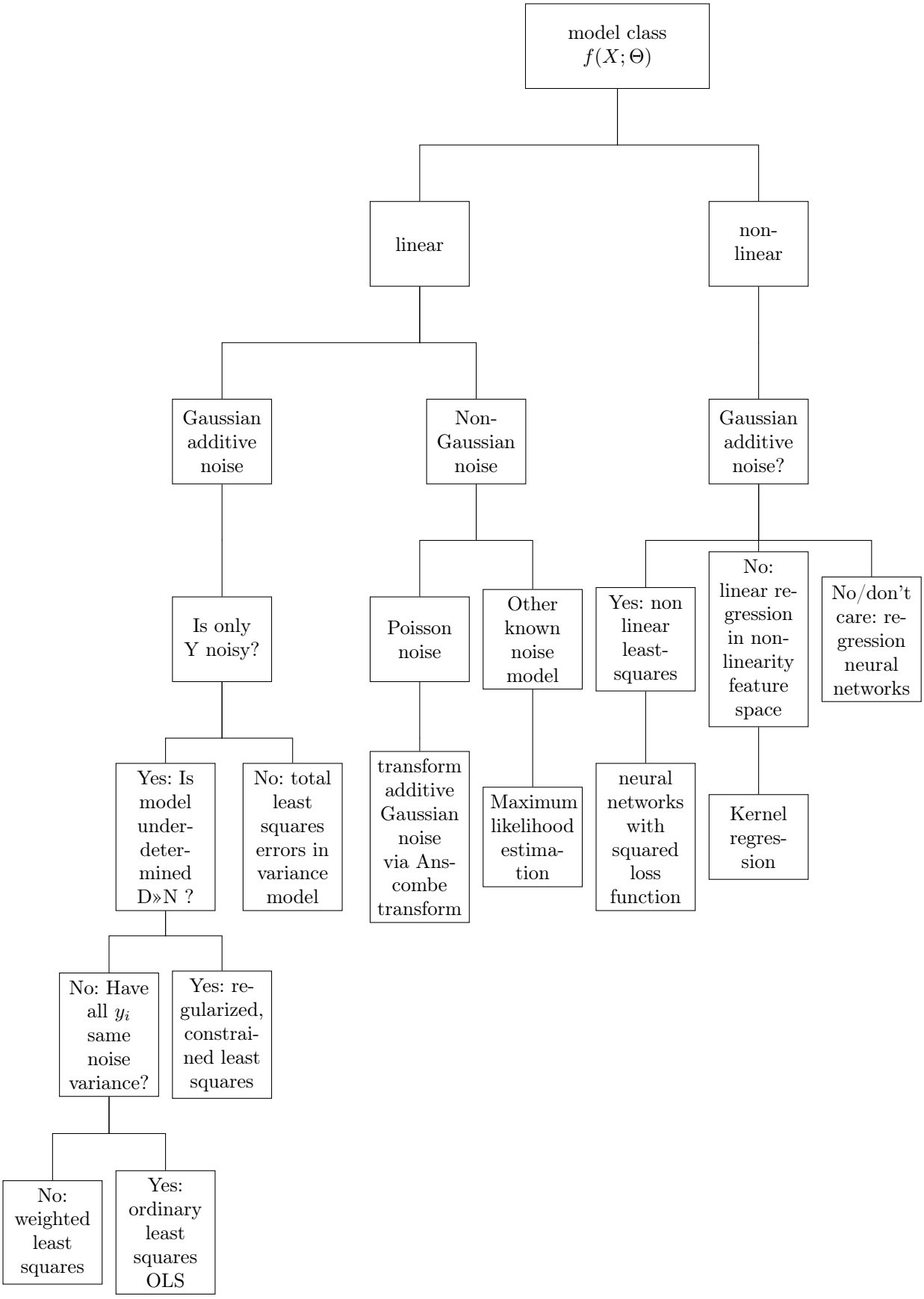
density trees tend to overfit:

- traditional: pruning $\widehat{=}$ cut-off subtrees with high overfitting and replace by single leaf
- modern: density forest $\widehat{=}$ train many trees and take their average probability ('ensemble method' $\Rightarrow$ later)
  how to make the trees different:
  1. train every tree on a random subset of the training data (bootstrap sampling)
  2. consider a random subset of the features inthe split: search algorithm

2 Regression

2.1 Introduction

- Learn model $y = f(x) \quad x \in \mathbb{R}^D \Rightarrow y \in \mathbb{R}^{D'} (D' = 1)$
- training set $\{(\underbrace{x_i}_{\substack{\text{D-dim} \\ \text{features}}} , \underbrace{y_i}_{\substack{\text{real-valued} \\ \text{true response}}})\}_{i=1}^N$ assume i.i.d. - matrix notation


model class
$f(X;\Theta)$
linear
non-
linear
Gaussian
additive
noise
Non-
Gaussian
noise
Gaussian
additive
noise?
Is only
Y noisy?
Poisson
noise
Other
known
noise
model
Yes: non
linear
least-
squares
No:
linear re-
gression
in non-
linearity
feature
space
No/don't
care: re-
gression
neural
networks
Yes: Is
model
under-
deter-
mined
D»N ?
No: total
least
squares
errors in
variance
model
transform
additive
Gaussian
noise
via Ans-
combe
transform
Maximum
likelihood
estima-
tion
neural
networks
with
squared
loss
function
Kernel
regres-
sion
No: Have
all y_i
same
noise
variance?
Yes: re-
gularized,
constrai-
ned least
squares
No:
weighted
least
squares
Yes:
ordinary
least
squares
OLS

2.2 Ordinary Least Squares (OLS)

- linear model with additive Gaussian noise, X is noise-free, all Y have same noise variance

$$Y = \underbrace{X}_{\substack{\text{Row vector}\\ \text{D-dim}\\ \text{feature}}} \cdot \underbrace{\beta}_{\substack{\text{column vector}\\ \text{of D-dim weights}\\ \text{activations}}} + \underbrace{\varepsilon}_{\substack{\text{Gaussian}\\ \text{distributed}\\ \text{scalar}}}$$

$$\varepsilon \sim N(0, \sigma^2) \iff Y \sim N(X\beta, \sigma^2)$$

- find best $\hat{\beta}$ via Maximum Likelihood principle $\hat{=}$ make training set typical under the model
  compute the residuals

$$r_i = y_i - x_i\beta$$

$$\text{If the model is correct } (\hat{\beta} = \beta^*): \quad r_i \sim N(0, \sigma^2)$$

  If model is correct and we know the truth: $\beta = \beta^* \to r_i = \varepsilon_i$, we only have $\beta = \hat{\beta} \to r_i \sim \varepsilon_i$

- ML principle

$$\begin{aligned}
\hat{\beta} &= \arg\max_{\beta} p(\{y_1, ..., y_N\} | \{x_1, ..., x_N\}; \beta) \\
&= \arg\max_{\beta} \prod_{i=1}^{N} \underbrace{p(y_i|x_i;\beta)}_{y * e^{\frac{-(y_i - x_i\beta)^2}{2\sigma^2}}} \\
&= \arg\min_{\beta} -\sum_{i=1}^{N} \log p(y_i|x_i;\beta) \\
&= \arg\min_{\beta} \sum_{i=1}^{N} \frac{(y_i - x_i\beta)^2}{2\sigma^2} - N \log v \\
&= \arg\min_{\beta} \sum_{i=1}^{N} (y_i - x_i\beta)^2 \quad \text{least-squares objective}
\end{aligned}$$

