Machine Learning for Natural and Life Sciences

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Contents

Machine Learning for Natural- and Life-Science

- Goal: Teach the background of ML, not just recipes.
  ⇒ help you understand ML literature
- Setting: – we are interested in properties or quantities Y, but these are ~~hard to~~ impossible or impractical to measure directly ≙ "response"
  – properties / quantities X are related to Y and are easier to measure / observe ≙ "features"

  ⇒ approximate Y^* (true values, "ground truth") by a formula $\hat{Y} = f(X) \approx Y^*$

  ↑ approximate responses of our model, "predictions"

  – problem: the formula $f(X)$ is not known

  ⇒ collect training data and fit the model to $f(X)$ reproduce the behavior of that data

  – supervised learning: we cannot measure Y under normal field conditions, but we can obtain it in an experimental setting
    - example: crash test to determine car safety

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

N training instances

i: instance index

X_i, Y_i: features and response of instance i

X ≙ feature matrix is simply a table

Instance	Instance index	Height	Weight	Gender	
Alice	$i=1$	1.60	80	f	
Bob	$i=2$	1.85	85	m	...
Carol	$i=3$	1.70	70	f	
⋮			×3,2		$\hat{=} X$
Feature index →		$j=1$	$j=2$	$j=3$	

$j \in 1, \dots, D$ D-dimensional feature space

Problem: for simplicity of the math and software, we want X to be real-valued, but many features are discrete / categorial, e.g. gender

⇒ "one-hot encoding": one flag per label

modified table/matrix

	...	gender: male	gender: female
Alice		0	1
Bob		1	0
Carol		0	1

⇒ $X \in \mathbb{R}^{N \times D}$, likewise Y

[if only two labels, we need only ~~one~~ encode one, because the other is implied, e.g. male = 1 − female]

- simple solutions to the problem

– threshold classifier:

- e.g. ~~bmi~~ $Y = \begin{cases} 0 & \text{patient is healthy} \\ 1 & \text{patient suffers from diabetes} \end{cases}$

cannot be measured directly ⇒ measure a bio-marker

~~X: sugar content in blood~~

X: blood sugar concentration

classifier: $Y = \begin{cases} 0 & \text{if } X < 100 \text{ mg/dl} \\ 1 & > \end{cases}$

(simplified for illustration purposes)

- problem: often, there is no single feature that indicates the response

⇒ combine several features in some formula referring a "score"

e.g. $Y = \begin{cases} 0 & \text{person is normal} \\ 1 & \text{person is ~~obese~~ overweight} \end{cases}$

$$\text{score} = \frac{\text{weight [kg]}}{\text{height}^2\ [\text{m}^2]} \quad \text{"body mass index"}$$

$$Y = \begin{cases} 0 & \text{if BMI} < 25 \\ 1 & \text{BMI} > 25 \end{cases}$$

- problem: hand-crafted features have disadvantages
  - hard to find, expensive (may require decades)
  - in complex situations, simplifications are necessary
    ⇒ loss of accuracy

⇒ overcome these difficulties using <u>machine learning</u>
(downside: machine learning is often less explainable than an explicit formula ⇒ explainable ML is last research area)

- nearest-neighbor classifier
  - classify a new instance x_{test} like the most similar instance in the training set
  - define similarity by a distance function of the features

$$dist(x, x') = \begin{cases} \text{small} & \text{if } x \text{ and } x' \text{ are similar} \\ \text{large} & \text{— " — different} \end{cases}$$

e.g. Euclidean distance between features

$$dist(x, x') = \sqrt{\sum_{j=1}^{D} (x_j - x'_j)^2}$$

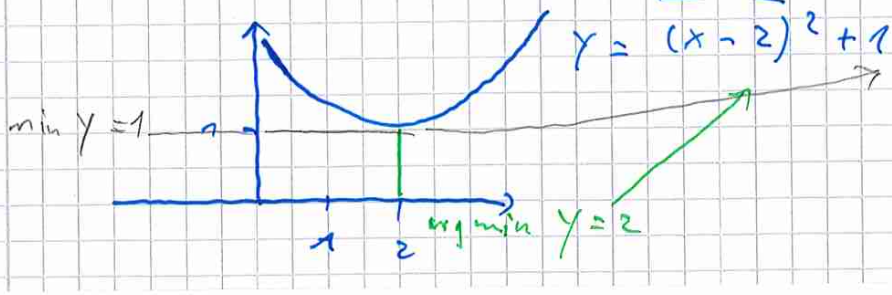
↑ sum over features = index j

- arg min - Notation:

$$i_{nearest} = \arg\min_{i=1}^{N} dist(x_{test}, x_i)$$

[$\min_{i=1}^{N} dist(x_{test}, x_i)$: - iterate over all training inst.
- compute distance
- return the minimal distance]

$\arg\min_{i=1}^{N}$ - iterate over all training instances
- compute distance
- return <u>index</u> of instance with minimal distance



$\Rightarrow \hat{y}_{test} = y^*_{nearest} = y_{i_{nearest}}$ classifier response

- often works pretty well, but has a number of shortcomings
  - need to memorize TS and search with $O(N)$ in each query $\Rightarrow$ scales poorly to large TS
    - ~~steed~~ memorize only important training instances $\Rightarrow$ hard to identify
    - speed-up by approximate nearest-neighbor search
  - $\hat{y}$ is not guaranteed to converge toward y^* even if $N \to \infty$ (error may be twice as big as the best achievable)
    - k-nearest neighbor $\Rightarrow$ more expensive
  - requires hand-crafted distance function
    $\Rightarrow$ same problems as hand-crafted stores
    $\Rightarrow$ metric learning (Bjön Ommer)
    - human similarity judgements are hard to model
- show Voronoi diagram (animation)

Loss functions

classical models: – define a specific formula for every situation
(e.g. physics: Newtons laws, law of gravity, Maxwells laws, etc.)
– theoreticians hand-craft these models

machine learning – use generic model families that apply to many situations and have free parameters Θ : $Y = f_\Theta(X)$

e.g. Linear: $Y = aX + b$
$\hookrightarrow \Theta = (a, b)$

– among all possible choices for Θ, pick $\hat{\Theta}$ such that $Y_i \approx f_{\hat{\Theta}}(X_i)$ works as well as possible for the TS $\{(X_i; Y_i)\}_{i=1}^{N}$
"model fitting / training"

⇒ need a way to quantify the "goodness of fit",
i.e. to compare the performance of different choices of Θ

let $\hat{Y} = f_\Theta(X)$ the prediction for a data set X, given Θ
$Y^* = f^*(X)$ the ~~function~~ true relationship
(we know Y^*, but not f^*)

$\text{loss}(Y^*, \hat{Y}) \longrightarrow \mathbb{R}^+$ measures the difference between truth and predictions

$$\begin{cases} \approx 0 & \text{if } Y^* \approx \hat{Y} \\ \text{big} & \text{otherwise ("loss")} \end{cases}$$

if the data instances are iid (independent of each other, but generated from the same true model f^*)
this simplifies to ~~a~~ additive loss over all instances

$$\text{loss}(Y^*, \hat{Y}) = \frac{1}{N} \sum_{i=1}^{N} \text{loss}(Y_i^*, \hat{Y}_i)$$

The particular formula for the $Loss(..)$ determines what is considered a good fit and must be selected by the model designer / data scientist according to the application.

- most common choice: squared loss

$$Loss(Y^*, \hat{Y}) = \frac{1}{N} \sum_{i=1}^{N} (Y_i^* - \hat{Y}_i)^2$$

$$= 0 \iff Y_i^* = \hat{Y}_i \text{ for all } i$$

e.g. for 2-class classification

$$Y = \begin{cases} 0 & \text{if healthy} \\ 1 & \text{if diabetes} \end{cases}$$

$$(Y_i^* - \hat{Y}_i)^2 = \begin{cases} 0 & \iff Y_i^* = \hat{Y}_i \quad \text{correct prediction} \\ 1 & \iff Y_i^* \neq \hat{Y}_i \quad \text{wrong prediction} \end{cases}$$

$\hat{=}$ count the wrongly predicted instances $\hat{=}$ 0/1 error

- $\hat{Y}_i = f_\Theta(X_i)$ depends on the choice of Θ, and so will the loss $\Rightarrow$ choose Θ to minimize the loss ~~of~~ on the TS

$$\hat{\Theta} = \arg\min_{\Theta} \frac{1}{N} \sum_{i=1}^{N} Loss(Y_i^*, \hat{Y}_i = f_\Theta(x_i))$$

Finding the optimal $\hat{\Theta}$ is in general a complicated optimization problem $\Rightarrow$ later.

The loss after optimizing $\hat{\Theta}$ is the "training error"

$$\hat{err} = \frac{1}{N} \sum_i Loss(Y_i^*, \hat{Y}_i = f_{\hat{\Theta}}(x_i))$$

$$= \min_{\Theta} \frac{1}{N} \sum_i Loss(Y_i^*, Y_i = f_\Theta(x_i)) \Big] =$$

Because we chose $\hat{\Theta}$ such that it achieves the minimum

- what we are actually interested in is the performance of our model in the field, i.e. on arbitrary data beyond the TS

$$Err = \mathbb{E}_{X,Y^* \sim p^*(X,Y)} \left[Loss(Y^*, \hat{Y} = f_{\hat{\Theta}}(X)) \right]$$

"generalization ~~error~~ error"

- fundamental insight of ML and statistics:

$$Err > \hat{Err}$$

generalization error is usually bigger than training error, sometimes much bigger $\hat{=}$ "overfitting"

$\Rightarrow$ take home message: fundamental insight 1

> IT MAKES NO SENSE TO REPORT MODEL PERFORMANCE IN TERMS OF THE TRAINING ERROR $\hat{Err}$

- Instead we must estimate and report the generalization error. In practice, empirical estimation works best. 2 possibilities:
  - independent test set $Test = \{(x_i^{test}, y_i^{test})\}_{i=1}^{N'}$

    Compute the average loss of the test set

$$\hat{Err} = \frac{1}{N'} \sum_{i=1}^{N'} Loss\left(y_i^{test}, \hat{f}(x_i^{test})\right)$$

    Note: - Never use the test data for training.
    - $\hat{\vartheta}$ remains fixed now.
  - cross-validation: if no independent test set is available, create it from the training set:

    Create k ~~set~~ random subsets ("folds"), here $k = 5$
    $\Rightarrow$ "k-fold cross-validation"
    Let TS_ℓ denote fold ℓ, $TS_{\setminus\ell}$ the remaining data for $\ell = 1 \dots k$
    - train on $TS_{\setminus\ell}$ to get $\hat{\vartheta}_\ell$
    - estimate $\hat{Err}_\ell$ on TS_ℓ, using $\hat{\vartheta}_\ell$ fixed

    estimate $\hat{Err} = \frac{1}{k} \sum_\ell \hat{Err}_\ell$

    typical values for k: 10, 5 (2 if training is very expensive); $K = N$ LOO-CV for theory

- Infrastructure for CV is available in all credible ML libraries (sk-learn, pytorch, ...)

⇒ don't implement it yourself (except as an exercise)

Bayes decision rule

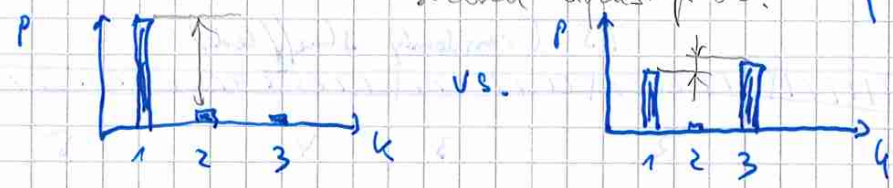
- instead of a hard class decision, we can return a soft response: the probability of each label, given the features

$$\forall k: \quad p(Y_i = k \mid X_i) \qquad \text{with} \sum_{k=1}^{C} p(Y_i = k \mid X_i) = 1$$

- a hard decision is easily obtained by deciding for the most probable class: $\hat{Y}_i = \arg\max_k p(Y_i = k \mid X_i)$

- many methods learn to approximate $\hat{p}(Y \mid X)$ (the "posterior probability" = after measuring the features) as well as possible ⇒ more information than a hard decision rule, e.g. uncertainty estimate via margin:

$$p(\hat{Y}_i \mid X_i) - \arg\max_{k \neq \hat{Y}_i} p(Y_i = k \mid X_i) = \begin{cases} \text{large} & \text{if no doubt} \\ \approx 0 & \text{if uncertain} \end{cases}$$



- the true posterior $p^*(Y_i \mid X_i)$ is called the "Bayesian ~~decision~~ posterior". The Bayes decision rule

$$\hat{y}_i = \arg\max_k p^*(Y_i = k \mid x_i)$$

is the theoretically best possible classifier

⇒ learning attempts to ensure $\hat{p}(Y_i \mid x_i) \approx p^*(Y_i \mid x_i)$

- the ~~limit~~ Bayesian posterior and thus the limit is generally unknown in practice, but plays an important role as a ~~upper~~ lower bound for the error in theoretical analysis

Explain confusion matrix, distance between false positives and false negatives ⇒ see later

