Regression and Classification Basics

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Contents

1 Machine Learning Modeling Basics

What Is Machine Learning (ML)?

- Lofty definition: make machines learn!!!
  - Have to make "machines" and "learn" more precise
- The machines of ML: mathematical input–output processes that lend themselves to some form of (numerical) parameterization
- The learning process: adjust the machine's parameters until a goal is reached
- New thing: "goal"?
  - At first sight, get something done
  - Ultimately, to minimize some error measure
- Summing things up: a ML process tries to find a concrete mathematical/algorithmic **input–output parameterized transformation** that **minimizes an error measure** by iteratively **adjusting the transformation's parameters**

Where Lies ML?

- In the middle of a possibly long process chain
- Before ML starts we must
  - Go from **raw to organized** data: accesing, gathering, cleaning, formatting, ...
  - Go from **organized to** (potentially) **informative** data: extracting basic and derived features
- After ML finishes we must perform
  - Outcome **evaluation**: how good/actionable it is
  - Outcome **exploitation**: collect, organize, act
  - **Individual model maintenance**: monitor performance, tune hyper–parameters
  - **Modeling life cycle maintenance**: discard old models, introduce new ones and **communicate** our work/results
- ML is in the middle of the global process chain but also in the middle of some subchains

Supervised/Unsupervised Models

- Model types: **supervised, unsupervised**
- Supervised models:
  - Targets y^p are known and the model tries to predict or estimate them
  - These known targets guide, or **supervise**, model building
  - Main emphasis here

- Unsupervised models:
  - There are no predetermined or supervising outputs
  - But nevertheless the model is supposed to learn relations or find structure in the data
  - Sometimes as a first step towards a supervised model

Regression and Classification

- Problems (usually) to be solved by models: regression, classification
- Patterns come in pairs (x, y)
  - x: inputs, predictors, features, independent variables
  - y: target, response, dependent variable; numerical in regression, class labels in classification
- **Regression**: the desired output y is regressed into the inputs x to derive a model $\widehat{y} = f(x)$
  - We want $y \simeq \widehat{y}$ so having $y - \widehat{y}$ "small" is the natural goal
- **Classification**: inputs are derived from several classes $C_1, \ldots, C_K$, to which labels ℓ_k are assigned
  - The model now assigns a label $\ell(x)$ to an input x
  - If x is derived from C_k we want to have $\ell(x) = \ell_k$
  - Here having $\ell(x) - \ell_k$ "small" may not make sense

The Boston Housing Problem

- This is a first "toy" problem
- We want to estimate the median of house values over an area from some information about it which we believe relevant
- Features x: several real estate–related variables of Boston areas
  - CRIM: per capita crime rate by town
  - RM: average number of rooms per dwelling
  - NOX: nitric oxides concentration (parts per 10 million)
  - AGE: proportion of owner-occupied units built prior to 1940
  - LSTAT: % lower status of the population
  - ...
- Target y: MEDV, median value of owner-occupied homes in $1,000's

Wind Energy Forecasting

- This is a second, real regression problem
- We want to estimate the hourly energy production of a wind farm from NWP variables which we believe relevant

- The **features** are the NWP variables
  - U, V surface wind components
  - U, V 100–meter wind components
  - Temperature
  - Pressure
  - ...
- The **target** is the energy produced during the outgoing hour

The ML Cycle in Wind Energy

- Raw data: historic wind energy production data plus NWP files from weather forecasters
  - Possibly huge files with special formats
  - We have to extract the relevant NWP information, organize them in a suitable way and pair it with the energy data
- The ML core: whatever set of (non–linear) regression algorithm which you may think useful
- After ML is finished
  - Collect, organize and save the different model outputs
  - Select one single model output or some combination (more ML) of them as your system's output
  - Compute uncertainty estimates
  - Combine your outputs with someone's else
  - And keep up the entire process

How to Build Regression Models

- In general we have a sample $S = \{x^p, y^p\}$, $1 \leq p \leq N$, with x^p the **features** and y^p the **targets**
- We want to build a model $\widehat{y} = f(x)$ so that $\widehat{y}^p = f(x^p) \simeq y^p$; i.e., we want to **regress** y to the x
- The concrete f is chosen within a certain family $\mathcal{F}$
  - Examples here: linear regression, multilayer perceptrons (MLPs), SVMs
  - And also: Random Forests (RF), Gradient Boosting (GB), nearest neighbor (NN)
- Natural option to ensure $f(x^p) \simeq y^p$: choose f to minimize the sample mean square error (MSE)

$$\widehat{e}(f) = \widehat{e}_S(f) = \frac{1}{2N}\sum_{p=1}^{N}(y^p - f(x^p))^2$$

- Thus, the model we select is $\widehat{f} = \widehat{f}_S = \arg\min_{f\in\mathcal{F}} \widehat{e}_S(f)$

Model Parameterization

- Usually individual models are selected through (ideally optimal) **parameter sets**
  - The parameters (weights) $W \in R^M$ select a concrete f in $\mathcal{F}$
- **Parametric** models have a fixed functional form $f(x) = f(x; W)$
- Simplest example: linear regression, where $M = d$ and $W = (w_0, w)$

$$f(x; w_0, w) = w_0 + \sum_{j=1}^{d} w_j x_j = w_0 + w \cdot x$$

- **Semi–parametric** models also use weights but without a predefined functional form; MLPs but also RF or GBR
- **Non parametric** models do not use weights nor follow any broad functional form; NN models