- example: fit a line in 2D $X \in \mathbb{R}$

$$Y = [X; 1] \begin{bmatrix} a \\ b \end{bmatrix} + \varepsilon$$

$$Y = aX + b + \varepsilon$$

$$\hat{a}, \hat{b} = \arg\min_{a,b} \underbrace{\sum_{i=1}^{N} (Y_i - aX_i - b)^2}_{\text{Loss}}$$

$$\frac{\partial \text{Loss}}{\partial b} = \sum \sum_{i=1}^{N} (Y_i - aX_i - b)(-1) \stackrel{!}{=} 0$$

$$\sum_i Y_i - a \sum_i X_i - \sum_i b = 0$$

$$\frac{1}{N} \sum_i Y_i = a \frac{1}{N} \sum_i X_i + b$$

$$\bar{Y} = a\bar{X} + b$$

Regressionline always goes through the origin $\Rightarrow$ always center data(i.e. $\bar{X} = 0, \bar{Y} = 0$)

- regression goes through origin $\Rightarrow$ no need for intercept b
- numbers get smaller $\Rightarrow$ regression is numerically more stable

$\Rightarrow$ assume $X \Rightarrow X - \bar{X}, Y \Rightarrow Y - \bar{Y}$

rewrite objective in matrix form

$$\hat{\beta} = \arg\min_{\beta} (Y - X\beta)^T (Y - X\beta)$$

$$\frac{\partial \text{Loss}}{\partial \beta} = 2X^T(Y - X\beta) \stackrel{!}{=} 0$$

$$\underbrace{X^T X}_{\text{scatter matrix}} \quad \beta = X^T Y \quad \text{linear system of equations 'normal equations'}$$

$\Rightarrow$ solve for β
possibilities to solve:

1. formal solution:

$$\underbrace{(X^T X)^{-1}(X^T X)}_{\mathbb{1}} \beta = (X^T X)^{-1} X^T Y$$

$(X^TX)^{-1}$ exists if X has full rank description

$$\hat{\beta} = \underbrace{(X^TX)^{-1}X^T}_{X^+}Y$$

$X^+ = (X^TX)^{-1}X^T$: Moore-Penrose pseudo-inverse, inverse to rectangular matrices

2. Cholesky factorization: X^TX is positive definite symmetric
for every such matrix, there is a decomposition:

$$R^TR = X^TX \quad R : D * D \text{ upper triangular}$$

$$R^TR\beta = X^TY \quad \text{define } Z = R\beta$$

$$R^TZ = X^TY = F \quad \text{linear equations in Z}$$

(a) solve for Z by forward substitution because R^T is lower triangular
(b) solve $R\beta = Z$ by backward substitution because R is upper triangular

advantages:

- easy to construct: $S = X^TX$, we don't have to construct X first
for k from 1 to D:
for l from 1 to D:
$s_{kl} = 0$
for i from 1 to N:
$s_{kl} += x_{ik}x_{il}$

disadvantages:

- Loss of precision: Condition number of metric X

$$\kappa = \|X\|_F\|X^+\|_F$$

$$\text{Frobenius norm:} \quad \|X\|_F = \sqrt{\sum_{k,l} X_{kl}^2}$$

- condition of $S = X^TX$
$\Rightarrow$ number of significant digits: $m\beta \approx \kappa^2\varepsilon$
ε : machine precision, type double: 10^{-16}

$$X^+ = (X^TX)^{-1}X^T \quad \text{pseudo inverse}$$

$\Rightarrow \kappa = 10^8 \Rightarrow \kappa^2 \varepsilon \approx 1$

3. **Singular Value Decomposition** (SVD) of X:
   Theorem: every matrix can be expressed as

$$\underbrace{X}_{N\times D} = \underbrace{U}_{\substack{N\times D \\ \text{orthogonal}}} \cdot \underbrace{\Lambda}_{\substack{D\times D \\ \text{diagonal matrix} \\ \text{of 'singular values'}}} \cdot \underbrace{V^T}_{\substack{\text{orthogonal} \\ D\times D}} \quad \text{orthogonal: } U^{-1} = U^T$$

   If x is square and symmetric: $X = U \cdot \underbrace{\Lambda}_{Eigenvalues} \cdot U^T$ 'Eigenvaluedecomposition'

$$X^T = (U \cdot \Lambda \cdot V^T)^T = (V^T)^T \cdot \Lambda^T \cdot U^T = V \cdot \Lambda \cdot U^T$$

$$S = X^T \cdot X = V \cdot \Lambda \cdot \underbrace{U^T}_{U^{-1}} \cdot U \cdot \Lambda \cdot V^T = V \cdot \Lambda^2 \cdot V^T$$

$$S^{-1} = (V^T)^{-1} \cdot (\Lambda^2)^{-1} \cdot V^{-1} = V \cdot \Lambda^{-2} \cdot V^T$$

$$\beta = S^{-1} \cdot X^T \cdot Y$$

$$\begin{aligned} S^{-1} \cdot X^T &= V \cdot \Lambda^{-2} \cdot \underbrace{V^T \cdot V}_{\mathbb{1}} \cdot \Lambda \cdot U^T \\ &= V \cdot \Lambda^{-2} \cdot V \cdot U^T \\ &= V \cdot \Lambda^{-1} \cdot U^T = X^T \end{aligned}$$

$$\boxed{\beta = V \cdot \Lambda^{-1} \cdot U^T \cdot Y}$$

   disadvantage: complicated algorithm to find U, V, Λ
   advantages:

   - numerically most stable method
   - also works if X does not have full rank (rank $D^* < D \Rightarrow D - D^*$ of the singular values Λ are 0)
     $\Rightarrow$ drop rows of U, columns of Λ and V^T with 0 singular value

4. **QR decomposition** (standard, because good compromise between numeric stability and effort)
   Theorem: every X has a decomposition

$$X = \underbrace{Q}_{\substack{N\times N \\ \text{orthogonal}}} \cdot \underbrace{R}_{\substack{N\times D \\ \text{upper triangular}}}$$

$$
\begin{aligned}
X^T &= R^T \cdot Q^T \\
X^T X &= R^T \cdot Q^T \cdot Q \cdot R = R^T \cdot R \\
(X^T \cdot X)^{-1} &= R^{-1} \cdot R^{-T} \\
(X^T \cdot X)^{-1} \cdot X^T &= R^{-1} \cdot R^{-T} \cdot R^T \cdot Q^T = R^{-1} \cdot Q^T \\
\beta &= R^{-1} \cdot Q^T \cdot Y \iff R \cdot \beta = Q^T \cdot Y
\end{aligned}
$$

solve by backwards substitution
algorithm: construct R one column at a time, immediatly apply the corresponding update to RHS (never construct Q)

5. if X doesn't fit into memory: LSQR algorithm
   - variant of conjugate gradient algorithm to solve linear systems of eg., modified for least squares probability
   - matrix X is only ever accessed via matrix-vector products $X \cdot U$ and $X^T \cdot V$ (only vectors M memory)
     ⇒ pass subroutines for these products to algorithm instead of matrix data structure
     ⇒ algorithm never sees matrix Y and its complicated handling

Theorem: Every X has a decomposition

$$
X = \underbrace{U}_{\text{orthogonal}} \cdot \underbrace{B}_{\substack{\text{bi-diagonal} \\ \text{matrix}}} \cdot \underbrace{V^T}_{\text{bi-diagonal}}
$$

⇒ solve the linear system by forward substitution and each iteration only needs z columns of β
⇒ construct $U \cdot B \cdot V^T$ one column/row at at time, immediately carry out next itereation of substitution
⇒ one only needs columns/rows t, t-1
⇒ never need full decomposition in memory