Linear Models

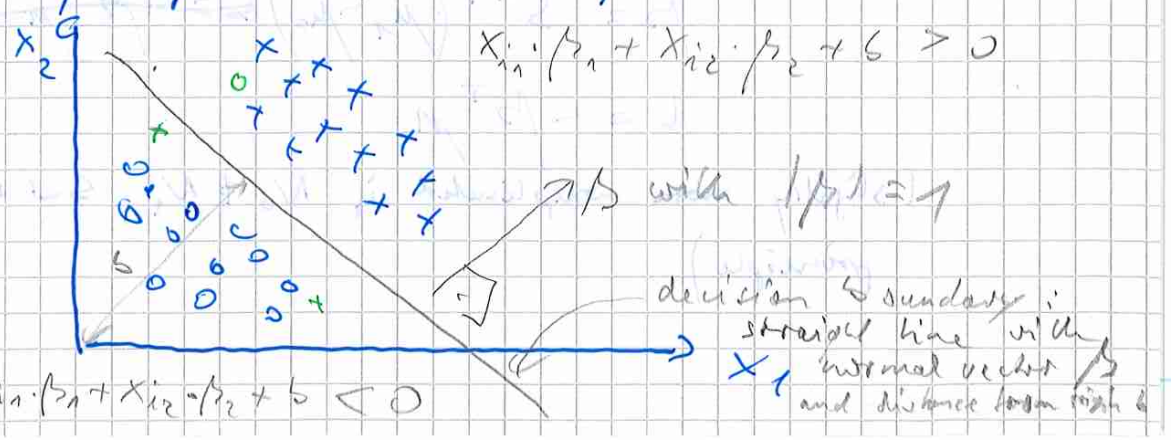
- simplest model family, applicable to
  - regression: $y_i \in \mathbb{R}$
  - classification ~~$y_i \in \{1, \dots, C\}$~~ $y_i \in \{0, 1\}$
    (extensions to more classes possible by coupling several linear models in one-against-the-rest fashion)
- computes a weighted sum of the feature values plus offset
  - matrix notation for regression $\hat{y}_i = x_i \cdot \beta + b$
    (β: column vector of D weights; b: offset)
    element notation $\hat{y}_i = \sum_{j=1}^{D} x_{ij} \cdot \beta_j + b$
    β_j: weight of feature j
    $|\beta_j| \begin{cases} \text{big}: & \text{feature } j \text{ is important} \\ \approx 0 & \text{— " — unimportant} \end{cases}$
  - matrix notation for classification $\hat{y}_i = \mathbb{1}[x_i \cdot \beta + b > 0]$

$$\mathbb{1}[\text{cond}] = \begin{cases} 1 & \text{if "cond" is true} \\ 0 & \text{if "cond" is false} \end{cases}$$

} simply converts true/false to numbers 0/1

$\Rightarrow x_i \cdot \beta + b$ should be positive if $y_i^* = 1$
negative if $y_i^* = 0$

  - the parameters are $\Theta = \{\beta, b\}$ ($D+1$ numbers)
- linear classification works well if data are linearly separable, or nearly so



- many ways to find good decision planes, e.g. optimal parameters $\hat{\beta}, \hat{b}$, controlled by the choice of loss function.
  - If the data are suitable for linear classification, all solutions will be similar.
  - squared loss: $\Rightarrow$ LDA (linear discriminant analysis)

define $\tilde{y}_i = \begin{cases} 1 & \text{if } y_i = 1 \\ -1 & \text{if } y_i = 0 \end{cases} = 2y_i - 1$

optimize $\hat{\beta}, \hat{b} = \underset{\beta, b}{\operatorname{argmin}} \frac{1}{N} \sum_{i=1}^{N} (\tilde{y}_i - x_i\beta - b)^2$

reduces learning to ordinary least squares and has a simple solution

(assuming balanced classes, i.e. $N_0 = N_1 = \frac{N}{2}$)

1) compute the class means

$$\mu_1 = \frac{1}{N_1} \sum_{i: y_i = 1} x_i \qquad \mu_0 = \frac{1}{N_0} \sum_{i: y_i = 0} x_i$$

2) and total mean

$$\mu = \frac{1}{N} \sum_i x_i = \frac{\mu_0 + \mu_1}{2} \quad (N_0 = N_1)$$

2) compute within-class covariance matrix

$$S = \frac{1}{N} \sum_i (x_i - \mu_i)(x_i - \mu_i)^T$$

↑ outer product

with $\mu_i = \begin{cases} \mu_1 & \text{if } y_i = 1 \\ \mu_0 & \text{if } y_i = 0 \end{cases}$ class-wise mean

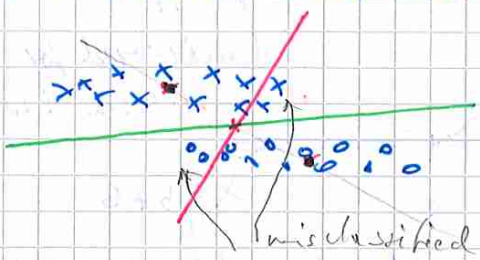
3) compute parameters

$$\beta = S^{-1}(\mu_1 - \mu_0) \qquad \cancel{b = \beta^T \mu}$$

$$b = -\beta^T \mu$$

(slightly more complicated if $N_0 \neq N_1$, but same principle)

- comparison between LDA and a naive rule: choose bisector between class means



normal vector of decision boundary

$\beta = S^{-1}(\mu_1 - \mu_0)$

↑

rotates decision boundary according to cluster shape

(no rotation if clusters are round)

- strong assumptions: – cluster shapes are close to Gaussian bell (elliptic)
  – both classes have same cluster shape
  – somewhat robust if not fulfilled exactly

Linear support vector machine (SVM)

- insight: features are not exact, but noisy ⇒ slightly perturbed TS is equally plausible

← decision boundary with maximum margin

⇒ decision should be robust against such perturbations

⇒ we should maximize the "safety margin" between data points and decision boundary

$$\hat{\beta}, \hat{b} = \underset{\beta, b}{\arg\min} \; \frac{\beta^T \beta}{2} + \frac{\lambda}{N} \sum_i \text{Hinge Loss}(y_i^*, x_i \beta + b)$$

$\frac{\beta^T\beta}{2}$: maximizes margin for possible TS perturbations; "regularization term"

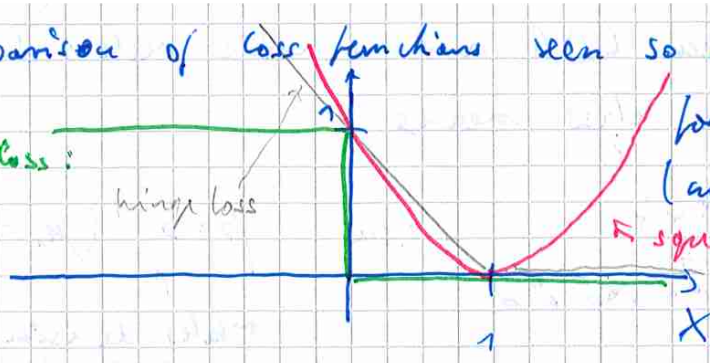
$\sum_i \text{Hinge Loss}(y_i^*, x_i\beta + b)$: measures quality of prediction on the TS; "data term"

λ: regularization parameter: adjusts trade-off between training error and robustness (hyperparameter, must be chosen by user)

$$\text{Hinge Loss}(y_i^*, x_i\beta + b) = \begin{cases} \max(0, 1 - (x_i\beta + b)) & \text{if } y_i^* = 1 \\ \max(0, 1 + (x_i\beta + b)) & \text{if } y_i^* = 0 \end{cases}$$

no analytic solution, but efficient iterative algorithms

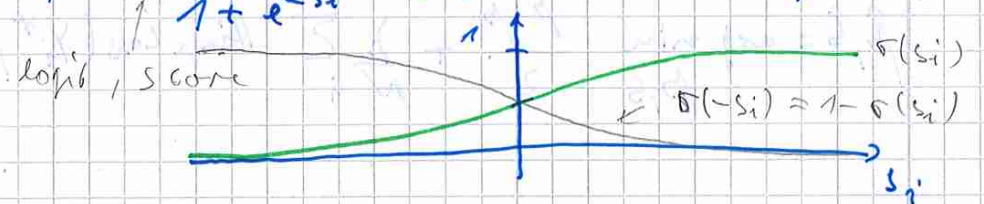
- comparison of loss functions seen so far:



- 0/1 loss: no penalty if correct sign (i.e. correct decision)
  constant penalty if wrong sign
- squared loss: quadratic penalty if $x_i\beta + \delta \neq 1$
  (i.e. over confident responses are also penalized)
- hinge loss: no penalty for sufficiently confident correct answers: $x_i\beta + \delta \geq 1$
  linearly increasing penalty for incorrect answers: $x_i\beta + \delta < 0$
  small penalty for correct answers with low confidence (i.e. small margin) $0 < x_i\beta + \delta < 1$

Logistic Regression (LR)

- learn an approximation $\hat{p}(y_i | x_i)$ of the true Bayesian posterior $p^*(y_i | x_i)$
- combine linear model $s_i = x_i\beta + \delta \in \mathbb{R}$ with subsequent non-linearity $\sigma(s_i) = \frac{1}{1 + e^{-s_i}} \in [0, 1]$ = "logistic sigmoid fct."



$$\hat{p}(y_i = 1 | x_i) = \sigma(x_i\beta + \delta)$$

$$\hat{p}(y_i = 0 | x_i) = 1 - \hat{p}(y_i = 1 | x_i) = 1 - \sigma(x_i\beta + \delta) = \sigma(-(x_i\beta + \delta))$$

- optimal decision:

$$\hat{y}_i = \begin{cases} 1 & \text{if } \hat{p}(y_i = 1 | x_i) > \hat{p}(y_i = 0 | x_i) \Leftrightarrow x_i\beta + \delta > 0 \\ 0 & < \end{cases}$$

⇒ posterior is non-linear, but decision rule is linear

- optimization problem: define $\hat{p}$, i.e. $\hat{\beta}$ and $\hat{b}$ such that the combined posterior of the training labels is maximized
  $\hat{=}$ maximum likelihood principle

$$\hat{\beta}, \hat{b} = \arg\max_{\beta, b} \underbrace{\prod_{i: y_i = 1} \hat{p}(y_i = 1 \mid x_i)}_{\text{due to i.i.d.}} \cdot \prod_{i: y_i = 0} \hat{p}(y_i = 0 \mid x_i)$$

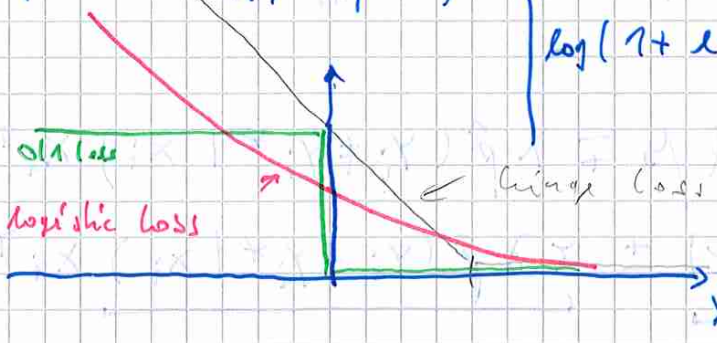
$$= \arg\max_{\beta, b} \prod_{i: y_i = 1} \sigma(x_i \beta + b) \cdot \prod_{i: y_i = 0} \sigma(-(x_i \beta + b))$$

- after some manipulations and introduction of regularization (i.e. maximization of safety margin), this results in

$$\hat{\beta}, \hat{b} = \arg\min_{\beta, b} \frac{\beta^T \beta}{2} + \frac{1}{\alpha} \sum_i \text{logistic Loss}(y_i, x_i \beta + b)$$

solve iteratively, similar to SVM

$$\text{logistic Loss}(y_i, x_i \beta + b) = \begin{cases} \log(1 + e^{-(x_i \beta + b)}) & \text{if } y_i = 1 \\ \log(1 + e^{x_i \beta + b}) & \text{if } y_i = 0 \end{cases}$$



for $y_i = 1$
(mirrored for $y_i = 0$)

⇒ logistic loss is a smooth version of the hinge loss, similar behavior

- for large dataset ($N > 10^4 \ldots 10^5$), stochastic gradient descent (SGD), or one of its improved variants, is the fastest optimization algorithm
  (for small datasets, $N \leq 10^3 \ldots 10^4$, Newton or quasi-Newton algorithms are faster)
  - SGD selects a single random instance or a mini-batch to estimate the loss in every iteration
    $i \sim \text{uniform}(1 \ldots N)$

loss in current iteration:

$$\text{loss}_i = \frac{\beta^T\beta}{2} + \lambda \log\left(1 + e^{\mp(x_i\beta + s)}\right)$$

with $-$ if $y_i = 1$ and $+$ if $y_i = 0$

$$\frac{\partial \text{loss}_i}{\partial \beta} = \frac{\beta}{\cancel{2}} + \frac{\lambda}{1 + e^{\mp(x_i\beta+s)}} \cdot e^{\mp(x_i\beta+s)} \cdot \left(\mp x_i^T\right)$$

$$= \beta \mp \lambda \cdot \underbrace{\sigma\left(\mp(x_i\beta + s)\right)}_{= 1 - \hat{p}(y_i = y_i^* \mid x_i)} x_i^T$$

$$= \hat{p}(y_i \neq y_i^* \mid x_i)$$

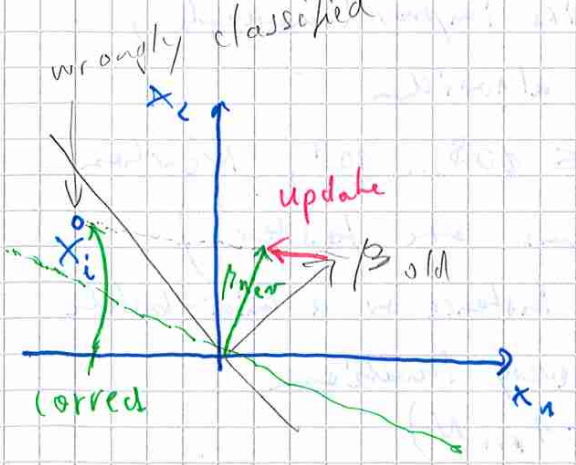
$$= \beta \mp \lambda \cdot \hat{p}(y_i \neq y_i^* \mid x_i)\, x_i^T$$

