

Regression and Classification Basics

Análisis de datos y su interpretación

Master en Big Data y Data Science

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Antes de empezar ...

- Contenido
 - ① Introducción al aprendizaje automático
 - ② Preprocesado de datos
 - ③ Clustering
 - ④ Redes Neuronales
 - ⑤ Máquinas de vectores soporte
 - ⑥ Conjuntos de clasificadores y árboles de decisión
 - ⑦ Deep Learning
- Evaluación:
 - Asistencia a clase: 10%
 - Evaluación continua: 50%
 - Examen final: 40%

Outline

- 1 Machine Learning Modeling Basics
- 2 Basic Regression
- 3 Bias, Variance and Cross Validation
- 4 Data and Model Analysis
- 5 Basic Classification
 - The Classification Model
 - Nearest Neighbor Classification
- 6 Logistic Regression
- 7 Practical Classification
 - Measuring Classifier Accuracy
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Modeling Basics

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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 $\hat{y} = f(x)$
 - We want $y \simeq \hat{y}$ so having $y - \hat{y}$ "small" is the natural goal
- **Classification:** inputs are derived from several classes C_1, \dots, 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 $\hat{y} = f(x)$ so that $\hat{y}^p = f(x^p) \simeq y^p$; 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)

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

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

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 $\hat{e}_S(f) = \hat{e}_S(W)$
- The problem to solve becomes

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

- In linear regression

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

which ends up in a simple quadratic form

- The regression problem reduces to **minimize** $\hat{e}_S(W)$
 - Something in principle well understood in mathematical optimization

Regression Basics

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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
$$\hat{\phi}(x) = \frac{1}{M} \sum_1^M y^j$$
 - 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 $e(w)$

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

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

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

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

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

- The optimal w^* solves $\hat{e}'(w) = 0$ 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 $(x^1, \dots, x^N)^t$, $(y^1, \dots, y^N)^t$

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

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

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

$$\nabla \hat{e}(w) = \frac{1}{N} X^t X w - \frac{1}{N} X^t Y = \hat{R} w - \hat{b}$$

Solving the Linear Equations

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

$$\hat{R} = \frac{1}{N} X^t X, \quad \hat{b} = \frac{1}{N} X^t Y$$

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

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

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

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

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

Finding Optimal Models

- For general regression models it may not be possible to solve analytically the equation $\nabla \hat{e}(W) = 0$
 - 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

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

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

Measuring Model Fit

- First option: **Root Square Error**

$$RSE = \sqrt{\frac{1}{N} \sum (y^p - \hat{y}^p)^2} = \sqrt{\frac{1}{N} RSS}$$

- OK, but how good is this? We must always have a **base model** to benchmark our results
- Simplest “model”: the mean $\bar{y} = \frac{1}{N} \sum_1^N y^p$, with square error

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

- We can compare our model against our base computing

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

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

Regularization

- Our regression solution $\hat{w}^* = (X^t X)^{-1} X^t Y$ won't work if $X^t X$ is not invertible
 - For instance, when some features are correlated
- We could fix this working instead with $X^t X + \alpha I$ for some $\alpha > 0$
- To make this practical, note that $\hat{w}^* = (X^t X + \alpha I)^{-1} X^t Y$ 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

Bias, Variance and Cross Validation

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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, \dots, S_M , it is natural to use as our best final model the averages of the $\hat{f}_{S_m}(x)$ models, i.e.,

$$\frac{1}{M} \sum_1^M \hat{f}_{S_m}(x) \simeq E_S[\hat{f}_S(x)] = \hat{f}_N(x)$$

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

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

Bias Versus Variance

- Ideally we would like to have a model such that

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

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

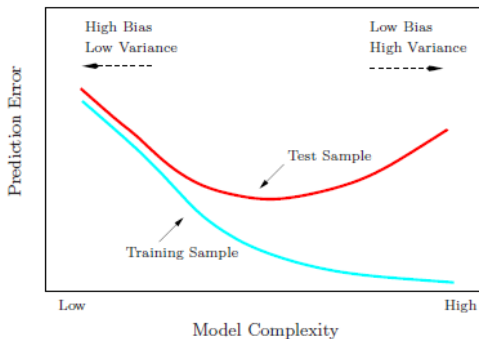
$$V_N(x) \simeq 0,$$

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)



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

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
 - Compute $\hat{f}_M(x) = \frac{1}{M} \sum_m \hat{f}_{S_m}(x) \simeq \hat{f}_N(x)$
 - Get the error estimate $\hat{e} = \frac{1}{N} \sum_p (y^p - \hat{f}_M(x^p))^2$ 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, \dots, 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**

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

- 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**

Data and Model Analysis

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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 viceversa
 - **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 \hat{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

Basic Classification

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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

$$\delta(x) = \arg \max_m P(m|x)$$

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

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

- 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 $F(x) = \int_a^x f(y)dy$,

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

- In d dimensions it becomes

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

- Putting everything together, we arrive

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

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 $\hat{\pi}_m = \frac{N_m}{N}$, 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

Nearest Neighbor Classification

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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

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

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

Logistic Regression (LR)

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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 $w_0 + w \cdot x < \delta_0$ and 1 otherwise
 - However, we may end up with probability estimates less than 0 or 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 \hat{w}_0^*, \hat{w}^* as

$$\hat{w}_0^*, \hat{w}^* = \arg \min_{w_0, w} -\ell(w_0, w; S)$$

- 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 $S = \{(x^1, y^1), \dots, (x^N, y^N)\}$, we define a **sample dependent loss function**

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

- $L(W)$ 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 **minibatch learning**
- Several such procedures will appear here in the coming weeks

Measuring Classifier Accuracy

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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 $\hat{y} = \hat{y}(x)$ the label predicted at x ; we say that x is a
 - **True Positive (TP)** if $y = \hat{y} = 1$
 - **True Negative (TN)** if $y = \hat{y} = 0$
 - **False Positive (FP)** if $y = 0$ but $\hat{y} = 1$
 - **False Negative (FN)** if $y = 1$ but $\hat{y} = 0$
- 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!!)

Practical Issues

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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

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

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

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