2.2.1 Computer Topography

Consider a single ray from X-ray source

$$
I = I_0 e^{-\int \mu(x) da}
$$

goal: use many different directions to find $\mu(x, y)$

$$
\boxed{I(b) = I_0 e^{-\int \mu(a,b) da}}
$$

Radon transform of $\mu(a, b)$
⇒ Task: invert Radon-transformation

$$
\log(I(b)) = \log(I_0) - \int \mu(a, b) da
$$

$$Y = \int \mu(a,b)da = -\log \frac{I}{I_0} + \underbrace{\varepsilon}_{Noise}$$

Y: response of least squares problem
get X (features) by discretizing the problem; a, b and integral

Wiederholung Computer Tomography

- estimate X-ray absorption as a function of location $\mu(a,b)$
- measure path integrals:

$$I = I_0 e^{\int_{ray} \mu(a,b)dray}$$

$$\iff \ln \frac{I_0}{I} = \int_{ray} \mu(a,b)dray$$

- to make this solvable, we need many rays
- to make this solvable with least squares, we must discretize

Step 1 use detector array and N_p parallel rays

Step 2 use N_0 different orientations $\Rightarrow$ # of measurements $N = N_p \cdot N_0$

$$\text{instance index} \quad i = \underbrace{i_p}_{detectorindex} + N_p \cdot \underbrace{i_0}_{angelindex}$$

Step 3 Discretize $\mu(a,b)$:

$$a = a_0 + j_a \Delta a$$
$$b = b_0 + j_b \Delta b$$

unknown:

$$\mu(j_a, j_b) \iff \beta_j \quad \text{with } j = j_a + D_a \cdot j_b \quad \text{'flattening of image'}$$

Step 4 Discretize Integral: relax $\delta((a,b) \in ray)$ to $\Rightarrow$ triangular shape $\iff$ change integral into sum:

$$\begin{aligned} y_i &= \int \mu(a,b)\delta((a,b) \in ray)dadb \\ &\approx \sum_{j_a, j_b} \underbrace{\mu(j_a, j_b)}_{\beta_j} \cdot \underbrace{\text{weight}((j_a, j_b), ray)}_{x_{ij}} + \underbrace{\varepsilon_i}_{\text{noise}} \end{aligned}$$

$$x_{ij} = \text{triangle}(\text{dist}(a = a_0 + j_a \Delta a, b = b_0 + j_b \Delta b), ray_i)$$

Matrix Notation:

$$Y = X\beta + \varepsilon$$

This is LSQ! Solve with your favorite LSQ method

2.2.2 Different Y_i have different noise level σ_i

Case 1: simple analytic formula for σ_i or σ_i^2 $\Rightarrow$ variance stabilizing transformation (almost equal). Example: Anscombe transform: $Y \sim \text{Poisson}(Y^*)$

$$\Rightarrow \text{mean} = Y^*, \text{variance} = Y^*$$

Transform:

$$\begin{aligned}\tilde{y} &= 2\sqrt{y + \frac{3}{8}} \sim \mathcal{N}(2\sqrt{y^* + \frac{3}{8}} - \frac{1}{4\sqrt{y^*}}, \sigma^2) \\ &= 1 + \underbrace{\mathcal{O}\left(\frac{1}{y^{*4}}\right)}_{\text{correction term}}\end{aligned}$$

$\Rightarrow$ apply OLS to $\tilde{y}$

But: If y is amplified:

$$y' = ay + b \quad a : \text{amplification factor} \quad b : \text{dark signal}$$

Anscomb (y') gives rubbish (not Poisson)

$$\Rightarrow \text{apply} \quad \text{Anscomb}\left(\frac{y' - b}{a}\right)$$

Case 2 We know σ_i for all i:

$$y_i = \left(b \pm \underbrace{0.4}_{\sigma_i}\right) cm$$

$$\Rightarrow \mathbb{E}|(x_i\beta^+ - y_i)^2| = \sigma_i^2 = \mathbb{E}(r_i^2)$$

$$\Rightarrow \mathbb{E}\left\lfloor \frac{r_i^2}{\sigma_i^2} \right\rfloor = 1 = const$$

non-parametric stabilization
⇒ weighted least squares:

$$\boxed{\hat{\beta} = \arg\min_{\beta} \sum_i \frac{(x_i\beta - y_i)^2}{\sigma_i^2}}$$

Matrix notation: covariance matrix:

$$S = \begin{bmatrix} \sigma_1^2 & & 0 \\ & \sigma_2^2 & \\ 0 & & \ddots \end{bmatrix}$$

$$\begin{aligned} \hat{\beta} &= \arg\min (X\beta - Y)^T S^{-1} (X\beta - Y) \\ &= \underbrace{(X^T S^{-1} X)^{-1} X^T S^{-1}}_{\text{weighted pseudo-inverse}} Y \end{aligned}$$

aquivalent to change of variables:

$$\begin{aligned} \tilde{X} &= S^{-\frac{1}{2}} X \\ \tilde{Y} &= S^{-\frac{1}{2}} Y \\ S^{-\frac{1}{2}} &= \begin{bmatrix} \frac{1}{\sigma_1} & & 0 \\ & \frac{1}{\sigma_2} & \\ 0 & & \ddots \end{bmatrix} \\ \beta &= (\tilde{X}^T \tilde{X})^{-1} \tilde{X}^T \tilde{Y} \end{aligned}$$

Case 3: We don't know σ_i ⇒ we need additional assumptions, e.g. noise independent for all:

⇒ cov-matrix s is diagonal, as in case 2

⇒ estimate σ_i together with β

⇒ Iteratively Re-weighted least squares

Mit: $\sigma_i^{(0)} = 1$

for $t = 1, ..., T_{max}$:

$$\begin{aligned} \hat{\beta}^{(t)} &= \arg\min_\beta \textstyle\sum_i \frac{(x_i\beta - y_i)^2}{(\sigma_i^{(t-1)})^2} \\ \sigma_i^{(t)} &= |x_i \hat{\beta}^{(t)} - y_i| \end{aligned}$$

in the limit $N \to \infty$

$$\sigma_i^{(2)} = \sigma_i^* \quad \text{(ture } \sigma_i \text{ found)}$$

for finite N (and slight violation of assumption):

use a few more iterations

2.3 If both Y and X are noisy - Total Least Squares (TLS)

$\hat{=}$ errors-in-variables-model

- standard interpretation of OLS: $X\beta = Y$ has no solution $\Rightarrow$ minimize difference between LHS ans RHS $(X\beta - Y)^2$
- alternative interpretation of OLS:
  - find $\tilde{Y}$ such that $X\beta = \tilde{Y}$ is solvable
  - make the difference between Y and $\tilde{Y} = Y + R$ small $\Rightarrow$ minimize the correction $\min_R \|R\|_2^2$
- if X is also noisy:
  - find $\tilde{X}$ and $\tilde{Y}$ such that $\tilde{X}\beta = \tilde{Y}$ is solvable
  - define $\tilde{X} = X + E, \quad \tilde{Y} = Y + R$
  - define correction matrix $T = [ER] \Rightarrow \min_T \|T\|_F^2$

Formal definition of optimization problem

$$\hat{T}, \hat{\beta} = \arg\min_{T,\beta} \|T\|_F^2 \text{ with } T = [ER] \text{ subject to } (X + E)\beta = Y + R$$