Since we want to minimize the loss, we perform gradient descent, i.e. the update goes in the opposite direction with step size τ:

$$\beta \leftarrow \beta - \tau\left(\beta \mp \lambda \hat{p}(y_i \neq y_i^* \mid x_i)\, x_i^T\right)$$

$$\beta \leftarrow \underbrace{\beta(1-\tau)}_{\text{regularization: reduce magnitude of } \beta} \pm \underbrace{\tau\lambda \hat{p}(y_i \neq y_i^* \mid x_i)\, x_i^T}_{\text{update weight}}$$

- if classification is already correct: $\hat{p}(y_i \neq y_i^* \mid x_i) \approx 0$ $\Rightarrow$ almost no update
- if classification is wrong: $\hat{p}(y_i \neq y_i^* \mid x_i) \approx 1$ $\Rightarrow$ move β towards x_i (if $y_i^* = 1$) or away from x_i (if $y_i^* = 0$)

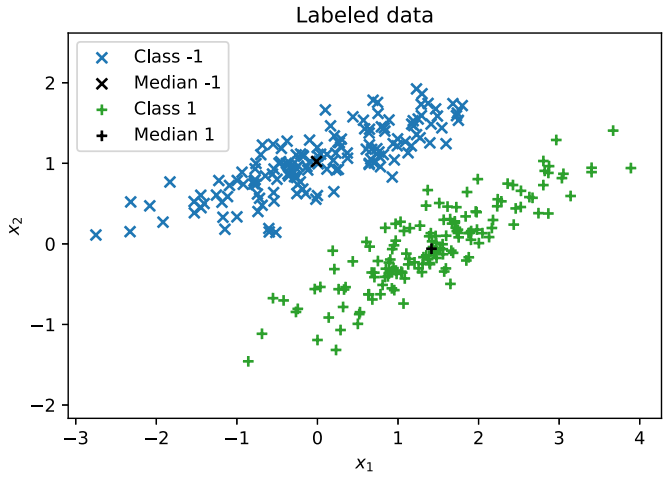


In [1]:
```
import numpy as np
import matplotlib.pyplot as plt
%config InlineBackend.figure_formats = ['svg']
from sklearn.discriminant_analysis import LinearDiscriminantAnalysis
from sklearn.linear_model import LogisticRegression
from sklearn.svm import SVC
```

Separable data

In [2]:
```
def generate_data(n_1, n_2, n_dim=2):
    # Skew the data
    mean_1 = np.array([0, 1])
    al_1 = 70 * 2 * np.pi / 360
    s_11 = 0.2
    s_12 = 1.0
    sigma_1 = np.array([[s_11 * np.cos(al_1), s_12 * np.sin(al_1)],
[-s_11 * np.sin(al_1), s_12 * np.cos(al_1)]])

    mean_2 = np.array([1.5, 0])
    al_2 = 60 * 2 * np.pi / 360
    s_21 = 0.2
    s_22 = 1.0
    sigma_2 = np.array([[s_21 * np.cos(al_2), s_22 * np.sin(al_2)],
[-s_21 * np.sin(al_2), s_22 * np.cos(al_2)]])

    # Generate uniform Gaussian distributions, then rotate and move
    data_1 = np.matmul(sigma_1, np.random.randn(n_1, n_dim, 1)).res
hape(-1, n_dim) + mean_1
    data_2 = np.matmul(sigma_2, np.random.randn(n_2, n_dim, 1)).res
hape(-1, n_dim) + mean_2

    # Dataset: Features and labels
    features = np.concatenate([data_1, data_2])
    labels = np.array([-1] * n_1 + [1] * n_2)

    return features, labels

np.random.seed(23905)
features, labels = generate_data(150, 150)
```

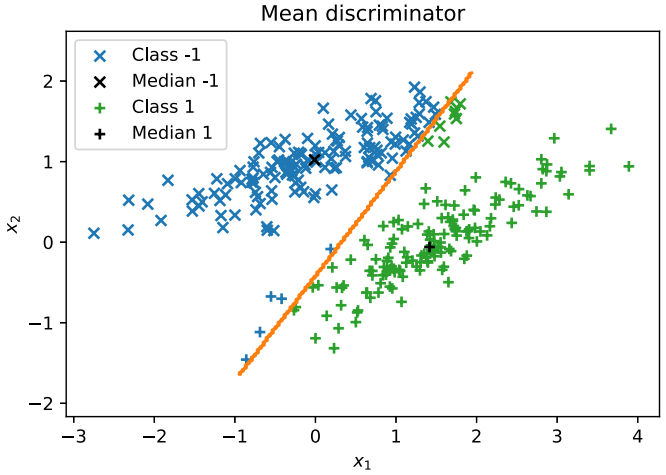

In [3]:
```
def plot_prediction(features, y_true, y_predicted):
    labels = np.unique(y_true)
    for i, (label, marker) in enumerate(zip(labels, "x+*.")):
        class_data = features[y_true == label]
        # Color is given by the predicted label
        colors = [f"C{predicted - labels.min()}" for predicted in y
_predicted[y_true == label]]
        plt.scatter(class_data[:, 0], class_data[:, 1], marker=mark
er, label=f"Class {label}", c=colors)
        # Median is more stable than mean
        median = np.median(class_data, axis=0)
        plt.scatter(median[0], median[1], c="black", marker=marker,
linewidths=10, label=f"Median {label}")
    plt.legend()
    plt.xlabel("$x_1$")
    plt.ylabel("$x_2$")
    plt.axis("equal")

plt.title("Labeled data")
plot_prediction(features, labels, labels)
x_range = plt.xlim()
y_range = plt.ylim()
```



In [4]:
```
def plot_decision_boundary(x_range, y_range, fit, samples=200, colo
r="C1", margin=False):
    x, y = np.meshgrid(np.linspace(*x_range, samples), np.linspace(
*y_range, samples))
    positions = np.stack((x.reshape(-1), y.reshape(-1)), axis=1).re
shape(-1, 2)
    if margin:
        prediction = fit.decision_function(positions)
        levels = [-1, 0, 1]
        linestyles = ['--', '-', '--']
    else:
        prediction = fit.predict(positions)
        levels = [0]
        linestyles = ["-"]
    cntr = plt.contour(x, y, prediction.reshape(samples, samples),
                       colors=color, levels=[-1, 0, 1],
                       linestyles=linestyles)
    return cntr.legend_elements()[0][1]

def plot_prediction_grid(x_range, y_range, fit, samples=100):
    x, y = np.meshgrid(np.linspace(*x_range, samples), np.linspace(
*y_range, samples))
    positions = np.stack((x.reshape(-1), y.reshape(-1)), axis=1).re
shape(-1, 2)
    prediction = fit.predict_proba(positions)[:, 1]
    plt.imshow(prediction.reshape(samples, samples), origin="lower"
, extent=(x.min(), x.max(), y.min(), y.max()),
               cmap="coolwarm", vmin=0, vmax=1, alpha=0.3)
    plt.colorbar(label="Predicted Probability class -1")
```

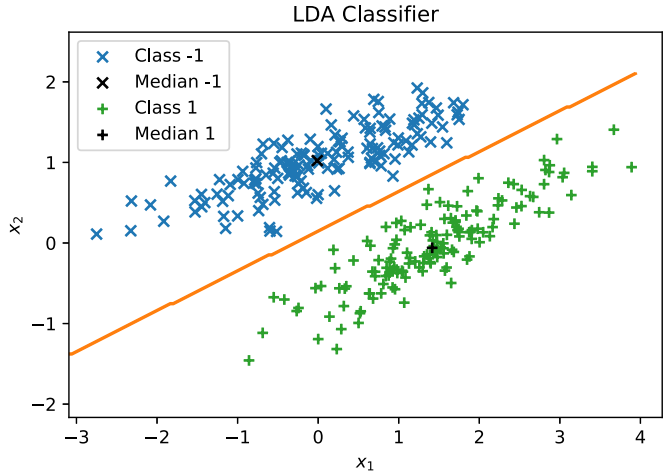
Mean discrimination

In [5]:
```
lmda = LinearDiscriminantAnalysis()
means = [np.median(features[labels == -1], axis=0), np.median(featu
res[labels == 1], axis=0)] * 20
lmda.fit(means, [-1, 1] * 20)

plt.title("Mean discriminator")
predicted_labels = lmda.predict(features)
plot_decision_boundary(x_range, y_range, lmda)
plot_prediction(features, labels, predicted_labels)
```



LDA

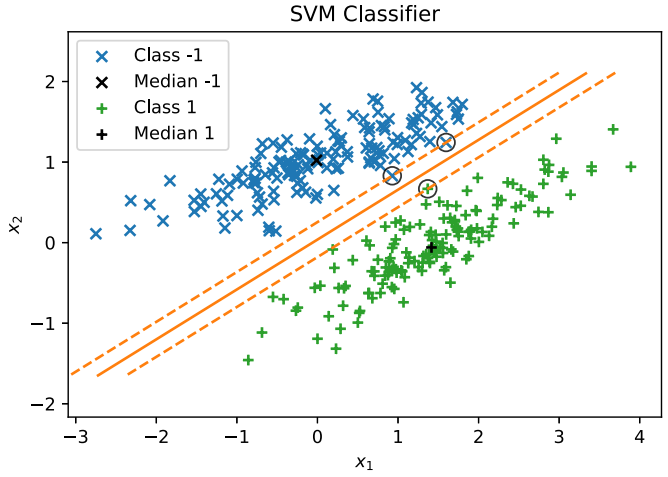
In [6]:
```
lda = LinearDiscriminantAnalysis()
lda.fit(features, labels)

plt.title("LDA Classifier")
predicted_labels = lda.predict(features)
plot_decision_boundary(x_range, y_range, lda)
plot_prediction(features, labels, predicted_labels)
```



Linear SVM

In [7]:
```
svm = SVC(gamma="scale", kernel="linear", C=1000)
svm.fit(features, labels)

plt.title("SVM Classifier")
predicted_labels = svm.predict(features)
plot_decision_boundary(x_range, y_range, svm, margin=True)
plot_prediction(features, labels, predicted_labels)
plt.scatter(svm.support_vectors_[:, 0], svm.support_vectors_[:, 1],
            s=100, linewidth=1, facecolors='none', edgecolors="k",
            alpha=0.8)
```

Out[7]: <matplotlib.collections.PathCollection at 0x1a1f991690>

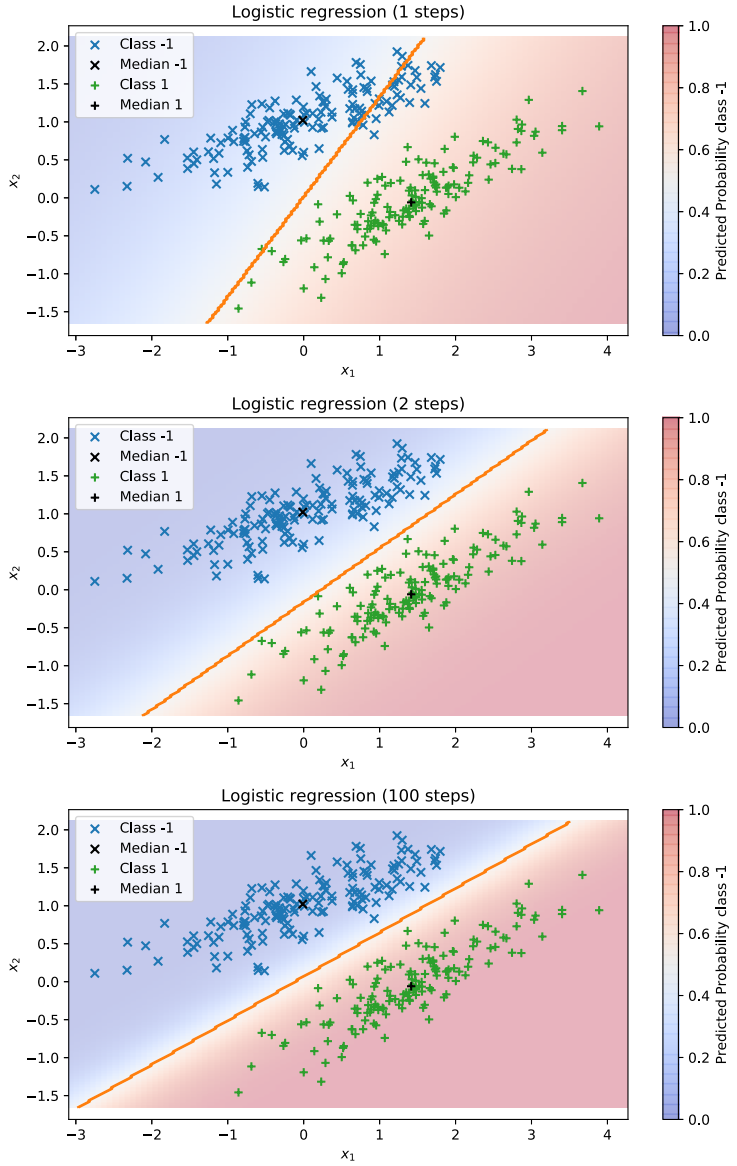


LR

In [8]:
```
def learn_and_show_lr(steps=100):
    lr = LogisticRegression(solver="lbfgs", max_iter=steps)
    lr.fit(features, labels)

    plt.title(f"Logistic regression ({steps} steps)")
    plot_prediction_grid(x_range, y_range, lr)
    plot_decision_boundary(x_range, y_range, lr)
    plot_prediction(features, labels, predicted_labels)
```

In [9]:
```
plt.figure(figsize=(8, 12))
plt.subplot(311)
learn_and_show_lr(1)
plt.subplot(312)
learn_and_show_lr(2)
plt.subplot(313)
learn_and_show_lr(100)
plt.tight_layout()
```

```
/Users/felix/miniconda3/envs/ml-tutorial/lib/python3.7/site-packag
es/sklearn/linear_model/logistic.py:947: ConvergenceWarning: lbfgs
failed to converge. Increase the number of iterations.
  "of iterations.", ConvergenceWarning)
/Users/felix/miniconda3/envs/ml-tutorial/lib/python3.7/site-packag
es/sklearn/linear_model/logistic.py:947: ConvergenceWarning: lbfgs
failed to converge. Increase the number of iterations.
  "of iterations.", ConvergenceWarning)
```