Model Estimation as Error Minimization

- For a parametric or semiparametric $f(x; W)$ we can write $\widehat{e}_S(f) = \widehat{e}_S(W)$
- The problem to solve becomes

$$\widehat{W}^* = \widehat{W}_S^* = \arg\min_W \widehat{e}_S(f(\cdot; W)), \quad \text{i.e., } \widehat{e}_S(\widehat{W}^*) \leq \widehat{e}_S(W) \; \forall W$$

- In linear regression

$$\widehat{e}(w_0, w) = \frac{1}{2N} \sum_p \left(y^p - w_0 - w \cdot x^p\right)^2$$

  which ends up in a simple quadratic form
- The regression problem reduces to **minimize** $\widehat{e}_S(W)$
  - Something in principle well understood in mathematical optimization

2 Basic Regression

Regression Assumptions

- **Key assumption**: x and y are related as $y = \phi(x) + n$ where
  - $\phi(x)$ is the **true** underlying function
  - n is **additive noise** with 0 mean and finite variance σ_N^2
- Our sample is just a particular instance of a deeper **sample generation process**
- Thus x, n are produced by **random variables** X, N
  - And so is y, given by $Y = \phi(X) + N$
- Moreover, X and N are **independent distributions** with densities $q(x)$, $\nu(n)$

- Thus, X and Y (or X and N) have a joint density

$$p(x, y) = p(x, \phi(x) + n) = q(x)\ \nu(n) = q(x)\ \nu(y - \phi(x))$$

The Best Regression Model

- It is easy to see that the best f is simply $f(x) = E_y[y|x]$, for

$$E_y[y|x] = E_n[\phi(x) + n] = \int (\phi(x) + n)\, \nu(n) dn = \phi(x)$$

- Have we finished? In theory yes; in practice, not at all!!!
  - We do not know ν and, thus, cannot compute the required integrals
  - If for any x we would have M values y^j, we could try $\widehat{\phi}(x) = \frac{1}{M} \sum_1^M y^j$
  - But this doesn't happen either
- So we forget about using $E[y|x]$ and get back to get an approximation $f \simeq \phi$ from the sample

Linear Models

- Assuming $x \in R^d$, the basic linear model is

$$f(x) = w_0 + \sum_1^d w_i x_i = w_0 + w \cdot x$$

- w_0 complicates notation; to drop it we center x and y so that $E[x_i] = E[y] = 0$; then $w_0 = 0$
- Then we are left with the simpler homogeneous model $f(x) = w \cdot x$
- In practice we will always **normalize** x, for instance to have 0 mean and 1 standard deviation (std) on each feature
  - But not y if we may help it
- But: how do we find w?

1–dimensional Linear Regression (LR)

- Assume that features X and target Y are **centered**, i.e., have 0 means
- For 1-dimensional patterns x the LR model then becomes

$$f(x) = w \cdot x$$

- And the error is then the function $e(w)$

$$\widehat{e}(w) \quad = \quad \frac{1}{2N} \sum_{p=1}^{N} (w \cdot x^p - y^p)^2 = \frac{1}{2N} \sum_p (\delta^p)^2$$

- The problem has obviously a minimum w^*
- To find it we just solve $\widehat{e}'(w) = 0$

Solving $\widehat{e}'(w) = 0$

- To compute $\widehat{e}'(w)$ we have

$$\begin{aligned}\widehat{e}'(w) &= \frac{1}{2N}\sum_p x^p\delta^p = \frac{1}{2N}\sum_p \left(w(x^p)^2 - x^p y^p\right)\\ &= w\left(\frac{1}{2N}\sum_p (x^p)^2\right) - \frac{1}{2N}\sum_p x^p y^p\end{aligned}$$

- The optimal w^* solves $\widehat{e}'(w) = 0$ and is given by

$$w^* = \frac{\frac{1}{2N}\sum_p x^p y^p}{\frac{1}{2N}\sum_p (x^p)^2} = \frac{\frac{1}{2N}X\cdot Y}{\frac{1}{2N}X\cdot X} = \frac{\frac{1}{N}X\cdot Y}{\text{var}(x)}$$

  where X and Y denote the N dimensional vectors $(x^1,\ldots,x^N)^t$, $(y^1,\ldots,y^N)^t$

General Linear Regression

- Assume again that X and Y are centered
- The LR model becomes now $f(x) = \sum_1^d w_i x_i = w\cdot x$
- If Y is the $N\times 1$ **target** vector and we organize the sample S in a $N\times d$ **data matrix** X, the sample mse is given by

$$\begin{aligned}\widehat{e}(w) &= \frac{1}{2N}\sum_p (w\cdot x^p - y^p)^2 = \frac{1}{2N}(Xw-Y)^t(Xw-Y)\\ &= \frac{1}{2N}(w^tX^tXw - 2w^tX^tY + Y^tY)\end{aligned}$$

- Now we have to solve $\nabla\widehat{e}(w) = 0$, i.e., $\frac{\partial\widehat{e}}{\partial w_i}(w) = 0$
- It is easy to see that

$$\nabla\widehat{e}(w) = \frac{1}{N}X^tXw - \frac{1}{N}X^tY = \widehat{R}w - \widehat{b}$$