Theorem: Let $Z = [XY] \leftarrow N \times (D+1)$ <u>after</u> centralization of X and Y

$$\text{SVD of} \quad Z = \underbrace{U}_{\substack{\text{orthogonal} \\ N\times(D+1)}} \cdot \underbrace{\Lambda}_{\substack{\text{diagonal} \\ (D+1)\times(D+1)}} \cdot \underbrace{V^T}_{\substack{\text{orthogonal} \\ (D+1)(D+1)}}$$

$$\begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_{D+1} \end{pmatrix}$$

$$\text{Then } \min \|T\|_F^2 = \min_j (\lambda_j^2)$$

$$\text{Let } \hat{j} = \arg\min_j \lambda_j^2 \quad \Rightarrow \quad \hat{v} = v_{\hat{j}} \text{of matrix V}$$

$$\text{corresponding singular vector} \quad \hat{v} = \begin{bmatrix} w \\ \alpha \end{bmatrix}$$

$$\Rightarrow \quad \boxed{\hat{\beta} = -\frac{w}{\alpha}}$$

2.4 Total Least Squares

If Y and X are noisy:

- find corrections $\tilde{X} = X + E, \tilde{Y} = Y + R$ such that $\tilde{X}\beta = \tilde{Y}$ is solvable
- minimize corrections
- algorithm:
  1. centralize X and Y
  2. concatenate $[XY] = Z$
  3. find the singular value of Z with smallest magnitude and corresponding singular vector $\hat{v}$
  4.

$$\hat{\beta} = -\frac{\hat{v}_{1\ldots D}}{v_{1+D}} \quad \hat{v} = \begin{bmatrix} \hat{v}_{1\ldots D} \\ v_{1+D} \end{bmatrix}$$

OLS: Only Y noisy ⇒ correct only Y (move values in Y-directions)

TLS: X and Y must be corrected (move points in X,Y direction). Correction must be perpendicular to regression line ⇒ best correction direction is the smallest singular vector

Intuitive Interpretation: Fit the data cloud with an ellipsoid (as in QDA) defined by the SVD (singular vector decomposition) of Z (or eigendecomposition of $Z^T Z$) ⇒ correction direction ≙ normal of regression hyperplane ≙ smallest ellipsoid radius

2.5 The linear system is underdetermined ⇒ Regularization

What is underdetermined?

$$\beta \in \mathbb{R}^D \Rightarrow \text{want to find D unknown numbers}$$

But the data doesn't have enough information to find D unknowns

Case 1: $X \in \mathbb{R}^{N \times D}$ with $N < D$

$$\text{In general:} \quad \text{rank}(X) \leq \min(N, D) = N < D$$

Rank measures the amount of information contained in X

Case 2: $D \geq N$, but $\kappa(X)$ (condition number) is bad ≙ several columns of X are almost linearly dependent ≙ effective rank $D^* < D$, D^*≙ number of singular values of X that are significantly different from zero ≙$D - D^*$ singular calues are effectively 0
⇒ we need additional information to compute D numbers ⇒ refularization provides this info

2.5.1 Bias-Variance Trade-Off:

Bias (systematic errors): intrinsic error of the model, doesn't disappear for $N \to \infty$. **Variance** (random errors): error caused by finite N
Intuition:

- modeling training effort is mose efficiently spend when both errors are about equal
- let TS_N be a training set of size N.

$$\text{If data are i.i.d. :} \quad p(TS_N) = \prod_i p(X_i, Y_i) = p(X, Y)^N$$

- let β^* be the (unknown) optimal model parametes, $\hat{\beta}$ solution from TS_N
- suppose we can repeat experiment with many random TS_N
- determine the expected squared error of $\hat{\beta}$:

$$\mathbb{E}_{TS_N}[(\hat{\beta} - \beta^*)^2] \quad \text{'Mean squared error (MSE) of } \hat{\beta}\text{'}$$

$$\begin{aligned}\mathbb{E}_{TS_N}[(\hat{\beta} - \beta^*)^2] &= \mathbb{E}[((\hat{\beta} - \mathbb{E}[\hat{\beta}])^2 + (\mathbb{E}[\hat{\beta}] - \beta^*))^2] \\ &= \underbrace{\mathbb{E}[(\hat{\beta} - \mathbb{E}[\hat{\beta}])^2]}_{\text{variance of } \hat{\beta}} + \underbrace{\mathbb{E}[(\mathbb{E}[\hat{\beta}] - \beta^*)^2]}_{\text{squared bias of } \hat{\beta}} + 2\mathbb{E}[(\hat{\beta} - \mathbb{E}[\hat{\beta}])(\mathbb{E}[\hat{\beta}] - \beta^*)]\end{aligned}$$

$$\mathbb{E}[(\hat{\beta} - \mathbb{E}[\hat{\beta}])(\mathbb{E}[\hat{\beta}] - \beta^*)] = \mathbb{E}[\hat{\beta}](\mathbb{E}[\hat{\beta}] - \beta^*) - \underbrace{\mathbb{E}[\mathbb{E}[\hat{\beta}]]}_{\mathbb{E}[\hat{\beta}]}(\mathbb{E}[\hat{\beta}] - \beta^*) = 0$$

$$\Rightarrow \boxed{\mathbb{E}[(\hat{\beta} - \beta^*)^2] = \mathbb{E}[(\hat{\beta} - \mathbb{E}[\hat{\beta}])^2] - \mathbb{E}[(\mathbb{E}[\hat{\beta}] - \beta^*)^2]}$$

Application of OLS:

$$Y = X\beta + \varepsilon$$

$$\begin{aligned}\mathbb{E}[\hat{\beta}] &= \mathbb{E}[(X^T X)^{-1} X^T Y] \\ &= \underbrace{\mathbb{E}[\underbrace{(X^T X)^{-1} X^T X}_{\mathbb{1}} \beta^*]}_{\mathbb{E}(\beta^*) = \beta^*} + \underbrace{\mathbb{E}[(X^T X)^{-1} X^T \varepsilon]}_{= (X^T X)^{-1} \underbrace{\mathbb{E}[\varepsilon]}_{0}} \\ &= \beta^*\end{aligned}$$

$$\Rightarrow \mathbb{E}[(\mathbb{E}[\hat{\beta}] - \beta^*)^2] = \mathbb{E}[(\beta^* - \beta^*)^2] = 0$$

$\Rightarrow$ OLS is unbiased. Covariance matrix of β:

$$\begin{aligned}\mathbb{E}[(\hat{\beta}-\mathbb{E}[\hat{\beta}])(\hat{\beta}-\mathbb{E}[\hat{\beta}])^T] &= \mathbb{E}[(\hat{\beta}-\beta^*)(\hat{\beta}-\beta^*)^T] \\ &= \mathbb{E}[(X^TX)^{-1}X^T\varepsilon\varepsilon^TX(X^TX)^{-1}] \\ &= (X^TX)^{-1}X^T \underbrace{\mathbb{E}[\varepsilon\varepsilon^T]}_{\substack{\text{covariance of noise} \\ =\sigma^2\mathbb{1}}} X(X^TX)^{-1} \\ &= \sigma^2\underbrace{(X^TX)^{-1}X^TX}_{\mathbb{1}}(X^TX)^{-1}\end{aligned}$$

$$\Rightarrow \boxed{\mathbb{E}[(\hat{\beta}-\beta^*)(\hat{\beta}-\beta^*)^T] = \sigma^2(X^TX)^{-1}}$$

This is the error propagation formula from Y to $\hat{\beta}$. We used:

$$\begin{aligned}\hat{\beta} &= (X^TX)^{-1}X^T(X\beta^*+\varepsilon) \\ \beta^* &= (X^TX)^{-1}X^TX\beta^* \\ \hat{\beta}-\beta^* &= (X^TX)^{-1}X^T\varepsilon\end{aligned}$$