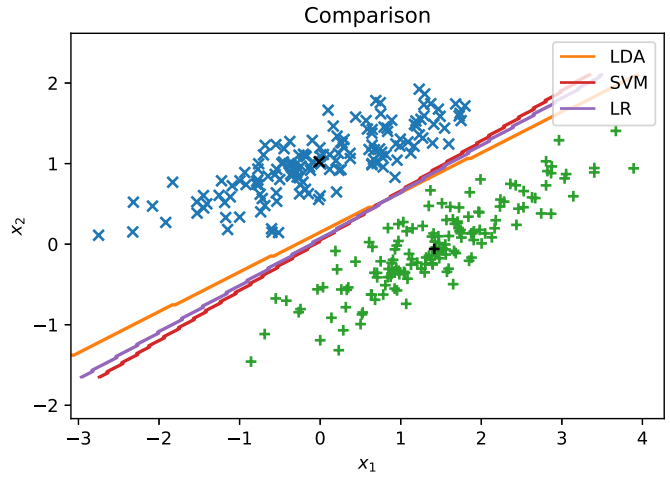
In [10]:
```
lr = LogisticRegression(solver="lbfgs")
lr.fit(features, labels)
```

Out[10]:
```
LogisticRegression(C=1.0, class_weight=None, dual=False, fit_inter
cept=True,
                   intercept_scaling=1, l1_ratio=None, max_iter=10
0,
                   multi_class='warn', n_jobs=None, penalty='l2',
                   random_state=None, solver='lbfgs', tol=0.0001,
verbose=0,
                   warm_start=False)
```

Comparison

In [11]:
```
plt.title("Comparison")
plot_prediction(features, labels, labels)
lda_line = plot_decision_boundary(x_range, y_range, lda, color="C1"
)
svm_line = plot_decision_boundary(x_range, y_range, svm, color="C3"
)
lr_line = plot_decision_boundary(x_range, y_range, lr, color="C4")

plt.legend([lda_line, svm_line, lr_line], ["LDA", "SVM", "LR"])
```

Out[11]:
```
<matplotlib.legend.Legend at 0x1a2049be50>
```



unbalanced loss functions / classes

- in two-class problems, there are two kinds of errors:
  - false positive $\hat{y}_i = 1$, $y_i^* = 0$
  - false negative $\hat{y}_i = 0$, $y_i^* = 1$
- often, consequences of these errors are very different, e.g. access control to a bank safe
  - false negative: authorized person is rejected:
    ⇒ annoying, but simply retry (cf. fingerprint sensor on cell phones)
  - false positive: burgler is admitted
    ⇒ very expensive

⇒ weight each loss term with its cost

$$\hat{\beta}, \hat{s} = \underset{\beta, s}{\operatorname{argmin}} \frac{1}{N} \sum_i w_i \, \text{loss}(y_i^*, x_i \beta + s)$$

for access control: $w_i = \begin{cases} \text{big} & \text{if } y_i^* = 0 \text{ (false positive)} \\ \text{small} & \text{if } y_i^* = 1 \end{cases}$

choose weights according to application

- unbalanced classes: one class (e.g. positive ≙ disease) is much more rare than the other (e.g. healthy)

⇒ errors may be misleading

- consider test for a disease with 1% false positives and 1% false negatives – sounds pretty good
- positive to negative ratio is 1/100
- simple calculation shows that if

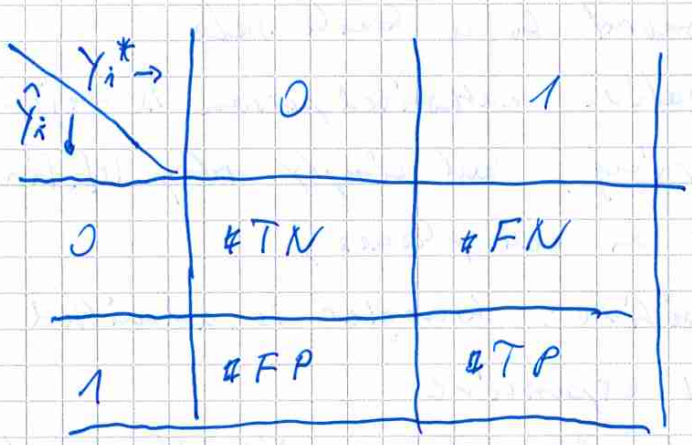
$$\hat{y}_i = 1 \text{ (suspected disease)}, \; p(y_i^* = 1 \mid x_i) = 0.5 \text{ (actual disease)}$$

⇒ many patients are unnecessarily scared

⇒ report precision and recall instead of error rates

more ...

- even worse: if only true positive rate (e.g. 99%) false negative rate (e.g. 1%) is reported, but not the false positive rate, the test quality cannot be judged at all! (cf. ~~blood~~ breast cancer blood test scandal)
- confusion matrix for $C=2$ ($C>2$ analogously)



should be diagonal

true positive rate $\hat{=}$ sensitivity: $\hat{=}$ recall

$$\frac{\#TP}{\#P} = \frac{\#TP}{\#TP + \#FN}$$

true negative rate $\hat{=}$ specifity:

$$\frac{\#TN}{\#N} = \frac{\#TN}{\#TN + \#FP}$$

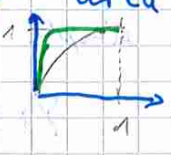
precision:

$$\frac{\#TP}{\#TP + \#FP}$$

- If we have a score or posterior, we can freely choose the threshold, e.g. $\hat{p}(y_i = 1 \mid x_i) > 0.5$ (balanced)
  $\hat{p}(y_i = 1 \mid x_i) > 0.9$ (avoid false positives)

  ⇒ precision, recall, specifity change according to threshold

  ⇒ ROC curve and precision/recall curve depict this dependency ⇒ judge quality of results by "area under curve" (AUC)



fundamental insight 2:

DEFINING APPROPRIATE LOSS FCT. FOR AN APPLICATION IS A MAJOR PART OF A MACHINE LEARNING DESIGN.

⇒ easier than hand-crafted model, because only a critic, not a constructive solution

Regression

- classification: Y is discrete (e.g. C classes)
  regression: Y is a real number
- closely related: $s_i = x_i \beta + \delta$ is a real-valued score
  $\hat{y}_i = \text{sign}(x_i \beta + \delta)$ a discrete class
  ⇒ regression is often an intermediate part of classification and often a goal of its own

(example)

- linear regression is most basic approach
  ⇒ ordinary least squares (OLS) method

$$\hat{\beta}, \hat{\delta} = \arg\min_{\beta, \delta} \frac{1}{N} \sum_{i=1}^{N} \left(y_i^* - \underbrace{(x_i \beta + \delta)}_{= \hat{y}_i} \right)^2$$

y_i^*: arbitrary real number

~~$= \arg\min_{\beta, \delta = N}$~~

- we can eliminate δ by centralizing the data

$$\tilde{x}_i = x_i - \mu \qquad \mu = \frac{1}{N} \sum_i x_i \quad \text{mean}$$

($\tilde{x}_i$ has now zero mean)

$$\hat{\beta} = \arg\min_{\beta} \frac{1}{N} (y^* - X\beta)^T (y^* - X\beta)$$

(matrix notation)

- find the optimum by setting the derivative to zero

~~$\frac{\partial}{\partial \beta} \frac{1}{N} (y^* - X\beta)^T (y^* - X\beta) = \frac{2}{N} (-y^* X + X^T X \beta) \doteq 0$~~

$$\frac{\partial}{\partial \beta} \frac{1}{N} (X^T y^* - X^T X \beta)^T (y^* - X\beta) = \frac{2}{N} (-X^T y^* + X^T X \beta)$$

$$\doteq 0$$

$$X^T X \beta = X^T y^*$$

$$\hat{\beta} = \underbrace{(X^T X)^{-1} X^T}_{=: X^+} y^*$$

"pseudo-inverse"
Moore-Penrose inverse
generalization of inverse for rectangular matrices

- in order to give all features equal influence in the loss, it makes sense to standardize features ⇒ unit-free quantities

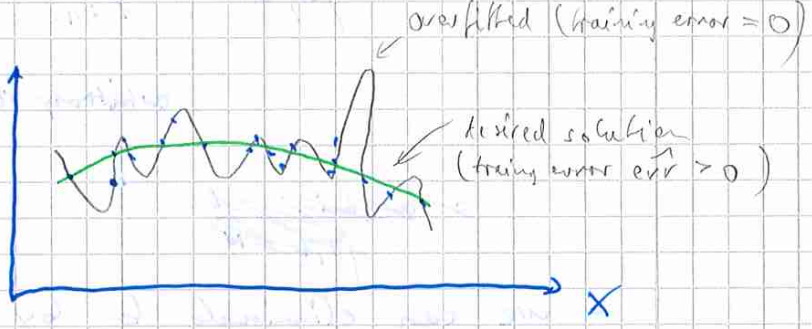
$$\tilde{x}_i = \frac{x_i - \mu}{\sigma}$$ ← element-wise division

σ: vector of standard deviations (σ_j: stddev of feature j)
(this is also helpful in classification, standard data preprocessing)

- numeric solution of OLS: re-usable algorithms in all ML libraries, using QR decomposition or singular value decomposition (SVD)

Overfitting

- non-linear example



- effective counter-measure: regularization of parameters, e.g. penalize large values of β-coefficients
most common: L2 regularization: restrict Euclidean (squared) norm

$$\|\beta\|_2^2 = \sum_j \beta_j^2 = \beta^T \beta$$

⇒ ridge regression

$$\hat{\beta} = \arg\min_{\beta} \frac{\beta^T \beta}{2} + \frac{\lambda}{n} \sum_i (y_i^* - x_i \beta)^2$$

identical to support vector machine, but with squared loss ⇒ robustness against noise

- L1 regularization: restrict L1 norm

$$\|\beta\|_1 = \sum_j |\beta_j|$$

⇒ LASSO regression

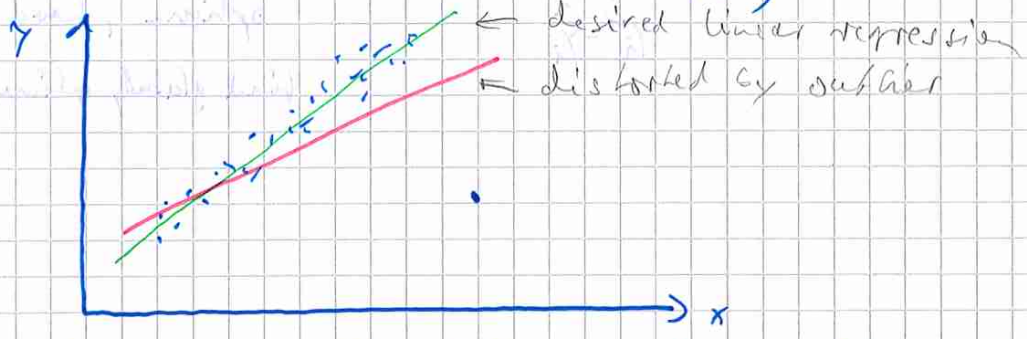
$$\hat{\beta} = \arg\min_{\beta} \|\beta\|_1 + \frac{\lambda}{N} \sum_i (y_i^* - x_i \beta)^2$$

⇒ sparsity enforcing: many coefficients $\beta_j = 0$
non-zero coefficients denote important features
⇒ feature selection

- regularization parameter λ must be manually chosen for each application as a hyper-parameter to optimize the bias-variance trade-off

robust regression

- results can be severely distorted when training data is contaminated by outliers ⇒ grossly wrong data points (e.g. satellite data: transmission errors as opposed to measurement noise)

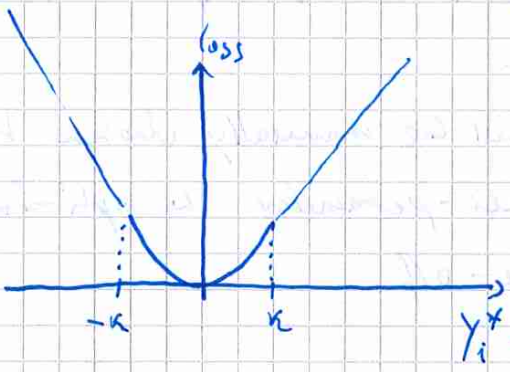


- solution 1: identify inliers and ignore outliers
⇒ RANSAC algorithm
- solution 2: modify the loss function to become robust against outliers

- squared loss: outliers are highly weighted, because error term is squared
- absolute loss: $\text{Loss}(y_i^*, \hat{y}_i) = |y_i^* - \hat{y}_i|$
  - much more robust, influence of outliers greatly reduced
  - disadvantages: • often no unique solution for $\hat{\beta}$
    • higher generalization error on new data

- Huber loss: best of both worlds
  - squared loss for small errors ⇒ high accuracy, uniqueness
  - absolute loss for high errors ⇒ robustness

$$\text{Huber Loss}(y_i^*, \hat{y}_i) = \begin{cases} (y_i^* - \hat{y}_i)^2 & \text{if } |y_i^* - \hat{y}_i| \leq \kappa \\ 2\kappa |y_i^* - \hat{y}_i| - \kappa^2 & \text{else} \end{cases}$$



- biweight functions: loss for high errors saturates, there is no distinction between "very wrong" and "extremely wrong"

advantage: even more robust
disadvantage: has many poor local optima, hard to find globally optimal

- outlier handling $\hat{=}$ out-of-distribution detection $\approx$ novelty detection $\hat{=}$ robustness against adversarial attacks / samples