Solving the Linear Equations

- The optimal $\widehat{w}^*$ must verify $\nabla\widehat{e}(\widehat{w}) = \widehat{R}\,\widehat{w} - \widehat{b} = 0$, where

$$\widehat{R} = \frac{1}{N}X^tX,\ \ \widehat{b} = \frac{1}{N}X^tY$$

- Over the original, non–centered data matrix we have

$$\widehat{R} = \frac{1}{N}(X-\overline{X})^t(X-\overline{X});$$

  i.e., $\widehat{R}$ is the **sample covariance matrix**

- If $\widehat{R}$ is invertible, we just solve the linear system $\widehat{R}\,\widehat{w} - \widehat{b} = 0$
- And obtain the sample–dependent optimal $\widehat{w}^*$ as

$$\widehat{w}^* = \widehat{R}^{-1}\widehat{b} = \left(X^t X\right)^{-1} X^t Y$$

Finding Optimal Models

- For general regression models it may not possible to solve analytically the equation $\nabla\widehat{e}(W) = 0$
  - For LR and big data, covariance matrices over large datasets or dimensions may not be computed
  - Numerical methods are needed
- The simplest numerical alternative is **gradient descent**:
  - Starting from some random W^0 we iteratively compute

$$W^{k+1} = W^k - \rho_k \nabla\widehat{e}(W^k) = W^k - \frac{\rho}{N}\left(X^t X W^k - X^t Y\right)$$

  - Component wise: $w_i^{k+1} = w_i^k - \rho_k \frac{\partial\widehat{e}}{\partial w_i}(W^k)$
  - ρ_k is the **learning rate**
- If $W^k \to W^*$, then $\nabla\widehat{e}(W^*) = 0$
  - Since our problems have obviously minima, this should be enough

Measuring Model Fit

- First option: **Root Square Error** $RSE = \sqrt{\frac{1}{N}\sum(y^p - \widehat{y}^p)^2} = \sqrt{\frac{1}{N}RSS}$
- OK, but how good is this? We must always have a **base model** to benchmark our results
- Simplest "model": the mean $\overline{y} = \frac{1}{N}\sum_1^N y^p$, with square error

$$\frac{1}{N}\sum(y^p - \overline{y})^2 = \frac{1}{N}TSS = \text{Var}(y)$$

- We can compare our model against our base computing

$$\frac{RSE^2}{\text{Var}(y)} = \frac{\sum(y^p - \widehat{y}^p)^2}{\sum(y^p - \overline{y})^2} = \frac{RSS}{TSS}$$

- The widely used R^2 coefficient is simply $R^2 = 1 - \frac{RSS}{TSS}$

Regularization

- Our regression solution $\widehat{w}^* = (X^t X)^{-1} X^t Y$ won't work if $X^t X$ is not invertible
  - For instance, when some features are correlated

- We could fix this working instead with $X^tX + \alpha I$ for some $\alpha > 0$
- To make this practical, note that $\widehat{w}^* = (X^tX + \alpha I)^{-1} X^tY$ minimizes

$$e_R(w) = \frac{1}{2N}\sum_p (y^p - w \cdot x_p^p)^2 + \frac{\alpha}{2}\|w\|^2,$$

- This is the **Ridge Regression** problem
  - Our first example of **regularization**, a key technique in Machine Learning
  - **All ML models must be regularized in some way**
- Important issue: how to find the right choice for α?

Takeaways on Linear Regression

1. We introduced **supervised** models
2. We have reviewed the essentials of the **linear regression model** (always the first thing to try)
3. We have considered model estimation as a problem on **error minimization**
4. We have seen how to build linear models analytically and numerically
5. We have defined how to measure model fit
6. We have introduced regularization

3 Bias, Variance and Cross Validation

Sample Dependence

- Important: **everything is sample dependent** for if we change S we get a different model
- We get sample–dependent weights $\widehat{W} = \widehat{W}_S$ and model $\widehat{f}_S(x) = \widehat{f}(x; \widehat{W}_S)$
- We must control their dependence on the concrete S sample used to build it
- Moreover, we must apply our model on new, **unseen** samples
- We must have a sample generating procedure that ideally gives homogeneous samples and a robust model building methodology
- Both together should (reasonably) guarantee that, for two S, S',

$$\widehat{f}_S(x) \simeq \widehat{f}_{S'}(x)$$

Sample Bias and Variance

- With several **independent** samples $S_1, \ldots, S_M$, it is natural to use as our best final model the averages of the $\widehat{f}_{S_m}(x)$ models, i.e.,

$$\frac{1}{M}\sum_{1}^{M}\widehat{f}_{S_m}(x) \simeq E_S[\widehat{f}_S(x)] = \widehat{f}_N(x)$$

  - The expectation $E_S[\widehat{f}_S(x)]$ is taken over all possible samples S of size N
  - $E_S[\widehat{f}_S(x)]$ is our ideally best model