$\varepsilon \mathrel{\widehat{=}}$ vector of independent zero-mean Gaussian noise values with variance σ^2

$$\Rightarrow \hat{\beta} \sim \mathcal{N}(\beta^*, \sigma^2(XX^T)^{-1})$$

$\Rightarrow \hat{\beta}$ of OLS has high variance when codition $\kappa(X)$ is bad (effective rank of X is $<$ D)

- If X has bad condition, two (one more) columns are almost linearly dependent, e.g. j and j'
  OLS can learn parameters β_j and $\beta_{j'}$ such that

  $$\sum_i (X_i\beta_j + X_i\beta_{j'}) = 0$$

  on the training set but β_j and $\beta_{j'}$ are big numbers that cancel on training set

  $$\Rightarrow \sum_i (X_i\beta_j + X_i\beta_{j'}) \text{ on } \underline{\text{test set}} \text{ is huge} \Rightarrow \text{overfitting}$$

- Intuition: To reduce overfitting we must prevent big coefficients β_j
- restricting the magnitude of β may mean, that $\hat{\beta} \approx \beta^*$ is no longer achievable $\Rightarrow$ introduced bias. But if the bias is less then variance, this doesn't matter, 'trade-off'
- penalize such that both error contributions are roughly equal
- only meaningful if the β_j have equal importance/scale to make penalties comparable

- always standardize X beforehand

$$X_j \to \frac{X_j}{\text{stdDev}[X_j]}$$

  $\Rightarrow$ each column now has unit variance $\widehat{=}$ comparable scales

- combine this with centralization $\Rightarrow$ data have zero mean, unit variance (standard data preprocessing)
- apply inverse transform to β at the end

Allow some bias to achieve a big reduction in variance, total error reduction

2.5.2 Ridge Regression

Solve constrained least squares problem:

$$\hat{\beta} = \arg\min_{\beta}(X\beta - Y)^2 \quad s.t. \quad \|\beta\|_2^2 = \beta^T\beta \leq t$$

Mathematically aquivalent formulation: Add constraint to the loss via Lagrange multiplier τ

$$\hat{\beta}_\tau = \arg\min_{\beta} \underbrace{(X\beta - Y)^2}_{\text{data term}} + \underbrace{\tau\beta^T\beta}_{\text{regularization term}}$$

Theorem: For each t from the original problem, there is a τ such that the solutions are the same. There are different solution methods

1. via regularized pseudo-inverse

$$\frac{\partial Loss}{\partial \beta} = 2X^T(X\beta - Y) + 2\tau\beta \stackrel{!}{=} 0$$

$$(X^TX + \tau\mathbb{1})\beta = X^TY$$

$$\boxed{\hat{\beta} = \underbrace{(X^TX + \tau\mathbb{1})^{-1}X^T}_{X_\tau^+}Y}$$

X_τ^+ : regularized pseudo-inverse

2. via reduction to OLS, define:

$$\tilde{X} = \begin{bmatrix} X \\ \sqrt{\tau}\mathbb{1} \end{bmatrix} \quad \tilde{Y} = \begin{bmatrix} Y \\ 0 \end{bmatrix}$$

$$(\tilde{X}\beta - \tilde{Y})^T(\tilde{X}\beta - \tilde{Y}) = (X\beta - Y)^T(X\beta - Y) + \tau\beta^T\beta$$

$$\Rightarrow \hat{\beta}_\tau = \arg\min_\beta (\tilde{X}\beta - Y)^2 \quad \text{This is OLS problem}$$

Now just use any OLS solver

3. via Singular Value Decomposition:

$$X = U\Lambda V^T \quad X^T = V\Lambda U^T \quad X^T X = V\Lambda^2 V^T$$

$$\begin{aligned} X^T X + \tau\mathbb{1} &= V\Lambda^2 V^T + VV^T\tau\mathbb{1}VV^T \\ &= V(\Lambda^2 + \tau V^T\mathbb{1}V)V^T \\ &= V\underbrace{(\Lambda^2 + \tau\mathbb{1})}_{diag(\lambda_j^2+\tau)}V^T \end{aligned}$$

$$(X^T X + \tau\mathbb{1})^{-1} = V diag\left(\frac{1}{\lambda_j^2 + \tau}\right)V^T$$

$$(X^T X + \tau\mathbb{1})^{-1}X^T = V diag\left(\frac{\lambda_j}{\lambda_j^2 + \tau}\right)\cancel{V^T V\Lambda U^T}$$

$$\boxed{(X^T X + \tau\mathbb{1})^{-1}X^T = V diag\left(\frac{\lambda_j}{\lambda_j^2 + \tau}\right)U^T = X_\tau^+}$$

If $\lambda_j \approx 0$: OLS($\tau = 0$) $\quad \frac{1}{\lambda_j} \approx \infty \Rightarrow$ instable solution.
Ridge Regression($\tau > 0$) $\quad \frac{\lambda_j}{\lambda_j^2+\tau} \approx \frac{\lambda_j}{\tau} \approx 0 \Rightarrow$ no exploding singular values, stable

4. Solution via the dual optimization problem $\Rightarrow$ next week

Bayesian interpretation of ridge regression:

Let $p(\beta|Y)$ be the probability for the solution β given data Y

We want the maximum likelihood $\hat{\beta} = \arg\max_\beta p(\beta|Y) = \arg\min_\beta -\log p(\beta|Y)$. Now we expand p by Bayes theorem:

$$\begin{aligned}
\hat{\beta} &= \arg\max_\beta p(\beta|Y) \\
&= \arg\min_\beta -\log p(\beta|Y) \\
&= \arg\min_\beta -\log p(Y|\beta)p(\beta) \\
&= \arg\min_\beta -\log \underbrace{p(Y|\beta^*)}_{\mathcal{N}(X\beta^*,\sigma^2)} - \log \underbrace{p(\beta^*)}_{\text{prior belief}} \\
&= \arg\min_\beta (X\beta^* - Y)^2 + const
\end{aligned}$$

We used the uninformative prior: $p(\beta^*) = const \Rightarrow -\log p(\beta^*) = const$

Gaussian prior: $p(\beta^*) = \mathcal{N}(0, \frac{1}{\tau})$

$$\Rightarrow -\log p(\beta^*) = \tau\beta^T\beta + const$$

2.5.3 Sparse Regression

We change the regularization term: either use threshhold $\|\beta\|_p \leq t$ or use $+\tau\|\beta\|_p$ lagrange multiplier:

- $p = 2 \Rightarrow$ ridge regression.
- $p = 1 \Rightarrow$ L1 regularization$\widehat{=}LASSO$
- $p = 0$ counting regularization

$$\|\beta\|_0 = \sum_j \mathbb{1}[\beta_j \neq 0] \quad \text{count non-zero elements}$$

Optimizing the problem under the L_0 ist NP-hard. The L_1 is always sparse if t is small enough, because optimum is at the corner of teasible region.