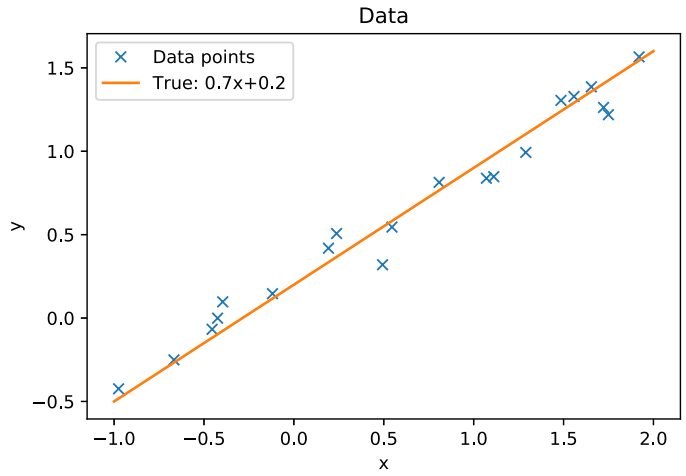
is still a hot research topic ⇒ show adversarial examples

In [1]:
```
import numpy as np
import matplotlib.pyplot as plt
%config InlineBackend.figure_formats = ['svg']
from sklearn.linear_model import LinearRegression, HuberRegressor
```

In [2]:
```
def plot_data_and_prediction(x, y, x_test, m_true, t_true, y_true,
m_pred=None, t_pred=None, y_pred=None):
    plt.xlabel("x")
    plt.ylabel("y")
    plt.plot(x, y, "x", label="Data points")
    plt.plot(x_test, y_true, label=f"True: {m_true}x+{t_true}")
    if y_pred is not None:
        plt.plot(x_test, y_pred, label=f"Fit: {m_pred:.2f}x+{t_pred
:.2f}")
    plt.legend()
```

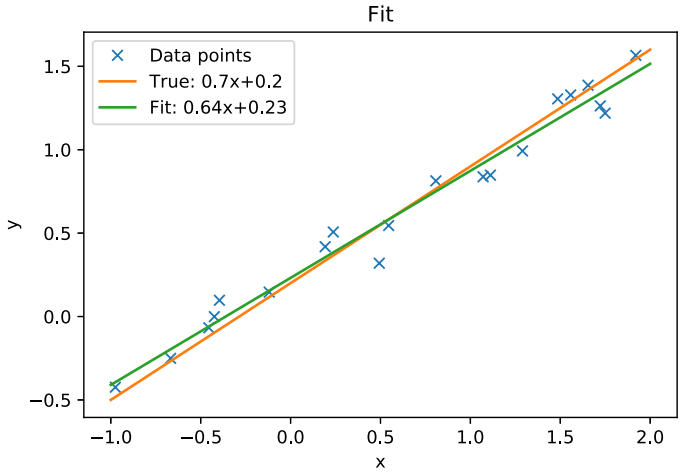
Data: m * x + t + noise

In [3]:
```
t = 0.2
m = 0.7
noise_std = 0.1

# Evaluate the true model at the edges
x_test = np.array([[-1], [2]])
y_test_true = m * x_test + t

n = 20
np.random.seed(537)
# samples x positions uniformly
x = np.random.rand(n) * 3 - 1
# sample noise from Gaussian
noise = noise_std * np.random.randn(n)
y = m * x + t + noise

plt.title("Data")
plot_data_and_prediction(x, y, x_test, m, t, y_test_true)
```



Linear model

In [4]:
```
model = LinearRegression()
model.fit(x.reshape(-1, 1), y)

plt.title("Fit")
y_test = model.predict(x_test)
plot_data_and_prediction(x, y, x_test, m, t, y_test_true,
                         model.coef_[0], model.intercept_, y_test)
```

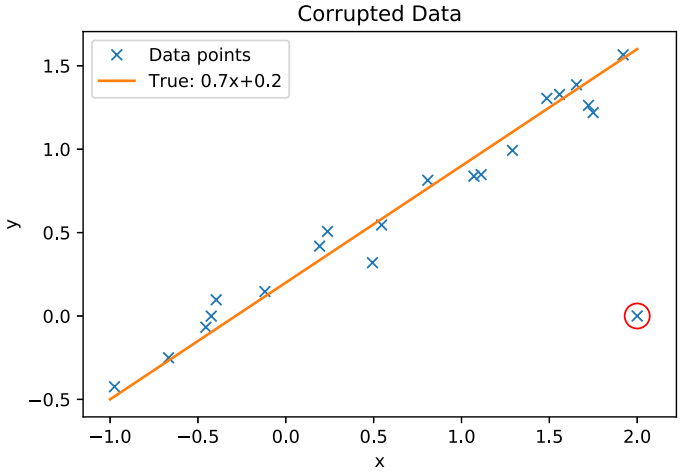


Corrupt data

Add one datapoint which is an outlier

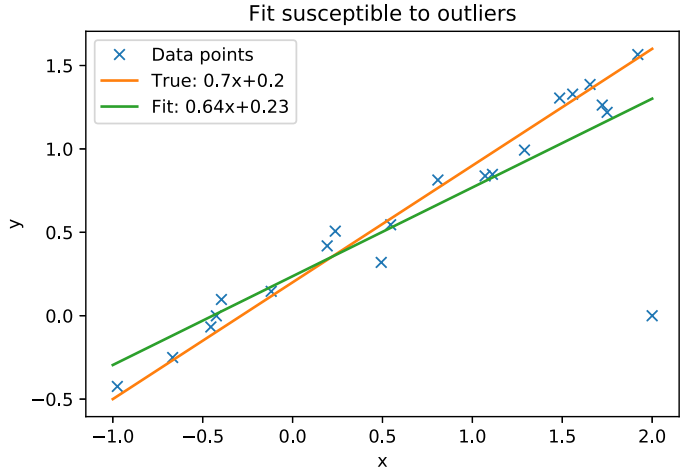
In [5]:
```
x_corrupt = np.concatenate((x, [2.0]))
y_corrupt = np.concatenate((y, [0.0]))

plt.title("Corrupted Data")
plot_data_and_prediction(x_corrupt, y_corrupt, x_test, m, t, y_test
_true)
plt.scatter(x_corrupt[-1], y_corrupt[-1], s=200, linewidth=1, facec
olors='none', edgecolors="r")
```

Out[5]: <matplotlib.collections.PathCollection at 0x1a1c0e5950>



Fit a linear function to the data: It is heavily corrupted by the corrupt data point

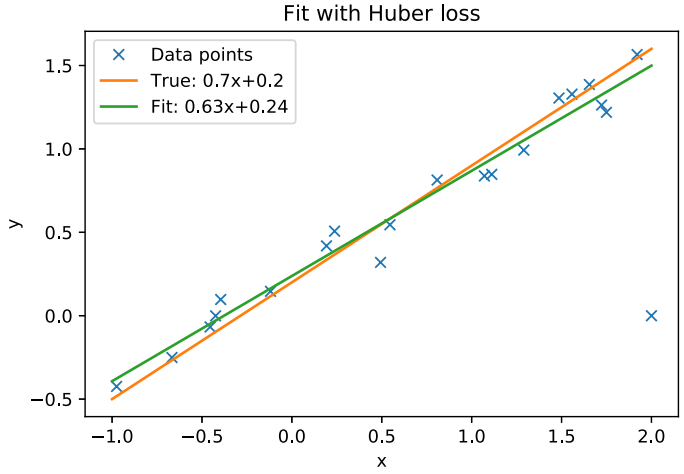
In [6]:
```
corrupt_model = LinearRegression()
corrupt_model.fit(x_corrupt.reshape(-1, 1), y_corrupt)

plt.title("Fit susceptible to outliers")
y_corrupt_test = corrupt_model.predict(x_test)
plot_data_and_prediction(x_corrupt, y_corrupt, x_test, m, t, y_test
_true,
                         model.coef_[0], model.intercept_, y_corrup
t_test)
```



Change the loss to Huber loss

This loss is less susceptible to outliers

In [7]:
```
huber_model = HuberRegressor()
huber_model.fit(x_corrupt.reshape(-1, 1), y_corrupt)

plt.title("Fit with Huber loss")
y_huber_test = huber_model.predict(x_test)
plot_data_and_prediction(x_corrupt, y_corrupt, x_test, m, t, y_test
_true,
                         huber_model.coef_[0], huber_model.intercep
t_, y_huber_test)
```



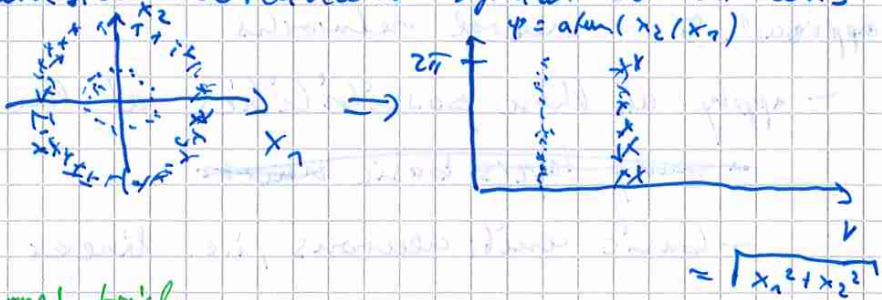
In [ ]:

Non-linear Methods

- most data are not adequately represented by linear models
- approach 1: manually design non-linear model and fit its parameters, e.g. non-linear least squares, Levenberg-Marquardt algorithm.
  problems: • has many poor local optima, good initial guess required to find best $\hat{\theta}$
  • manual model design is difficult, esp. for highly complex problems (e.g. medicine, biology, social sciences)
- approach 2: ~~cleverly combine several linear models into a non-linear model~~
- approach 2: augmented feature spaces
  (1) calculate new features by non-linear functions of the given original features
  (2) apply a linear model in this augmented feature space

example: body mass index = ~~height~~ weight / height^2

example: Cartesian coordinates ⇒ polar coordinates



- access features via Gram matrix $G = XX^T$ instead of directly via X
- replace G with kernel matrix K using $x_i x_j^T \rightarrow k(x_i, x_j)$ ⇒ non-linear kernel function

Kernel trick

variant: rewrite loss and regularization in terms of a non-linear kernel function ⇒ augmented feature space needs not be constructed explicitly, can have high and even infinite dimension

advantage: - training (i.e. finding optimal $\hat{\theta}$) is easier than in approach 1, good optimization algorithms

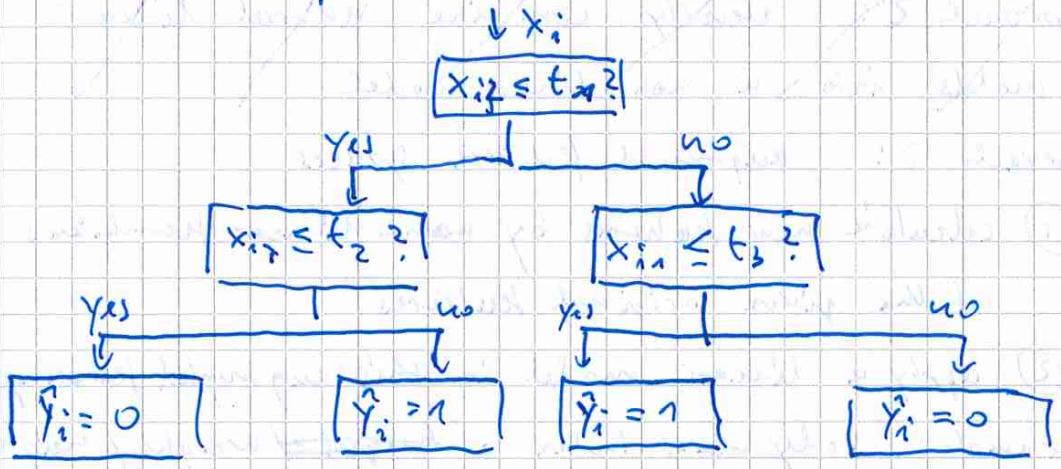
disadvantage: - manual design of good non-linear transformations or kernels is difficult

- approach 3: boosting
  - run several linear models in parallel, then take a weighted vote

$$\hat{y}_i = \text{sign}\left(\frac{1}{L}\sum_{\ell=1}^{L} w_\ell \cdot \text{sign}\left(x_i \beta_\ell + b_\ell\right)\right)$$

$$\Theta = \left\{(\beta_1, b_1, w_1), \ldots, (\beta_L, b_L, w_L)\right\}$$

- approach 4: decision trees
  - run several linear models in series ⇒ split feature space into subregions, where each subregion behaves simpler than the whole.



- approach 5: neural networks
  - apply all those possibilities at the same time

~~many layers~~ basic ~~neurons~~

  - basic unit: neurons, i.e. linear models, followed by simple non-linearity
  - sequential processing: arrange neurons in layers
  - parallel processing: each layer contains many independent neurons

why does this solve the problems?