- The **variance** of the $\widehat{f}_S(x)$ estimates is then

$$V_N(x) = E_S\left[(\widehat{f}_S(x) - \widehat{f}_N(x))^2\right]$$

Bias Versus Variance

- Ideally we would like to have a model such that

$$\widehat{f}_N(x) - \phi(x) \simeq 0,$$

  i.e., a model with small **bias**

  - This should be achievable with rich, highly flexible models
  - Or with essentially no regularization

- But we would also like to have a model such that

$$V_N(x) \simeq 0,$$

  i.e., a model with small **variance** $V_N(x)$

  - This should be achievable with simple models with few parameters
  - Or with more severe regularization

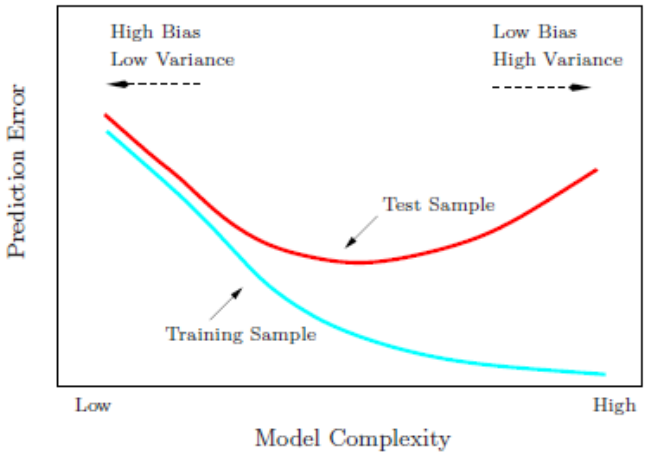
- But obviously both goals are contradictory to a large extent

The Bias–Variance Tradeoff

- There is thus a **tradeoff** between bias (low for complex models) and variance (low for simple models)

Evaluating Expected Performance

- It is obvious that before we start applying a model, we should have a reasonably accurate idea of its performance in practice
- I.e., we want to estimate the model's **generalization performance**
- Estimating the generalization performance **only over the sample S used for training results in misleading error values**
- The preceding suggests to have M independent subsamples S_m and



Taken from *Hastie et al., p. 38*

  - Compute $\widehat{f}_M(x) = \frac{1}{M}\sum_m \widehat{f}_{S_m}(x) \simeq \widehat{f}_N(x)$
  - Get the error estimate $\widehat{e} = \frac{1}{N}\sum_p (y^p - \widehat{f}_M(x^p))^2$ over a new, **unseen** sample $S' = \{(x^p, y^p)\}$

- But since usually we only have a single S, we apply **Cross Validation** (CV) to get our first realistic generalization error estimates

Cross Validation

- In Cross Validation (CV) we
  - Randomly split the sample S in M subsets $S_1, \ldots, S_M$
  - Work with M **folds**: pairs (S_m, S_m^c), with

$$S_m^c = S - S_m = \cup_{i \neq m} S_i$$

  - Build M different models **using the S_m^c as training subsets**
  - Compute their errors e_m on the folds' **validation subsets** S_m
  - Use these errors' average as a first estimate of the true model performance
- CV can and **must be used** in any model building procedure
- Most data science packages have tools to simplify this
- We will also use CV to find an **optimal model hyper–parameter** α in Ridge Regression

Grid Hyper–parameter Selection

- Build M **folds**: pairs (S_m, S_m^c) and use S_m^c as training and S_m as the validation subsets

- Fix a hyper–parameter range $[0, A]$
  - $\alpha = 0$: no penalty and, thus, small bias and high variance
  - $\alpha = A$: large penalty and, thus, small variance but high bias
- Select an $L + 1$ point **grid**

$$G = \left\{0, \frac{A}{L}, \frac{2A}{L}, \ldots, \frac{\ell A}{L}, \ldots, \frac{LA}{L} = A\right\}$$

- At each $\alpha_\ell = \frac{\ell}{L}A$, $0 \leq \ell \leq L$
  - Train M models on the S_m^c using the hyper–parameter α_ℓ
  - Average their M validation errors e_m on the S_m to get the error $e(\alpha_\ell)$ at α_ℓ
- Finally choose the (hopefully) optimal hyper–parameter α^* as

$$\alpha^* = \arg\min_{0 \leq \ell \leq L} \; e(\alpha_\ell)$$

Takeaways on Bias, Variance and CV

1. We have stressed that **any model estimation is sample–dependent** and that this has to be controlled
2. We have introduced the **bias** and **variance** as the two key components of any model error
3. We have discussed **bias–variance trade–off**
4. We have introduced **Cross Validation** here as a tool to estimate a **model's generalization performance**
5. We have also introduced **Cross Validation** as a tool to estimate a **model's hyper–parameters**

4 Data and Model Analysis

And So What?

- Key question: what are models for?
  - First answer: to be used to derive new predictions
  - Better answer: to extract knowledge and to make inference on the underlying problem
- In this light, LR models are simple, perhaps not too powerful, but certainly useful
  - They are the first tool to apply in (almost) any problem analysis
- Some questions are easier to answer for them:
  - Which variables do influence the target and which do not?
  - What are the strongest predictive variables?
  - Are there related/redundant variables?

  - Is the relationship actually linear?