Approximation algorithm: Orthogonal Matching Pursuit OMP Init:

- $X \in \mathbb{R}^{ND}, Y \in \mathbb{R}^N, T$: threshold for number of non-zero elements of β.
- set of active column indices of X: $A^{(0)} = \emptyset$
- set of inactive column indices of X: $B^{(0)} = \{j : j = 1...D\}$
- initial residual: $r^{(0)} = y$

Iteration:

- for $t = 1, ..., T$:
  - find $\hat{j}^{(t)} = \arg\max_{j \in B^{(t-1)}} |x_j^T \cdot r^{(t-1)}|$
  - move $\hat{j}^{(t)}$ from B to A
  - define active matrix $x^{(t)}$ containing all indices from $A^{(t)}$
  - solve OLS problem $\hat{\beta}^{(t)} = \arg\min_\beta \|x^{(t)}\beta - y\|$
  - update residual: $r^{(t)} = y - x^{(t)}\hat{\beta}^{(t)}$

Application of sparse regression - Topic discovery

- index i (rows of x) corresponds to words, index j (columns of x) corresponds to topicd each column x_j is word frequency hostogramm for topic j $\Rightarrow x_{ij} \widehat{=}$ relative frequency of word in document that only talks about topic j
- Y: word frequency histogram of new document
- task: find out, what topic(s) Y talks about by comparison of word counts
- linear model: $Y = X\beta + \varepsilon$
- β must be positive and sparse
- Solution: apply non-negative LASSO (L_1 regularization) or non-negative orthogonal matching pusuit to get β, non-zwor elements of $\beta \widehat{=}$ topics that best explain Y's word frequencies
- Extensions: to learn matrix X ('Dictionary') along with β of training set, 'dictionary learning'

2.6 Non-linear Regression

Non-linear model with additive gaussian noise $Y = f(X;\beta) + \varepsilon$ (linear regression is a special case: $f(X;\beta) = X\beta$). There are two approaches:

- find optimal β directly:
  - non-linear alg. (Levenberg-Marquort Algorithm)
  - regression tree/forest
- Write:

$$f(X;\beta) = \phi(X) \cdot \beta \quad \phi(X) : \mathbb{R}^D \to \mathbb{R}^{D'} \quad \text{non-linear mapping}$$

$$\tilde{X} = \phi(X) \quad \text{'augmented feature'}$$

how to find ϕ?

- hand crafted
- kernel trick/methods
- learn $\phi(X;\theta)$, e.g. neural network

Example 1 - XOR Problem True model: $Y = X_1 \text{ XOR } X_2 \neq [X_1, X_2] \cdot \beta + b$
Solution: Find new axis:

$$\begin{aligned}
\tilde{X_1} &= 2X_1 - 1 \in \{-1, 1\} \\
\tilde{X_2} &= 2X_2 - 1 \in 1, 1\} \\
\tilde{X_3} &= \tilde{X_1} \cdot \tilde{X_2} \\
Y &= \frac{\tilde{X_3} + 1}{2} = \tilde{X}\beta = \left[\tilde{X_1}, \tilde{X_2}, \tilde{X_3}\right] \cdot \begin{bmatrix} 0 \\ 0 \\ \frac{1}{2} \end{bmatrix} + \frac{1}{2}
\end{aligned}$$

Example 2 - Fitting a circle

$$\text{model:} \quad y_1 = c + \begin{bmatrix} cos(\phi_i) \\ sin(\phi_i) \end{bmatrix} \cdot (r + \varepsilon_i)$$

Free variable ϕ, parameters r (radius) and c (center).

$$\begin{aligned}
\text{Least squares problem:} \quad \hat{c}, \hat{r} &= \arg\min_{c,r} \sum_i (\|y_i - c\| - r)^2 \\
&= \arg\min_{c,r} \sum_i (\underbrace{\sqrt{(y_{i1} - c_1)^2 + (y_{i2} - c_2)^2}}_{\text{non-linear}} - r)^2
\end{aligned}$$

Solution 1: non-linear least squares (homework?) Solution 2: work in an augmented space by means of algebraic loss

$$\begin{aligned}
\hat{c}, \hat{r} &= \arg\min_{c,r} \sum_i (\|y_i - c\|^2 - r^2)^2 \\
&= \arg\min_{c,r} \sum_i ((y_{i1} - c_1)^2 + (y_{i2} - c_2)^2 - r^2)^2 \\
&= \arg\min_{c,r} \sum_i (y_i^2 - 2c^T \cdot y_i + c^2 - r^2)^2
\end{aligned}$$

$$\begin{aligned}
\tilde{x_i} &= [y_{i1}, y_{i2}, 1] \\
\tilde{y_i} &= y_i^T y_i \\
\beta &= [2c_1, 2c_2, r^2 - c^T c]^T \\
\hat{\beta} &= \arg\min_{\beta} \sum_i (\tilde{y_i} - \tilde{x_i}\beta)^2
\end{aligned}$$

$$\hat{c_1} = \frac{\hat{\beta}_1}{2} \quad \hat{c_2} = \frac{\hat{\beta}_2}{2} \quad \hat{r} = \sqrt{\hat{\beta}_3 + \hat{c}^T \hat{c}}$$

2.6.1 Levenberg-Marquart Algorithm

Problem: $\hat{\beta} = \arg\min_\beta \sum_i (Y_i - f(X_i;\beta))^2$ has no closed form solution because $f(X_i;\beta)$ is non-linear

- linearize f in the neighborhood of a current guess $\beta^{(t)}$ and find an improvement

$$\beta^{(t+1)} = \beta^{(t)} + \Delta^{(t)} \text{by } \underline{\text{linear least squares}}$$

  $\Rightarrow$ Iterate until convergence

- Linearization by Taylor expansion:

$$f(X;\beta+\Delta) = f(X;\beta) + \left.\frac{\partial f}{\partial \beta}\right|_\beta \cdot \Delta + \mathcal{O}(\Delta^2)$$

$$\text{Loss } (\beta+\Delta) \approx \sum_i \underbrace{(Y_i - f(X_i;\beta)}_{\tilde{Y}} - \underbrace{\left.\frac{\partial f}{\partial \beta}\right|_\beta}_{\tilde{X}} \cdot\Delta)^2$$

$\Rightarrow$ Gauss-Newton algorithm:
Initialization:

- find initial guess $\beta^{(0)}$
- for f=1...T (or until convergence):

$$\hat{\Delta}^{(t)} = \arg\min_\Delta \sum_i (\tilde{Y}_i^{(t)} - \tilde{X}_i^{(t)} \cdot \Delta)^2$$

$$\text{with } \tilde{Y}_i^{(t)} = Y_i - f(X_i;\beta^{(t-1)}), \tilde{X}^{(t)} = \left.\frac{\partial f}{\partial \beta}\right|_{\beta=\beta^{(t-1)}}$$

$$\beta^{(t)} = \beta^{(t-1)} + \hat{\Delta}^{(t)}$$

- Solution via pseudo-inverse

$$\tilde{\Delta}^{(t)} = (\tilde{X}^T\tilde{X})^{-1}\tilde{X}^T\tilde{Y}$$

- problem: Gauss-Newton easily overfitts/$\tilde{X}$ may have bad condition $\Rightarrow \Delta^{(t)}$ eplodes (no convergence)
- Lovenberg uses ridge regression to regularize

$$\hat{\Delta}^{(t)} = (\tilde{X}^T\tilde{X} + \tau\mathbb{1})^{-1}\tilde{X}^T\tilde{Y}$$

effect if τ small (relative to $\tilde{X}^T\tilde{X}$)
$\Rightarrow$ behaves like unregularized regression
$\Rightarrow$ fast convergence
If τ big (relative to $\tilde{X}^T\tilde{X}$)

$$\Rightarrow \tilde{\Delta}^{(t)} \approx \frac{1}{\tau}\tilde{X}^T\tilde{Y}$$

$\Rightarrow$ gradient decent, with step size $\frac{1}{\tau}$, slow but numerically stable

- problem: regularization should be applied to standardized data, but we cannot standardize $\tilde{X}$ because it mus be Jacobian
- Marquarts trick: weight τ with the diagonal elements of $\tilde{X}^T\tilde{X}$

$$\hat{\Delta}^{(t)} = (\underbrace{\tilde{X}^T\tilde{X} + \tau diag(\tilde{X}^T\tilde{X})}_{\text{multiply diagonal of} X^T X \text{with} (1+\tau)})^{-1}\tilde{X}\tilde{Y}$$

- how to choose τ automatically:
  $\Rightarrow$ Stepsize control: start with initial $\tau = \tau_0 (= 0.1)$
  - solve current iteration with current τ, if residual decreases
    $\Rightarrow$ accept $\hat{\beta}^{(t)}$ and use loss regularization in next iteration if residual increases $\Rightarrow$ reject $\hat{\beta}^{(t)}$, increase $\tau \leftarrow \sqrt{2}\tau$, retry current iteration.