- scales to very complex models ("deep" networks, "wide" networks)
- outputs of inferior layers are "learned augmented feature spaces"
- most local minima are reasonably good ⇒ robust optimization
- hand-crafting good architecture and non-linearities is still hard, but performance is relatively robust against sub-optimal solutions

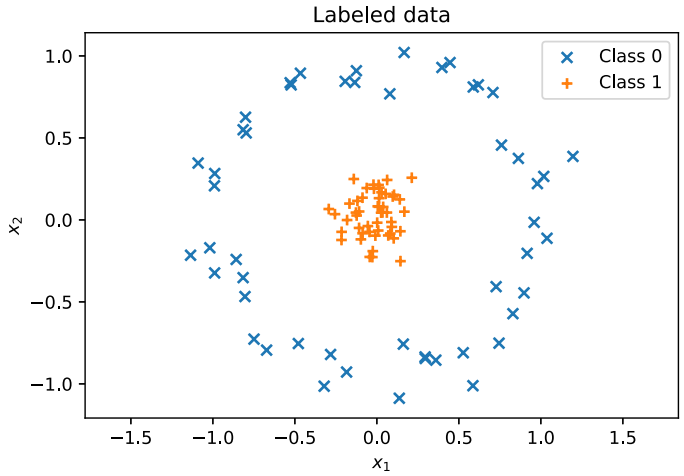
Non-linear methods

In [1]:
```
import numpy as np
%config InlineBackend.figure_formats = ['svg']
import matplotlib.pyplot as plt
from sklearn.datasets.samples_generator import make_circles
from sklearn.svm import SVC
```

The Data

In [2]:
```
features, labels = make_circles(100, factor=.1, noise=.1)
```

In [3]:
```
def plot_prediction(features, y_true, y_predicted):
    labels = np.unique(y_true)
    for i, (label, marker) in enumerate(zip(labels, "x+*.")):
        class_data = features[y_true == label]
        # Color is given by the predicted label
        colors = [f"C{predicted - labels.min()}" for predicted in y
_predicted[y_true == label]]
        plt.scatter(class_data[:, 0], class_data[:, 1], marker=mark
er, label=f"Class {label}", c=colors)
    plt.legend()
    plt.xlabel("$x_1$")
    plt.ylabel("$x_2$")
    plt.axis("equal")

plt.title("Labeled data")
plot_prediction(features, labels, labels)
x_range = plt.xlim()
y_range = plt.ylim()
```

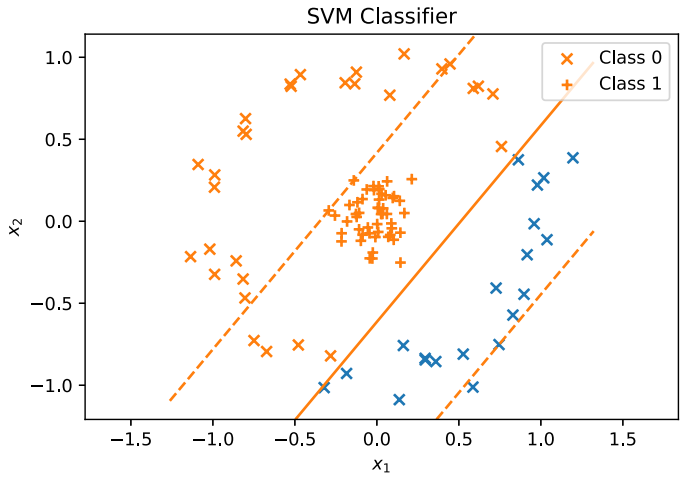



Fit the data

In [4]:
```
def plot_decision_boundary(x_range, y_range, fit, samples=200, colo
r="C1", margin=False):
    x, y = np.meshgrid(np.linspace(*x_range, samples), np.linspace(
*y_range, samples))
    positions = np.stack((x.reshape(-1), y.reshape(-1)), axis=1).re
shape(-1, 2)
    if margin:
        prediction = fit.decision_function(positions)
        levels = [-1, 0, 1]
        linestyles = ['--', '-', '--']
    else:
        prediction = fit.predict(positions)
        levels = [0]
        linestyles = ["-"]
    cntr = plt.contour(x, y, prediction.reshape(samples, samples),
                       colors=color, levels=[-1, 0, 1],
                       linestyles=linestyles)
    return cntr.legend_elements()[0][1]

def plot_prediction_grid(x_range, y_range, fit, samples=100):
    x, y = np.meshgrid(np.linspace(*x_range, samples), np.linspace(
*y_range, samples))
    positions = np.stack((x.reshape(-1), y.reshape(-1)), axis=1).re
shape(-1, 2)
    prediction = fit.predict_proba(positions)[:, 1]
    plt.imshow(prediction.reshape(samples, samples), origin="lower"
, extent=(x.min(), x.max(), y.min(), y.max()),
               cmap="coolwarm", vmin=0, vmax=1, alpha=0.3)
    plt.colorbar(label="Predicted Probability class -1")
```

Linear SVM

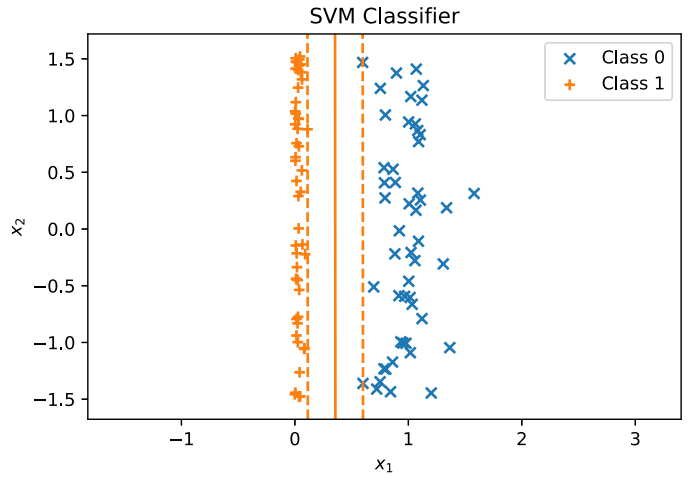
In [5]:
```
svm = SVC(gamma="scale", kernel="linear", C=10)
svm.fit(features, labels)

plt.title("SVM Classifier")
predicted_labels = svm.predict(features)
plot_decision_boundary(x_range, y_range, svm, margin=True)
plot_prediction(features, labels, predicted_labels)
```



Use new features

In [6]:
```
radius = np.sum(features ** 2, axis=1)
phi = np.arctan(features[:, 1] / features[:, 0])

mod_features = np.stack([radius, phi], 1)

svm = SVC(gamma="scale", kernel="linear", C=10)
svm.fit(mod_features, labels)

plt.title("SVM Classifier")
predicted_labels = svm.predict(mod_features)
plot_prediction(mod_features, labels, predicted_labels)
plot_decision_boundary(plt.xlim(), plt.ylim(), svm, margin=True)
```

Out[6]: <matplotlib.collections.LineCollection at 0x1a18d73850>

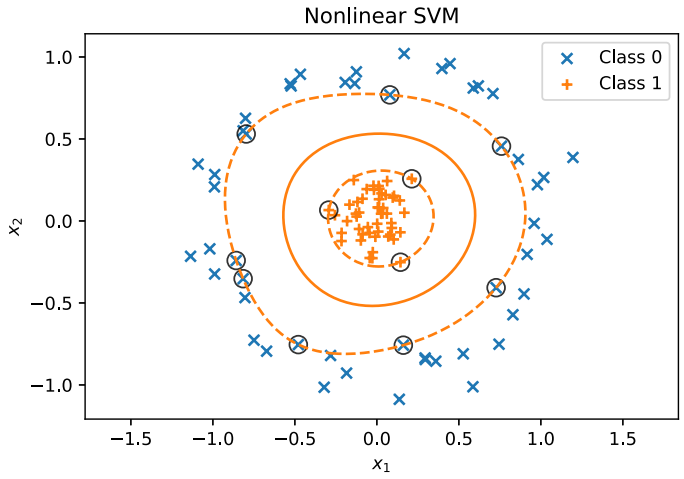


Non-linear SVM

Use a radial basis function kernel

In [7]:
```
svm = SVC(gamma="scale", kernel="rbf", C=20)
svm.fit(features, labels)

plt.title("Nonlinear SVM")
predicted_labels = svm.predict(features)
plot_decision_boundary(x_range, y_range, svm, margin=True)
plot_prediction(features, labels, predicted_labels)
plt.scatter(svm.support_vectors_[:, 0], svm.support_vectors_[:, 1],
            s=100, linewidth=1, facecolors='none', edgecolors="k",
            alpha=0.8)
```

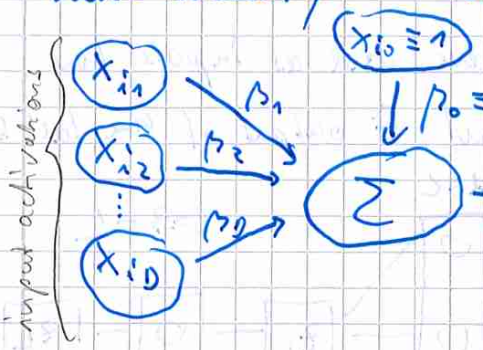
Out[7]: <matplotlib.collections.PathCollection at 0x1a1885b710>



In [ ]:

Neural Networks

- neurons are simple linear models, followed by a 1-dimensional non-linearity — very crude approximation of biological neurons



bias neuron: add feature 0, which is constant = 1

$\Rightarrow$ absorb bias parameter b into β as β_0

$(\beta \in \mathbb{R}^{D+1}, \; j = 0 \dots D)$

output of the neuron:

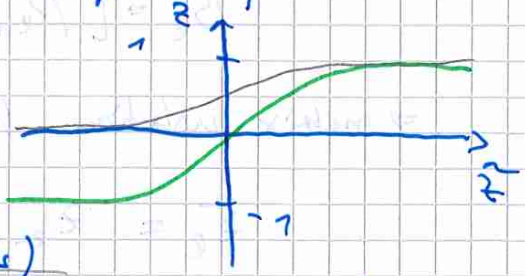
$$z_i = \varphi\left(\sum_{j=0}^{D} x_{ij} \cdot \beta_j \right) \qquad \text{row vector}$$

- activation fct. should be almost everywhere differentiable, so that we can train by gradient descent, (sign(z) is not suitable)

- traditional choices:

$$z = \varphi(\tilde{z}) = \frac{1}{1 + e^{-\tilde{z}}}$$

logistic sigmoid

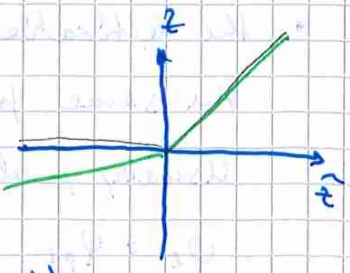


$$z = \varphi(\tilde{z}) = \tanh(\tilde{z})$$

~~$z = \tilde{z}$ (for linear layers e.g. regression outputs)~~

- modern choices

$$z = \varphi(\tilde{z}) = \mathrm{ReLU}(\tilde{z}) = \max(\tilde{z}, 0)$$



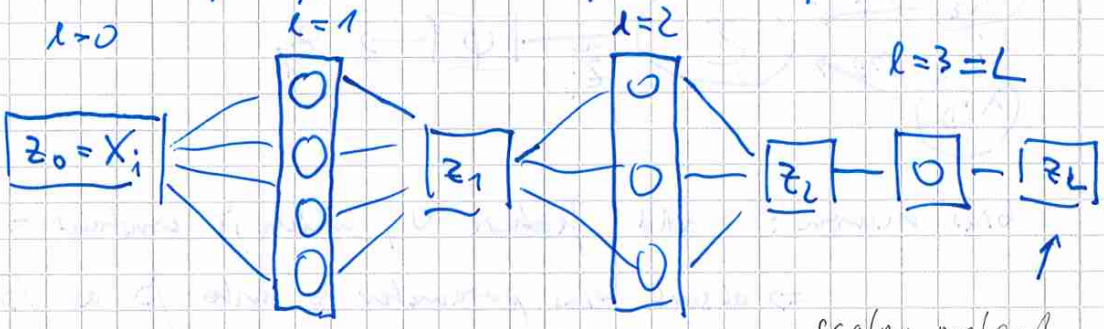
$$z = \mathrm{LeakyReLU}(\tilde{z}) = \begin{cases} \tilde{z} & \text{if } \tilde{z} \geq 0 \\ a \cdot \tilde{z} & \text{if } \tilde{z} < 0, \end{cases} \quad (a \ll 1 \text{ fixed})$$

$z = \mathrm{PReLU}(\tilde{z})$: like leaky ReLU, but a is learned

$$z = \mathrm{ELU}(\tilde{z}) = \begin{cases} \tilde{z} & \text{if } \tilde{z} > 0 \\ a(e^{\tilde{z}} - 1) & \text{otherwise} \end{cases} \quad (a \text{ fixed})$$

Fully connected networks

- consist of the input layer ($\hat{=}$ the original feature vector x_i) and L ~~compute~~ neuron layers
- all outputs of the previous layer are used as inputs for the next layer ; network output $\hat{=}$ output of the last layer



scalar output,
e.g. • regression in 1-D
• posterior probab. $\hat{p}(\hat{y}_i = 1 | x_i)$

- layer l contains H_l (M_l) neurons (+ bias neuron - not shown)
(here $H_1 = 4$ (M_1), $H_2 = 3$ (M_2), $H_3 = 1$ (M_3))
⇒ each layer needs H_l different weight vectors β:

$$\beta_{lm}, \quad l = 1 \dots L, \quad m = 1 \dots H_l \ (M_l)$$

Combine the weight vectors of each layer into matrix

$$B_l = [\beta_{l1} \dots, \beta_{lM_l}]$$

⇒ matrix notation for pre-activations of layer l:

$$\tilde{z}_l = z_{l-1} \cdot B_l$$

- the activation functions φ (non-linearities) are usually the same for all neurons in a given layer: φ_l.
Usually, all inner layers have the same activation $\varphi_l = \varphi_{l'}$, except for last layer φ_L, whose activation depends on the application

output of a 3-layer network for feature vector x_i: (35)

$$\hat{y}_i = z_{L3} = \varphi_3\Big(\varphi_2\big(\varphi_1\big(\underbrace{z_0}_{=x_i}\cdot B_1\big)\cdot B_2\big)\cdot B_3\Big)$$

(non-linearities; parallel processing; serial processing)

[note: the bias channels $z_{\ell 0} \equiv 1$ is always implicitly present, even if not shown explicitly]

- by increasing L and M_ℓ, we can adapt model complexity to the application
- output activation functions depend on the task:
  - regression: y_i is real or real-valued vector
    $$\varphi_L(\hat{z}_L) = \hat{z}_L \quad \text{linear activation}$$
    $\Rightarrow$ last layer performs linear regression, using penultimate activations z_{L-1} as augmented feature space
  - classification with $C = 2$: estimate posterior for positive class
    $$z_L = \hat{p}(y_i = 1 \mid x_i) = \sigma(\hat{z}_L) \quad \text{sigmoid fct.}$$
    [$\hat{p}(y_i = 0 \mid x_i) = 1 - z_L$ is trivial, doesn't have to be learned]