Issues with LR

- Before building any model we must perform a prior data analysis to keep under control important issues:
  - **Collinearity**: predictor variables that are redundant
  - **Outliers**: points (x^p, y^p) with a "normal" pattern x but an unlikely target value y^p, or vicev-ersa
  - **High-leverage points**: points (x^p, y^p) with an unlikely pattern x^p and a reasonable target value y^p
- And after a model is built we must check if its results agree with its assumptions
  - **Linearity** of the response–predictor relationships: if not, the LR will be poor
  - **No correlation of error terms**, i.e. our basic model assumption does hold
  - **No heteroscedasticity**, i.e., no non-constant variance of error terms, that varies on several x regions

Detecting and Handling Data Issues

- Before **any** model is built we **must** try detect possible data inconsistencies and/or redundancies
- Feature collinearity: look at least at the correlation matrix
- Analyze feature–target scatterplots; if possible, look also at the two–predictor scatterplots (though there are $d(d-1)/2$ of them)
- Outliers: will cause (x^p, y^p) to be far from the line fit or the residual to be out of range
  - Can detect them with box plots
- High-leverage points: x^p outside the main x range; harder to spot in multidimensional models
- We consider all this over the Boston Housing dataset

Housing: First Conclusions on the Data

- Collinearity: some predictor variables may be redundant
  - AGE–DIS: proportion of units built prior to 1940 and weighted distances to five employment centres
  - RAD–TAX: accessibility to radial highways and full-value property-tax rate
  - NOX–INDUS
- Outliers: points (x^p, y^p) with a normal pattern x but an unlikely target value y^p
  - ???
- High-leverage points (HLPs): perhaps at variables

  - ZN: proportion of residential land zoned for lots over 25,000 sq.ft.
  - CHAS: 1 if tract bounds Charles river; 0 otherwise
  - B: $1000(Bk - 0.63)^2$, with Bk the proportion of blacks by town
  - But have to look at HLPs as D-dimensional points and not features

Detecting and Handling Model Issues

- After the model is built we check whether it supports the basic LR assumptions
- Linearity: a residual plot should not have any structure
- Uncorrelated error terms: residuals do not change rather smoothly
- Error histograms should be symmetric and sharp at 0
- Heteroscedasticity: residual plots do not show a "funnel" like structure
- **Always address these possible problems**: if not, we may be fooling ourselves with an untenable model
- Let's build LR models over the Boston Housing data

Housing: First Conclusions on the Linear Model

- Recall the first things to look at after LR model building:
  - Linearity of the response-predictor relationships?
  - No correlation of residuals?
  - No heteroscedasticity?
- Linearity of the response-predictor relationships: not bad
  - If perfect fit, y and $\widehat{y}$ in diagonal; here in near diagonal
- Correlation of residuals only for large targets
  - Perhaps we should think about two separate models
- No heteroscedasticity, i.e., constant variance of residuals
  - No funnel appears in target-residual representation but there is still a bias
- Build a second model?

Takeaways on Data and Model Analysis

1. Before any model building we must analyze and understand our data
2. We must understand the assumptions our model implies on the data
   - If they aren't true the model won't be very good
3. This must be checked after the model is built

4. LR models are simple but their assumptions are of interest to any other model
5. LR are the first models to build, to have a benchmark and to better understand the problem and its data
6. And
    - Always tune the hyperparameters for our models
    - Always try out many different models
    - Always explore several feature representations for our data

5 Basic Classification

5.1 The Classification Model

Regression vs Classification

- Recall that in regression we have numerical continuous targets y and want our predictions $\hat{y}$ to be as close to y as possible
    - Given that there are infinitely many such approximations, closeness is a natural quality criterion
- But in classification we have a finite number of labelled targets for which "selection by closeness" doesn't make sense
- Natural alternative: select the **most probable** label given the pattern x we have just received
    - The concrete labels used for targets do not matter anymore
    - Model learning should thus be "target" agnostic
    - And good probability estimates should be quite useful
- Let's analyze this in an example

A First Problem: Pima Indian Diabetes

- We want to diagnose whether a person may have diabetes from some clinical measures
- Features x: clinical measures
    - `'numPregnant'`
    - `'bloodPress'`
    - `'massIndex'`
    - `'age' ...`
- Target y: 0 (no diabetes), 1 (diabetes)
- Clear goal but perhaps too radical
- Better: try to estimate the probability $P(1|x)$ of having diabetes depending on the features x we measure

Classification Setup

- We have random patterns ω from M classes, $C_1, \dots C_M$
- Over each pattern we "measure" d features $x = x(\omega) \in \mathbb{R}^d$
  - x inherits the randomness in ω and becomes a random variable
- A ω has a **prior probability** π_m of belonging to C_m
- Inside each class C_m there is a **conditional class density** $f(x|m)$ that "controls" the appearance of a given x
- The π_m and $f(x|m)$ determine the **posterior probability** $P(m|x)$ that x comes from class C_m
- **Intuition:** we should assign x to the class with the largest $P(m|x)$, that is, work with the classifier

$$\delta(x) = \text{arg max}_m P(m|x)$$

Computing Posterior Probabilities I

- **Bayes rule**: $P(B|A) = \frac{P(A \cap B)}{P(A)}$
- This requires to work with probabilities, not densities: $P(\{x\}) = P(m \cap \{x\}) = 0$ and