We did OLS in hand-crafted augmented data space:

$$\tilde{X} = \phi(X) \quad \tilde{Y} = \psi(Y)$$

2.6.2 Regression trees & forests

Almost equal to density tree, adapted to regression problem. Idea:

$$Y = f(X) + \varepsilon \quad \text{is approximated by a piecewise constant function}$$

$$\hat{Y} = \hat{f}(X) \quad \text{with} \quad \hat{f}(X) = \sum_l f_l \mathbb{1}\lfloor X \in \text{bin}_l \rfloor$$

If bins are fixed, determine

$$\hat{f}_l = \arg\min_{\{f_l\}} \sum_i (Y_i - \hat{f}(X_i))^2$$

$$\Rightarrow \hat{f}_l = \frac{1}{N_l} \sum_{i \in \text{bin}_l} Y_i \quad i \in \text{bin} \widehat{=} X_i \in \text{bin}_l$$

Define bins by recursive subdivision, as in density tree, but two differences:

- to determine the best split of bin l, search exhaustively or randomly over all possible splits of bin l, and than choose the best split $\widehat{=}$ minimize the redidual after splitting

$$\text{residual} \quad = \sum_{i \in \text{bin}_l} (Y_i - \hat{f}_\lambda)^2 + \sum_{i \in \text{bin}_\rho} (Y_i - \hat{f}_\rho)^2$$

- in each iteration, split the bin with highest score:

$$\text{score}_l \quad = \sum_{i \in \text{bin}_l} (Y_i - \hat{f}_l)^2 - \sum_{i \in \text{bin}_l} (Y_i - \hat{f}_{\lambda_l})^2 - \sum_{i \in \text{bin}_l} (Y_i - \hat{f}_{\rho_l})^2$$

We also generalize into regression forest, train many trees with random variation:

- check a random subset of the possible candidate splits
- present a random subset of the training data to each tree
- during prediction: return average of all trees

2.6.3 Kernel Methods

Idea: replace handcrafted augmented feature space with a kernel function. We consider a fourth solution method for ridge regression via dual optimization problem. Recall:

$$\hat{\beta} = \arg\min_\beta \sum_i (Y_i - X_i\beta)^2 + \tau\beta^T\beta$$

This is the primal optimization problem of ridge regression. Now we will rewrite:

$$\hat{\beta}, \{\hat{r}_i\} = \arg\min_{\beta, \{r_i\}} \sum_i r_i^2 + \tau\beta^T\beta \quad \text{such that } \forall i : r_i = Y_i - X_i\beta$$

Define Lagrangian function:

$$L(\beta, \{r_i\}, \{\alpha_i\}) = \tau\beta^T\beta + \sum_i r_i^2 + 2\tau \sum_i \alpha_i(Y_i - X_i\beta - r_i)$$

Where α_i are the Lagrangian multipliers, also calles the dual variables. We can now optimize:

$$\boxed{\hat{\beta}, \{\hat{r}_i\}, \{\hat{\alpha}_i\} = \arg\max_{\{\alpha_i\}} \arg\min_{\beta, \{r_i\}} L(\beta, \{r_i\}, \{\alpha_i\})}$$

$$\frac{\partial L}{\partial \beta} = 2\tau\beta^T - 2\tau \sum_i \alpha_i X_i \stackrel{!}{=} 0$$

$$\Rightarrow \beta^T = \sum_i \alpha_i X_i = \alpha^T X$$

$$L = \tau\alpha^T XX^T\alpha + \sum_i r_i^2 + 2\tau\sum_i \alpha_i Y_i - 2\tau\sum_i \alpha_i r_i - 2\tau\underbrace{\sum_i \alpha_i X_i X^T\alpha}_{\alpha^T XX^T\alpha}$$

$$= -\tau\alpha^T XX^T\alpha + \sum_i r_i^2 + 2\tau\sum_i \alpha_i Y_i - 2\tau\sum_i \alpha_i r_i$$

$$\text{Gram Matrix} \quad G = XX^T \in \mathbb{R}^{N\times N}$$

$$\text{Elements} \quad G_{ii'} = X_i X_{i'}^T$$

This is the scalar product between features of instance i and i'.

$$\frac{\partial L}{\partial r_i} = 2r_i - 2\tau\alpha_i \stackrel{!}{=} 0 \quad r_i = \tau\alpha_i$$

$$\Rightarrow L = -\tau\alpha^T G\alpha + \tau^2\alpha^T\alpha + 2\tau\sum_i \alpha_i Y_i - 2\tau^2\alpha^T\alpha$$

$$= -\tau\alpha^T G\alpha - \tau^2\alpha^T\alpha + 2\tau\alpha^T Y$$

$$\frac{\partial L}{\partial \alpha} = -2\tau G\alpha - 2\tau^2\alpha + 2\tau Y \stackrel{!}{=} 0$$

$$= -G\alpha - \tau\alpha + Y \stackrel{!}{=} 0 \qquad (G + \tau\mathbb{1}_N)\hat{\alpha} = Y$$

$$\boxed{\hat{\alpha} = (G + \tau\mathbb{1})^{-1}Y} \quad \text{dual solution}$$

$$\Rightarrow \hat{\beta}^T = \hat{\alpha}^T X$$

Prediction for new instance X_{new}:

$$Y_{\text{new}} = X_{\text{new}}\hat{\beta} = \hat{\beta}^T X_{\text{new}}^T = \hat{\alpha}^T XX_{\text{new}}^T$$

$$\text{with Gram vector} \quad g = XX_{\text{new}}^T, \quad g_i = X_i X_{\text{new}}^T$$

$$\boxed{Y_{\text{new}} = \hat{\alpha}^T g_{\text{new}}}$$

Solve dual in augmented feature space: $\tilde{X} = \phi(X)$

$$\hat{\alpha} = (\tilde{G} + \tau\mathbb{1})^{-1}Y \quad \tilde{G} = \tilde{X}\tilde{X}^T$$

$$Y_{\text{new}} = \hat{\alpha}^T \tilde{g}_{\text{new}} \quad \tilde{g}_{\text{new}} = \tilde{X}\tilde{X}_{\text{new}}^T$$

Kernel trick: we can construct $\tilde{G}$ and $\tilde{g}_{\text{new}}$ without ever computing $\tilde{X}$ and $\tilde{X}_{\text{new}}$, namely via a kernel function k

$$\tilde{G}_{ii'} = \phi(X_i)\phi(X_{i'})^T := K(X_i, X_{i'})$$

K is chosen to be much simpler than ϕ.