    [class label easily obtained from posterior via
    $$\hat{y}_i = \begin{cases} 1 & \text{if } z_L > 0.5 \\ 0 & \text{if } z_L < 0.5 \end{cases}$$
    (or other threshold for asymmetric costs)]
  - classification with $C > 2$: z_L is a probability vector of length C, i.e.
    $$z_{Lk} = \hat{p}(y_i = k \mid x_i)$$
    with normalization $\sum_{k=1}^{C} z_{Lk} = 1$

soft max activation generalizes sigmoid for multi-class problem (reduces to $z_{L4} = \sigma(\vec{z}_{L1} \cdot \vec{z})$ if $C=2$)

$$z_{L4} = \frac{e^{\vec{z}_{L4}}}{\sum_{\nu=1}^{C} e^{\vec{z}_{L4'}}}$$

- illustration of how it works, using a 2-layer network with sign( ) activation (not suitable for gradient training, but easy to understand)

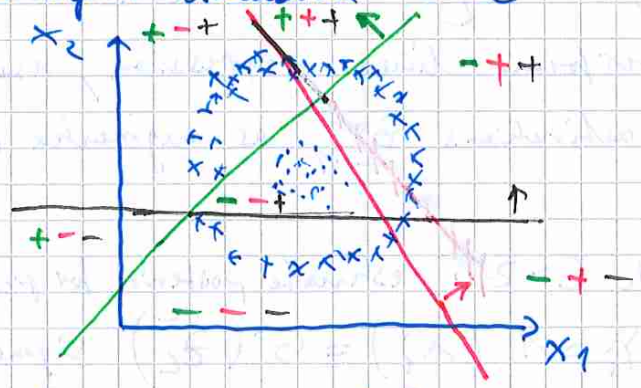
We have

$$z_2 = \varphi_2\left(\varphi_1(x_i \cdot B_1) \cdot B_2\right)$$

with $\varphi_{1,2}(\vec{z}) = \text{sign}(\vec{z}) = \{-, +\}$

- we use $M_1 = 3$, $M_2 = 1$ (4 neurons in total)

for input dimension $D = 2$



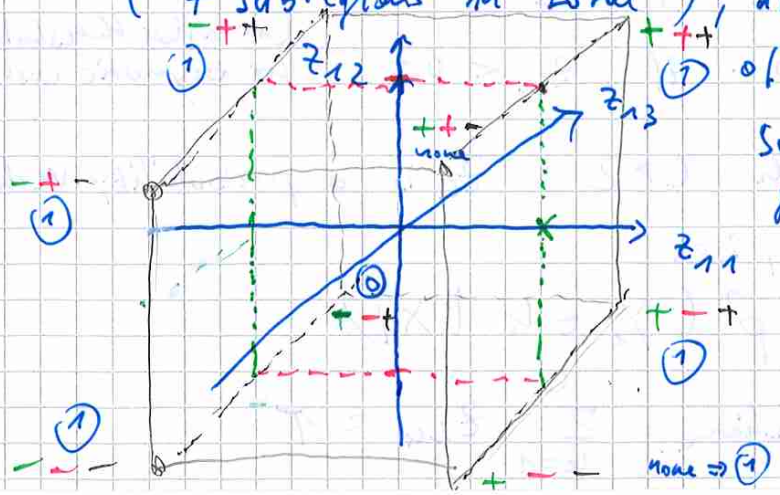
labels: $\times = 1$

$\cdot = 0$

first layer neurons define 3 decision planes ═ with arrows indicating the positive side

⇒ each subregion is assigned a particular sign combination (7 subregions in total), activations z_1 are corners of a cube.

Subregions are learned such that each contains a unique label.



second layer neuron must learn a decision plane that cuts off the corner $(-1,-1,+1)$ from the remaining corners of the cube,

e.g. $\beta_2 = (\underbrace{2}_{\text{bias weight}}, 1, 1, -1)$

with $\hat{y}_i = \begin{cases} 1 & \text{if } z_{11i} + z_{12i} - z_{13i} + 2 > 0 \\ 0 & \text{else} \end{cases}$

- loss functions are essentially the same as for linear models
  - regression: squared loss $\text{loss}(y_i^*, \hat{y}_i) = \| y_i^* - \hat{y}_i \|_2^2$
  - classification with $C=2$:

    $z_{Li} = \hat{p}(y_i = 1 \mid x_i)$ scalar posterior prob. value (sigmoid output)

    $(\hat{p}(y_i = 0 \mid x_i) = 1 - z_{Li}$ trivial$)$

    $\Rightarrow$ logistic loss

    $$\text{loss}(y_i^*, z_{Li}) = \begin{cases} -\log z_{Li} & \text{if } y_i^* = 1 \\ -\log(1 - z_{Li}) & \text{if } y_i^* = 0 \end{cases}$$

  - classification with $C > 2$

    $z_{Lik} = \hat{p}(y_i = k \mid x_i)$ full probability vector (softmax output)

    with $\sum_k z_{Lik} = 1$

    $\Rightarrow$ cross-entropy loss

    $\text{loss}(y_i^*, z_{Li}) = -\log z_{Lik}$ with $k = y_i^*$

    (reduces to logistic loss for $C=2$)

    $\hat{p}(y_i = y_i^* \mid x_i)$ should be close to 1 (and the loss close to 0)

    $-\log z_{Li,k=y_i^*} = \begin{cases} \approx 0 & \text{if } z_{Li,k=y_i^*} \approx 1 \\ \text{big} & \text{else} \end{cases}$

training by stochastic gradient descent

① pick a random instance i

② compute $\text{Loss}(y_i^*, \hat{z}_{Li})$ for current parameters $\Theta^{(t)}$

③ compute $\Delta\Theta = \frac{\partial \text{Loss}(y_i^*, z_{Li})}{\partial \Theta}$ (derivative of loss w.r.t. parameters)

④ update $\Theta^{(t+1)} = \Theta^{(t)} - \tau \Delta\Theta$

τ learning rate
subtraction, because we need descent to minimize loss

- step ③ is the critical part. The derivative is computed by back-propagation, i.e. by passing errors from output towards input.

Introduce auxilliary variable $\tilde{\delta}_\ell$ (row vector)

$$\tilde{\delta}_\ell = \frac{\partial \text{Loss}}{\partial \tilde{z}_\ell}$$

with $\tilde{z}_\ell = z_{\ell-1} B_\ell$ the pre-activations of layer ℓ (before applying nonlinearity $\varphi_\ell(\cdot)$)

- The chain rule gives

$$\tilde{\delta}_\ell = \frac{\partial \text{Loss}}{\partial \tilde{z}_\ell} = \frac{\partial \text{Loss}}{\partial \tilde{z}_{\ell+1}} \cdot \frac{\partial \tilde{z}_{\ell+1}}{\partial z_\ell} \cdot \frac{\partial z_\ell}{\partial \tilde{z}_\ell}$$

the RHS is simple:

$\frac{\partial \text{Loss}}{\partial \tilde{z}_{\ell+1}} =: \tilde{\delta}_{\ell+1}$ by definition of $\tilde{\delta}$. We already know this term because we work back to front.

$$\frac{\partial \tilde{z}_{\ell+1}}{\partial z_\ell} = \frac{\partial (z_\ell \cdot B_{\ell+1})}{\partial z_\ell} = B_{\ell+1}^T$$

$$\frac{\partial z_\ell}{\partial \tilde{z}_\ell} = \frac{\partial (\varphi_\ell(\tilde{z}_\ell))}{\partial \tilde{z}_\ell} = \text{diag}\left(\varphi_\ell'(\tilde{z}_\ell)\right)$$

$$\tilde{\delta}_\ell = \tilde{\delta}_{\ell+1} \cdot B_{\ell+1}^T \cdot \text{diag}\left(\varphi_\ell'(\tilde{z}_\ell)\right)$$

- The start of backpropagation is determined by the output activation:
  - regression: $\varphi_L(\tilde{z}_L) = \tilde{z}_L$

$$\text{Loss}(y_i^*, z_{Li}) = \frac{1}{2}(y_i^* - z_{Li})^2$$

$$= \frac{1}{2}(y_i^* - \tilde{z}_{Li})^2$$

$$\Rightarrow \frac{\partial \text{Loss}}{\partial \tilde{z}_L} = \tilde{\delta}_L = \tilde{z}_L - y_i^*$$

  - classification: $\varphi_L(\tilde{z}_L) = \text{softmax}(\tilde{z}_L)$

$$\text{Loss}(y_i^*, z_L) = \text{cross-entropy}(y_i^*, z_L)$$

$$\Rightarrow \left(\frac{\partial \text{Loss}}{\partial \tilde{z}_L}\right)_k = \begin{cases} z_{Lk} - 1 & \text{if } y_i^* = k \\ z_{Lk} & \text{if } y_i^* \neq k \end{cases}$$

- The derivative w.r.t. the parameters B_ℓ is easily computed from $\tilde{\delta}_\ell$

$$\frac{\partial \text{Loss}}{\partial B_\ell^T} = \left(\frac{\partial \text{Loss}}{\partial \tilde{z}_\ell}\right)^T \cdot \left(\frac{\partial \tilde{z}_\ell}{\partial B_\ell}\right)^T = \tilde{\delta}_\ell^T \cdot z_{\ell-1}$$

$$\left[\frac{\partial \tilde{z}_\ell}{\partial B_\ell^T} = \frac{\partial (z_{\ell-1} \cdot B_\ell)}{\partial B_\ell^T} = z_{\ell-1}\right]$$

⇒ gradient update with learning rate τ

$$B_\ell^{(t+1)} = B_\ell^{(t)} - \tau \cdot \left(z_{\ell-1}^T \cdot \tilde{\delta}_\ell\right)$$

outer product

- Fortunately, modern neural network libraries (pytorch, tensorflow) contain a module "autograd", which computes these (and more complex) derivatives automatically ⇒ you don't have to do these calculations by hand and implement the resulting algorithm
⇒ eliminated big source of bugs ~~and allows for very complex models~~

fundamental insight 3

NEURAL NETWORKS SUPPORT ~~MODELS~~ NON-LINEAR MODELS OF ALMOST ARBITRARY COMPLEXITY, BECAUSE:

- we can construct highly complex architectures by replicating a single basic unit (neuron = linear model plus non-linear activation) in parallel (layers) and in series (deep)
- auto grad allows to compute the gradients needed for training automatically, without additional programming
- modern GPUs make the forward and backward computation sufficiently fast.

Why do neural networks work so well?

- Theoretically not yet understood. NNs have so many parameters that they should overfit terribly (i.e. have small training error, but large generalization error). But this does not happen in practice.
- Theoretical guarantee: universal approximation theorems
  - 1-0 regression: $z_L \in \mathbb{R}$
    2-class classification $z_L = \hat{p}(y_i = 1 | x_i) \in [0,1]$
  Can be shown, that a 2-layer network ($L=2$) can approximate arbitrarily complicated true mappings ($y_i^* = f^*(x_i)$ or $p^*(y_i = 1 | x_i)$)
  If the hidden layer is sufficiently wide ($M_1 \to \infty$) and the weights B_1, B_2 are suitably chosen.
  However, this is a pure existence proof, gives no algorithm to determine M_1, B_1, B_2.
- Finding the globally optimal B_ℓ for any network is NP-hard (i.e. virtually impossible)

fundamental insight 4:

IF THE NETWORK IS SUFFICIENTLY LARGE (WIDE AND DEEP), AND WE HAVE ENOUGH TRAINING DATA, TYPICAL LOCAL OPTIMA TEND TO BE PRETTY GOOD (≙ CLOSE TO THE GLOBAL ONE, I.E. HAVE ~~GOOD~~ LOW GENERALIZATION ERROR).

This is an empirical finding, not yet theoretically understood, why this is the case.

Training tricks

- early stopping: regularly check generalization error during training on an independent validation set. Stop if this error estimate starts to increase (even if the training error would keep decreasing)
- training rate schedule: when training error saturates, decrease training rate $\tau \leftarrow \tau/10$. (repeat 2 or 3 times)
- mini-batch SGD: instead of estimating the loss from a single random instance, as in pure SGD, use the average over a random set of size k ("mini-batch") $k = 32 \ldots 10^4$, as GPU-RAM allows more ?
- ADAM optimizer (and similar relatives): Plain SGD uses uniform learning rate τ for all parameters. ADAM adjusts learning rate for each parameter ⇒ much faster convergence (or divergence, if unlucky).