$$P(m|x) = \pi_m \frac{P(m \cap \{x\})}{P(\{x\})} = \pi_m \frac{0}{0} = ...???$$

- But we can use the approximation

$$\begin{aligned} P(m|x) &\simeq P(m|B_r(x)) = \frac{P(C_m \cap B_r(x))}{P(B_r(x))} = \frac{P(B_r(x)|m)P(C_m)}{P(B_r(x))} \\ &= \frac{\pi_m P(B_r(x)|m)}{P(B_r(x))} = \pi_m \frac{\int_{B_r(x)} f(y|m)dy}{\int_{B_r(x)} f(z)dz} \end{aligned}$$

  where we assume that features x are measured independently from classes m

Computing Posterior Probabilities II

- Remember the Fundamental Theorem of Calculus:
  if $F(x) = \int_a^x f(y)dy$,

$$\lim_{\epsilon \to 0} \frac{1}{2\epsilon} \int_{x_0-\epsilon}^{x_0+\epsilon} f(y)dy = \frac{dF}{dx}(x_0) = f(x_0)$$

- In d dimensions it becomes

$$g(w) = \lim_{r \to 0} \frac{1}{|B_r(w)|} \int_{B_r(w)} g(z)dz$$

- Putting everything toghether, we arrive

$$\begin{aligned} P(m|x) &= \lim_{r\to 0} P(m|B_r(x)) = \pi_m \lim_{r\to 0} \frac{\int_{B_r(x)} f(y|m)dy}{\int_{B_r(x)} f(z)dz} \\ &= \pi_m \lim_{r\to 0} \frac{\frac{1}{|B_r(x)|}\int_{B_r(x)} f(y|m)dy}{\frac{1}{|B_r(x)|}\int_{B_r(x)} f(z)dz} = \frac{\pi_m\ f(x|m)}{f(x)} \end{aligned}$$

The Obviously Optimal Classifier

- Thus, we should decide according to a **classifier** function δ_B

$$\begin{aligned} \delta_B(x) &= \arg\max_m P(m|x) = \arg\max_m \frac{\pi_m\ f(x|m)}{f(x)} \\ &= \arg\max_m \pi_m\ f(x|m) \end{aligned}$$

- With some extra work we can show that this **Bayes Classifier** δ_B defines an optimal solution (in some precise sense) of the classification problem
- But ... This doesn't look too practical for we do not know either π_m or (much harder) $f(x|m)$

Approximating the Bayes Classifier

- To define δ_B we need to know the prior probabilities π_m and the prior densities $f(x|m)$
- A reasonable choice for π_m is $\widehat{\pi}_m = \frac{N_m}{N}$, where N_m is the number of patterns of C_m in the sample
- But effective multidimensional density estimates are rather difficult, because of the **curse of dimensionality**
  - Densities generalize histograms
  - Good histograms need accurate counts of elements nearby
  - But in high dimensions there won't be nearby elements!!
- Options:
  - Restrict possible density models: logistic regression
  - Assume no model and apply a Nearest Neighbor (NN) strategy

5.2 Nearest Neighbor Classification

The k–NN Classifier

- Very simple: at any x consider the subset $N_k(x)$ of its k closest sample points and
  - Let $n_m(x)$ the number of elements of class m in $N_k(x)$
  - Notice that $0 \leq n_m(x) \leq k$
  - Define $\delta_{kNN}(x) = \arg\max_m n_m(x)$

- That is, $\delta_{kNN}(x)$ assigns x to the class that has more patterns in $N_k(x)$
- We can partially justify this definition from a Bayesian point of view
- Assume that $B_r(x)$ is the smallest ball that contains $N_k(x)$ and consider the approximations
  - $|B_r(x)|\ f(x|m) \simeq \int_{B_r(x)} f(z|m)dz = P(C_m \cap B_r(x)) \simeq \frac{n_m(x)}{N_m}$
  - Similarly, $|B_r(x)|\ f(x) \simeq \int_{B_r(x)} f(z)dz = P(B_r(x)) \simeq \frac{k}{N}$
  - And $\pi_m \simeq \frac{N_m}{N}$

k–NN and the Bayes Classifier

- We then have

$$\begin{aligned} P(m|x) &= \pi_m \frac{f(x|m)}{f(x)} = \pi_m \frac{|B_r(x)|\ f(x|m)}{|B_r(x)|\ f(x)} \\ &\simeq \frac{N_m}{N} \frac{n_m(x)}{N_m} \frac{1}{\frac{k}{N}} = \frac{n_m(x)}{k} \end{aligned}$$

- Therefore δ_{kNN} should be close to δ_B, for

$$\begin{aligned} \delta_{kNN}(x) &= \text{arg max}_m\ n_m(x) = \text{arg max}_m \frac{n_m(x)}{k} \\ &\simeq \text{arg max}_m\ P(m|x) \end{aligned}$$

By the Way: k–NN Regression

- Sometimes the relation between features x and targets y doesn't justify a strong model $y = \phi(x) + n$
- k–NN Regression relies on a reasonable assumption: **Predictors that are close should give predictions that are also close**
- In k–NN Regression we fix a number k of neighbors to be considered and for an input x set

$$\hat{y} = Y_{kNN}(x) = \frac{1}{k} \sum_{x^p \in N_k(x)} y^p$$

  where $N_k(x)$ denotes again the k sample points closest to x
- **Weighted variants**: for instance, $Y_k^w(x) = \frac{1}{C_k(x)} \sum_{x^p \in N_k(x)} \frac{1}{\|x^p - x\|} y^p$
  - $C_k(x) = \sum_{x^p \in N_k(x)} \frac{1}{\|x^p - x\|}$ is a normalizing constant