Example

$$X_i = [X_{i1}, X_{i2}], \quad \tilde{X} = [X_{i1}^2, X_{i2}^2, \sqrt{2}X_{i1}X_{i2}, \sqrt{2}X_{i1}, \sqrt{2}X_{i2}, 1]$$

$$\begin{aligned}\tilde{G}_{ii'} = \tilde{X}_i\tilde{X}_{i'}^T &= X_{i1}^2X_{i'1}^2 + X_{i2}^2X_{i'2}^2 + 2X_{i1}X_{i2}X_{i'1}X_{i'2} + 2X_{i1}X_{i'1} + 2X_{i2}X_{i'2} + 1 \\ &= (X_iX_{i'}^T + 1)^2 = K(X_i, X_{i'})\end{aligned}$$

General condition that the kernel trick is applicable:

1. Solution of optimization problem only accesses features via scalar products. We achieve this by using the dual optimization problem with G.
2. Kernel function is positive definite (Mercer's condition)

$$\int_{\mathbb{R}^D}\int_{\mathbb{R}^D} K(X_i, X_{i'})f(X_i)f(X_{i'})d(X_i, X_{i'}) \geq 0$$

for arbitrary square integrable functions $f : \mathbb{R}^D \to \mathbb{R}^D$
Intuition: the matrix $\tilde{G} + \tau\mathbb{1}$ is always positive definite for $\tau > 0$ and invertible.

Popular Kernel functions

- Polynomial Kernels:

$$K(X_i, X_{i'}) = (X_iX_{i'}^T + 1)^q \quad q \in \mathbb{N}^+$$

- squared exponential (Gaussian) kernel

$$K(X_i, X_{i'}) = e^{-\frac{\|X_i - X_{i'}\|^2}{2\sigma^2}}$$

Example continued

$$K(X_i, X_{i'}) = (X_iX_{i'}^T + 1)^2$$

This is sufficient to solve the XOR problem. By choosing the right kernel, arbitrary non-linear relationships $Y = f(X)$ can be modeled. The disadvantage is that this is more expensive.

Inversion of $G+\tau\mathbb{1}$ takes $\mathcal{O}(N^3)$ if G is dense and $\mathcal{O}(N)$ if G is sparse. We also need prediction $\mathcal{O}(N \cdot D)$ to compute j_{new}. It also easily overfits, therefore carefully select regularization parameter τ and the properties q and σ of the kernel function via cross validation.
End.

Kernel Trick recalled: reformulate problems such that feautres are only accessed via scalar products $X_i X_{i'}^T$

- replace all scalar products with calls to kernel function $K(X_i, X_{i'})$
- choose kernel according to application, solve $\hat{alpha} = (G + \tau\mathbb{1})^{-1}Y$, predict $\hat{Y_{\text{new}}} = \hat{\alpha}^T g_{\text{new}} \quad G_{ii'} = K(X_i, X_{i'}), g_i = K(X_i, X_{\text{new}})$

Simplified version: Kernel regression without ridge - Nadaraya-Walson regression:

- no training
- prediction:

$$Y_{\text{new}} = \frac{\sum_i Y_i g_i}{\sum_i g_i} \hat{=} \alpha_{\text{new}} = \frac{Y}{\|g_{\text{new}}\|_1} = (\frac{1}{\|g_{\text{new}}\|_1}\mathbb{1})Y$$

- usually not as good as Kernel ridge regression but cheaper

2.7 Robust regression

2.7.1 Introduction

- Robust means that the regression still works when the data does not (exactly) conform to method's application
- 2 important types of deviation:
  1. contaminated data: True distribution has heavier tail then expected
  2. several independe model instances in the data $\Rightarrow$ inliers of one model are outliers of the other
- use robust regression wih care to not make up conclusions miss:
  - Ozone hole was discovered 1985 from the ground but shouls have been deected by Nimbus 7 satellite in 1983. The analysis software considered ouon concentration as low as in the hole as outliers and ignored hem
- 2 basic approaches:
  1. filer out the outliers, e.g. RANSAC algorithms
  2. use robust loss functions (implicit down weighted during optimization)

2.7.2 RANSAC algorithm

Application when:

- outlier funcino is medium $<$ 70% - 90% (more outliers - more expensive)
- data is superposition of several models
- regression problem has only few degrees of freedom (less than 10 unknown variables)

Idea: Let model have K unknowns. There is an algorithm that can fit the model with a minimal number of data points.
Examples:

- line fit in 2D: $N_{\min} = 2$
- circle in 2D: $N_{\min} = 3$
- hyperplane in n-D: $N_{\min} = n + 1$
- fundamentals matrix: $N_{\min} = 8$ (Transformation between two pictures of same scene)

Algorithm: Repeat for t=1...T:

- select instances at random and fi the model M_t.
- for all other insances compute the distance from the model d_{it} and count inliers $\widehat{=} d_{it} \leq \varepsilon$. $\varepsilon = 2\sigma \approx$ std. deviation without outliers.
- return model M with the most inliers (and corresponding inliers set).

Now imagine a model with data of two lines inside. Two find both lines we must find the first winner model. Then remove the inliers of the first model and run the RANSAC algorithm again. To improve the model: Use std. regression on the inliers set of the best fit - the random model is usually not the best fit.

- How often should we try? Define an acceptable prob. of failure, $\alpha \ll 1 \quad \alpha = 0.1\%$.
- must know the inlier function $\gamma = \frac{N_{in}}{N}$.

$$p(\text{pick only inliers in iteration t}) = \gamma^{\min} = p(\text{model } M_t \text{ is good})$$

$$p(\text{pick at least one outlier in iteration t}) = 1 - \gamma^{N_{\min}} = p(\text{model } M_t \text{ is bad})$$

$$p(\text{all T models are bad}) = (1 - \gamma^{N_{\min}})^T = 1 - p(\text{at least one model is good}) = 1 - \alpha$$

$$\Rightarrow T \geq \frac{\log(1-\alpha)}{\log(1-\gamma^{N_{\min}})}$$

application	$N_{\min}$	$\gamma = 90\%$	50%	30%
2D-line	2	3	17	49
3D-circle	3	4	35	169
fundam. matrix	8	9	1172	70188

Algorithm to find fundamental matrix

- detect characteristic points in both picturing ('interest points') with SIFT or HOG algorithm
- use RANSAC to create hypothesis about corresponding points - refer to same real world problem

2.7.3 Robust loss functions

Example: contaminated Gaussian distribution:

$$X \sim \underbrace{(1-\varepsilon)}_{\text{mixture prob.}} \underbrace{\mathcal{N}(0,\sigma^2)}_{\text{desired distrib.}} + \varepsilon\mathcal{N}(0,\tau^2))$$

$$\text{Mean: } \mu = 0 \quad \text{Variance of X: } var(\bar{X}) = \frac{1}{N}(1-\varepsilon)\sigma^2 + \varepsilon\tau^2) = \frac{\sigma^2}{N}(1-\varepsilon+\varepsilon\underbrace{\frac{\tau^2}{\sigma^2}}_{\leq 1})$$

If $\varepsilon > 0, \tau > 5$: Variance is increased. Traditional robust estimator median:

$$Med(X) = t \quad \text{such that} \quad \#\{x_i < t\} = \#\{x_i > t\}$$

Center of ordered set of observations.

$$var(Med(X)) = \frac{\sigma^2}{N}\frac{\pi}{2((1-\varepsilon)+\varepsilon\frac{\tau}{\sigma})^2}$$

$$\Rightarrow \frac{var(Med(x))}{var(Mean(X))} \overset{*}{=} \frac{\pi}{2} \simeq 1.57 \quad \text{if no contamination } (\varepsilon = 0)$$

$\Rightarrow$ need 57 % more data to achieve the accuracy with median. Median is more robust under outliers

$$\overset{*}{=} \begin{cases} 1 & \text{if } (\varepsilon = 5\%, \frac{\tau}{\sigma} = 4) \\ 0.29 & \text{if } (\varepsilon = 5\%, \frac{\tau}{\sigma} = 10) \\ 0.17 & \text{if } (\varepsilon = 10\%, \frac{\tau}{\sigma} = 10) \end{cases}$$