Some k–NN Issues

- **Q1: How do we choose k?** Using CV, of course

- There are no closed form solution and we have to balance again the bias–variance tradeoff
  - Small variance with large k: if $k = N$, k–NN regression returns the mean
  - Small bias with small k: if $k = 1$ a very close point should give a very close prediction
  - But also large variance: the nearest point to x in another sample may have a quite different target (or belong to another class)
- **Q2: Is k–NN always meaningful?**
- We have to modify our first assumption: Predictors that are close should give predictions that are also close, **provided that there are enough of them close by**
  - In fact, if x is away from the sample, the average over $N_k(x)$ may be meaningless

The Curse of Dimensionality

- This consideration reflects the **curse of dimensionality**:

  Even for low dimensions and large samples, **the sample space is essentially empty**
- Thus, for most problems, **there never will be enough close points**
- As a consequence, to get k observations we may go too far away from x and the average will not be meaningful
- Therefore, unless we deal with violently non–linear problems, a simple model such as linear or logistic regression (later) may be better than k–NN for moderate dimensions

6 Logistic Regression

Linear Regression for Classification?

- k–NN Classifier is simple but also crude; have to look elsewhere
- Building a regression model with targets some coding of class labels usually doesn't make sense
- But for a binary 0–1 response, it can be shown that the $w_0 + w \cdot x$ obtained using linear regression is in fact an estimate of $P(1|x)$
  - We may thus fix a threshold δ_0 and decide 0 if $w_0 + w\dot{x} < \delta_0$ and 1 otherwise
  - However, we may end up with probability estimates less than 0 o bigger than 1!!!
- We know that our goal should be to estimate $P(j|m)$; let's try to attain it!

Logistic Regression (LR)

- We assume
$$P(1|x) = \frac{1}{1 + e^{-(w_0 + w \cdot x)}}$$
  - Then $0 \leq P(1|x) \leq 1$ for any x

- We then have
$$P(0|x) = 1 - P(1|x) = \frac{e^{-(w_0+w\cdot x)}}{1+e^{-(w_0+w\cdot x)}} = \frac{1}{1+e^{w_0+w\cdot x}}$$
  - Notice that if $w_0 + w \cdot x = 0$, $P(1|x) = P(0|x) = 0.5$
- The ratio $\frac{P(1|x)}{P(0|x)} = e^{w_0+w\cdot x}$ is called the **odds** of x and its log the **log odds** or **logit**
- Thus, the basic assumption in LR is that the **logit is a linear function** $w_0 + w \cdot x$ of x
- We have the model $f(x; w)$; we need a loss function $L(w)$ to minimize for which we use the sample's **likelihood**

Sample's Likelihood

- Assume a sample $S = \{(x^p, y^p)\}$, with y^p either 1 or 0 and the (x^p, y^p) independent
- If the y^p labels are derived from a LR model with weights w_0, w, the probability of obtaining them S is

$$\begin{aligned} P(S|w_0, w) = P(\{(x^p, y^p)\}) &= \left\{\prod_{y^p=1} P(1|x^p)\right\}\left\{\prod_{y^p=0} P(0|x^p)\right\} \\ &= \prod_{p=1}^{N} P(1|x^p)^{y^p}\ P(0|x^p)^{1-y^p} \end{aligned}$$

because

  - If $y^p = 1$, $P(1|x) = P(1|x^p)^{y^p}\ P(0|x^p)^{1-y^p}$ and
  - If $y^p = 0$, $P(0|x) = P(1|x^p)^{y^p}\ P(0|x^p)^{1-y^p}$

Max Log–Likelihood Estimation

- The log–likelihood of w_0, w given S is then

$$\begin{aligned} \ell(w_0, w; S) &= \log P(S|w_0, w) \\ &= \sum_p \{y^p\ \log p(1|x^p) + (1-y^p)\ \log p(0|x^p)\} \\ &= \sum_p y^p\ \log \frac{p(1|x^p)}{p(0|x^p)} + \sum_p \log p(0|x^p) \\ &= \sum_p y^p\ (w_0 + w\cdot x^p) - \sum_p \log(1+e^{w_0+w\cdot x^p}) \end{aligned}$$

- We can thus estimate the optimal $\widehat{w}_0^*, \widehat{w}^*$ as
$$\widehat{w}_0^*, \widehat{w}^* = \arg\min_{w_0,w}\ -\ell(w_0, w; S)$$
- Extra bonus: ℓ is a convex differentiable function of (w_0, w) and, thus, it is enough to solve $\nabla\ell(w_0, w) = 0$

Newton–Raphson Solution

- However, $\nabla\ell(W) = \nabla\ell(w_0, w) = 0$ doesn't admit a closed form solution but only an iterative, numerical one
- We apply the **Newton–Raphson** iterative method, here equivalent to the general Newton method for function minimization
- Starting with an initial random W^0, Newton's iterations are

$$W^{k+1} = W^k - (\mathcal{H}_\ell(W^k))^{-1}\nabla\ell(W^k)$$

- $\mathcal{H}_\ell(W^k)$ denotes the Hessian of ℓ at W^k, which may or may not be invertible
  - Just as before, we can add a regularization term $\frac{\alpha}{2}\|W\|^2$ to avoid invertibility problems
  - Everything is fine if the W^k are close enough to the optimum W^* but far away things may get tricky
- The iterations in Logistic Regression are again typical of many of the model building methods used in Machine Learning

Learning in ML

- The general approach to **learning** is the following:
  - A **model** $f(x; W)$ is chosen
  - Given a sample $S = \{(x^1, y^1), \ldots, (x^N, y^N)\}$, we define a **sample dependent loss function**

$$L(W) = L(W|S) = L\left(y^1, \ldots, y^N, f(x^1; W), \ldots, f(x^N; W)\right)$$

- $L(W)$ is often minimized from some W^0 by **iterations**

$$W^{k+1} = W^k - \rho_k G(W^k, S)$$

  with ρ_k a **learning rate** and G some vectorial function
  - When $G(W) = \nabla L(W)$ we have **gradient descent**
  - When $G(W) = \mathcal{H}(W)^{-1}\nabla L(W)$ we obtain **Newton's method**
- When the entire sample S is used at each iteration, we speak of **batch learning**
- When only single patterns (x^p, y^p) or small subsamples are used, we speak of **on–line** or **mini-batch learning**
- Several such procedures will appear here in the coming weeks

7 Practical Classification

7.1 Measuring Classifier Accuracy

True/False Positives/Negatives

- Consider a two class problem with labels $y = 0, 1$
- We will call patterns with label 1 **positive** and those with label 0 **negative**
  - Usually the positive patterns are the interesting ones: sick people, defaulted loans, . . .
- Let $\widehat{y} = \widehat{y}(x)$ the label predicted at x; we say that x is a
  - **True Positive** (TP) if $y = \widehat{y} = 1$
  - **True Negative** (TN) if $y = \widehat{y} = 0$
  - **False Positive** (FP) if $y = 0$ but $\widehat{y} = 1$
  - **False Negative** (FN) if $y = 1$ but $\widehat{y} = 0$
- The standard way of presenting these data is through the **confusion matrix**

The Confusion Matrix

- Standard layout

	P' (Predicted)	N' (Predicted)
P (Actual)	True Positive	False Negative
N (Actual)	False Positive	True Negative

- Other layouts:
  - Positives (with label 1) at bottom (as done in `confusion_matrix` of `sklearn`)
  - Predicted values in rows, real values in columns

Classifier Metrics

- The classifier **accuracy** is $acc = \frac{TP+TN}{N}$
- acc is the first thing to measure but it may not be too significant: if the number N_0 of negatives is $\gg N_1$, the number of positives
  - The classifier $\delta(x) = 0$ will have a high accuracy $N_0/N \simeq 1$

  - But it will also be useless!!

- First variant: Precision, Recall
  - **Recall**: $TP/(TP+FN)$, i.e., the fraction of positives detected
  - **Precision**: $TP/(TP+FP)$, i.e., the fraction of true alarms issued
- Recall measures how many positive cases we recover, i.e., how effective is our method
- Precision measures the effort we need for that, i.e., its efficiency
- Ideal classifier: high recall, high precision (i.e., effective and efficient!!)

7.2 Practical Issues

What's New from Regression?

- Some things change from regression, some don't
- We should check feature correlations: they will affect most models
- Important: **positive and negative–class feature histograms**
  - Scatter plots (x_i, y) are usually less informative
- The **bias–variance trade–off** is subtler in classification
- Accuracy, recall, precision are the usual model quality measures
- We use CV with **stratified folds** to estimate generalization performance
- We also use CV for hyperparameter estimation, for regularization will also be needed
  - In LR we should minimize $-\ell(w_0, w; S) + \frac{\alpha}{2}\|w\|^2$

How to Handle Posterior Probabilities

- If possible, we don't want labels as model outputs but **posterior probabilities**
- Most models give them as pairs

$$(\widehat{P}(0|x), \widehat{P}(1|x)) = (\widehat{P}(0|x), 1 - \widehat{P}(0|x))$$

- In principle we would decide 1 if $\widehat{P}(1|x) > 0.5$ and viceversa, but this may be too crude
- It may be advisable to set a threshold θ and decide 1 if $\widehat{P}(1|x) > 1 - \theta$ and 0 if $\widehat{P}(1|x) < \theta$
- For **imbalanced** problems where $\pi_0 \gg \pi_1$ (usually the interesting ones) we would have $\widehat{P}(0|x) \simeq 1$ for most x
  - In this case we may choose another $\theta > 0.5$ and **suggest** 1 if $\widehat{P}(0|x) < \theta$

Takeaways on Basic Classification

1. We have introduced the classification problem as one of computing posterior probabilities
2. We have found the optimal Bayes classifier and approximated it by k–NN
3. We have introduced several measures of classifier performance
4. We have introduced Logistic Regression and the numerical minimization of its (minus) log–likelihood
5. We have introduced and analyzed some classification metrics
6. We have reviewed some practical issues of classification