  Let $g^{(t)} = \frac{\partial \text{loss}^{(t)}}{\partial B^{(t)}}$ the loss derivative in iteration t

  Plain SGD: $B^{(t+1)} = B^{(t)} - \tau\, g^{(t)}$

  ADAM maintains a running average of g and g^2!

$$G^{(t)} = \mu_1 G^{(t-1)} + (1-\mu_1) g^{(t)}$$

$$(G^2)^{(t)} = \mu_2 (G^2)^{(t-1)} + (1-\mu_2) (g^{(t)})^2$$

$(\mu_1 \approx 0.9, \quad \mu_2 \approx 0.999)$

$$\tilde{G}^{(t)} = \frac{G^{(t)}}{1-\mu_1^t} \qquad (\tilde{G^2})^{(t)} = \frac{(G^2)^{(t)}}{1-\mu_2^t}$$

"burn-in phase correction"

$$B^{(t+1)} = B^{(t)} - \tau \frac{\tilde{G}^{(t)}}{\sqrt{(\tilde{G^2})^{(t)}} + \varepsilon} \qquad \varepsilon = 10^{-8}$$

(avoid div-by-zero)

- batch normalization: normalize pre-activations z_l by their mean and std-dev within current mini-batch
  - standard network $z_l = z_{l-1} \cdot B_l \;,\; z_l = \varphi_l(z_l)$
  - batch norm:

$$z'_{l,i} = z_{l-1,i} \cdot B_l \quad \text{for } i \text{ in mini-batch}$$

$$\mu = \frac{1}{k} \sum_i z'_{l,i} \;,\; \sigma = \sqrt{\frac{1}{k} \sum_i (z'_{l,i} - \mu)^2 + \varepsilon}$$

$$z''_{l,i} = \frac{z'_{l,i} - \mu}{\sigma}$$

$$\tilde{z}_{l,i} = a_l \cdot z''_{l,i} + b_l$$

(a_l, b_l: learnable parameters)

$$z_{l,i} = \varphi_l(\tilde{z}_{l,i})$$

often significant improvements of training and generalization errors

- dropout: ~~random~~ deactivate part (e.g. 50%) of the network in every mini-batch:

  sample dropout masks $r_l \in \{0,1\}^{M_l}$ and replace activations $z_{l,i}$ with $z_{l,i} = r_l \cdot \varphi_l(\tilde{z}_{l,i})$

  ⇒ reduces overfitting, because subtle interactions between neurons are made impossible

during prediction, downscale weights B_ℓ by dropout factor (e.g. $B_\ell \leftarrow B_\ell \cdot 0.5$) and predict without dropout (33)

- weight initialization:

$$B_\ell \sim \mathcal{N}\left(0,\ \sigma^2 = \frac{1}{M_{\ell-1}+1}\right) \quad (\text{for } \tanh(\cdot))$$

$$\sim \mathcal{N}\left(0,\ \sigma^2 = \frac{2}{M_{\ell-1}+1}\right) \quad (\text{for } \mathrm{ReLU}(\cdot))$$

$\Rightarrow$ ensures that (expected) norm of the input weights of each neuron (incl. bias weight) is 1.

- piecewise linear activation functions (ReLU, PReLU, Leaky ReLU) tend to work better than δ and tanh, because they do not suffer from vanishing gradients when $\hat{z}_\ell \gg 0$.

- data augmentation: artificially increase training set size by applying random perturbations to the existing instances, e.g.: - mirror or rotate images
  - add slight noise
  - random (affine or non-rigid) morphing

$\Rightarrow$ make ~~training~~ network robust against those perturbations (because y_i^* remains unchanged or is perturbed accordingly)

- except for data augmentation, predefined modules for all these tricks are already available in NN libraries

- weight decay: add regularizer to loss that penalizes very large weights: L_2: $\lambda \sum_\ell \|B_\ell\|_F^2$

L_1: $\lambda \sum_\ell |B_\ell|$ (elementwise abs)

Convolutional Neural Networks

- in many applications, i.e. analysis of audio, images, videos, data are (approximately) translation invariant

human and dog

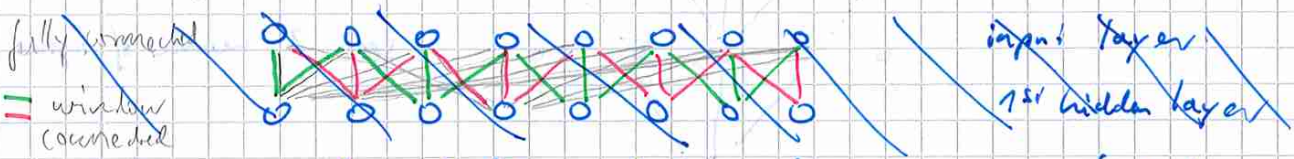
sliding window

~~⇒ important receptive fields should not~~

⇒ • should not only look at image as a whole, but also at every subregion of a certain (or various) size "receptive field"

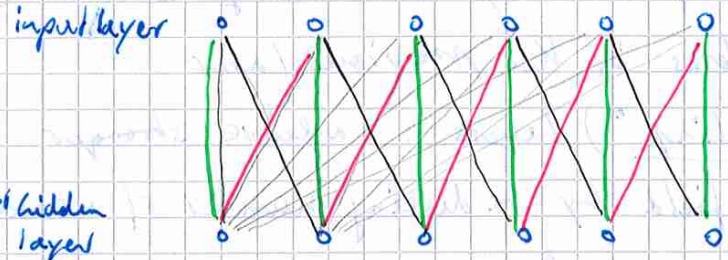
- these receptive fields should cover the entire image in a sliding window fashion

- consequences for network architecture (1D illustration)



– connections to the next layer become sparse (window of attention)

– connections of same color share weight (translation invariance)

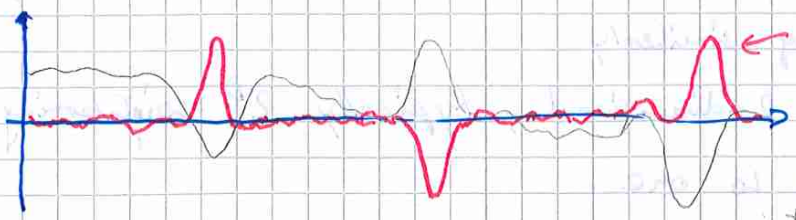


fully connected

= window connected

⇒ We do not need to repeat the redundant network architecture, but instead use a loop to actually move the window around. The weights in a window act as a filter that detect patterns of interest.

Matched filter with weights (+1) (−2) (+1)



← high response if local shape matches filter shape

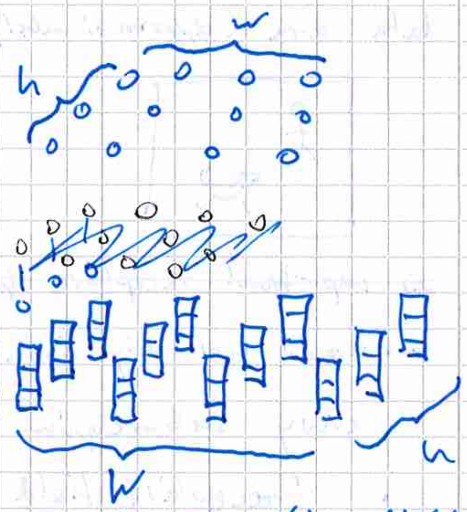
∈

ReLU: set negative response to zero

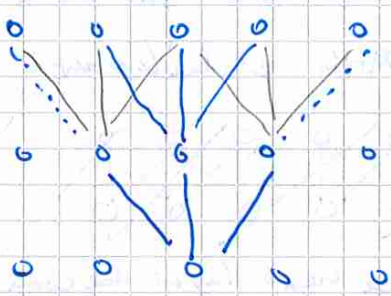
- images contain many different patterns of interest ⇒ run many filters in parallel. The output of each filter forms a <u>channel</u> of the next neuron layer.

  input layer (gray scale image)
  $w \times h$

  1st hidden layer after C filters:
  $C \times w \times h$



- deep networks: stacking layers with small receptive fields yields a larger receptive field



sees 3 neurons of input

sees 3 neurons of first layer
⇒ 5 neurons of input

⇒ complex patterns are formed by combining activation of several simple patterns in the previous layer

- downsampling ("<u>pooling</u>") layers: achieve stronger increase of receptive field by reducing number of neurons (≙ pixels). 1D example

  k^{th} layer values

max-pooling

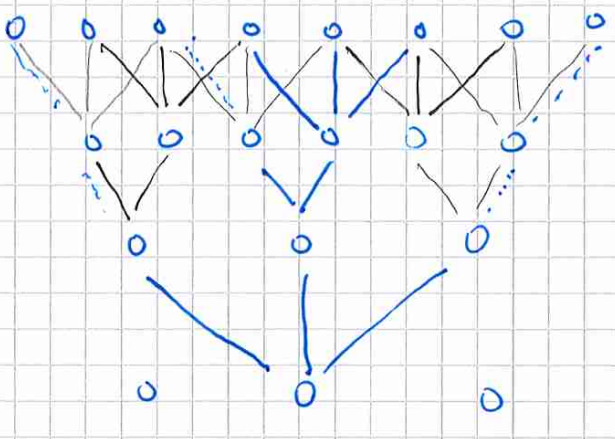
$z_{(k+1),1} = \max(z_{k,1}, z_{k,2})$

$z_{(k+1),2} = \max(z_{k,3}, z_{k,4})$

$z_{(k+1),3} = \max(z_{k,5}, z_{k,6})$

average pooling similarly

- if signal is 0-dimensional, typically 2^0 neighboring neurons elements are reduced to one.



neuron sees 8 neurons in the input layer

- strided convolution has a similar effect: don't move window to the next pixel, but skip one or more ≙ "stride"
  ⇒ downsampling according to how many pixels are skipped

- convolutional layers are specified by window size and number of filters:
  $5 \times 5 \times 8$: 8 filters of size 5×5
  $3 \times 3 \times 32$: 32 — " — 3×3
  $1 \times 1 \times 128$: 128 projections of the input channels (just scalar products of the center pixel)

- show famous networks on slides
  - classification networks (detect objects in image)
    LeNet, AlexNet, GoogLeNet, VGG, ResNet
  - segmentation networks: U-net, fully convolutional networks

- show applications on slides

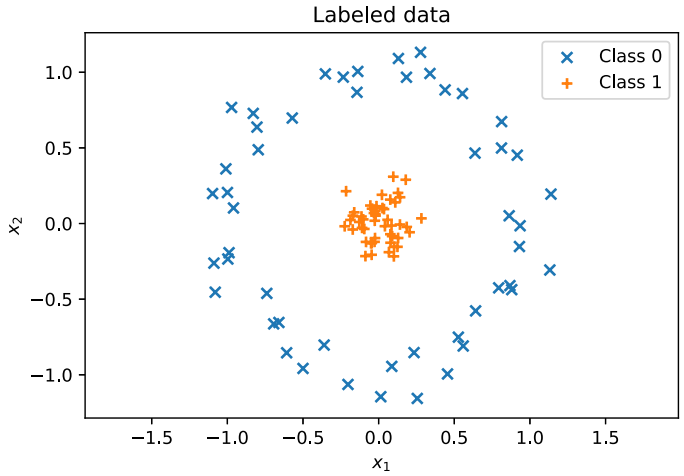
Neural Networks

In [1]:
```
import numpy as np
%config InlineBackend.figure_formats = ['svg']
import matplotlib.pyplot as plt
from sklearn.datasets.samples_generator import make_circles

import torch
from torch.optim import SGD
from torch import nn
```

The data

In [2]:
```
features, labels = make_circles(100, factor=.1, noise=.1)
```

In [3]:
```
def plot_prediction(features, y_true, y_predicted):
    labels = np.unique(y_true)
    for i, (label, marker) in enumerate(zip(labels, "x+*.")):
        class_data = features[y_true == label]
        # Color is given by the predicted label
        colors = [f"C{predicted - labels.min()}" for predicted in y
_predicted[y_true == label]]
        plt.scatter(class_data[:, 0], class_data[:, 1], marker=mark
er, label=f"Class {label}", c=colors)
    plt.legend()
    plt.xlabel("$x_1$")
    plt.ylabel("$x_2$")
    plt.axis("equal")

plt.title("Labeled data")
plot_prediction(features, labels, labels)
x_range = plt.xlim()
y_range = plt.ylim()
```

Interactive training with TensorFlow Playground

A linear classifier (https://playground.tensorflow.org/#activation=relu&batchSize=10&dataset=circle&regDataset=reg-gauss&learningRate=0.03&regularizationRate=0&noise=0&networkShape=&seed=0.97720&showTestData= cannot separate the data.

Can you modify the architecture so that the orange becomes separated from the blue? Check the solution (https://playground.tensorflow.org/#activation=relu&batchSize=10&dataset=circle&regDataset=reg-gauss&learningRate=0.03&regularizationRate=0&noise=0&networkShape=3&seed=0.97720&showTestData

... or start with a fresh TensorFlow Playground (https://playground.tensorflow.org/)

Build it yourself with PyTorch

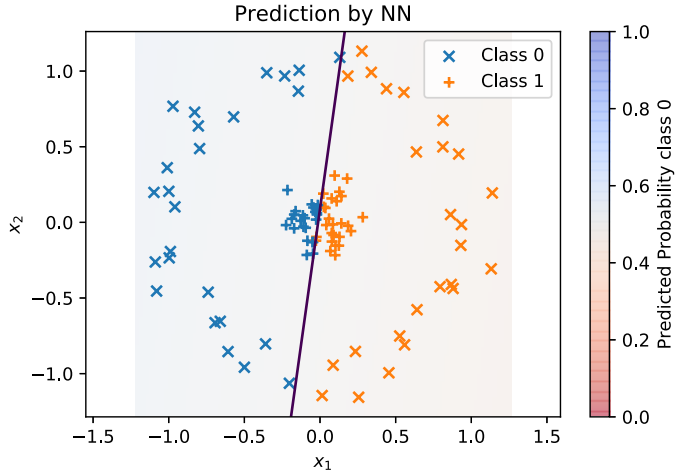
In [4]:
```
def build_model(depth, width):
    models = []

    prev_width = 2
    for d in range(depth):
        # Each layer is a linear transformation and a non-linearity
        models.append(nn.Linear(prev_width, width))
        models.append(nn.ReLU())
        prev_width = width

    # Final layer computes 2d log-softmax
    models.append(nn.Linear(prev_width, 2))
    models.append(nn.LogSoftmax(1))

    return nn.Sequential(*models)

def predict_label(model, x):
    if not torch.is_tensor(x):
        x = torch.tensor(x).float()

    with torch.no_grad():
        y_pred = model(x)
        # This computes the argmax of y_pred
        return y_pred.data.sort(1, True)[1][:, 0]


def train_model(model, x, y, epochs, lr=0.03):
    sgd = SGD(model.parameters(), lr=lr)
    loss = nn.NLLLoss()

    x = torch.tensor(x).float()
    y = torch.tensor(y)

    for epoch in range(epochs):
        sgd.zero_grad()

        # Predict and compute loss
        y_pred = model(x)
        loss_value = loss(y_pred, y)

        # Run gradient computation
        loss_value.backward()
        sgd.step()

        if epoch % 25 == 0:
            hard_pred = predict_label(model, x)
            hard_pred_correct = hard_pred == y
            error = 1 - hard_pred_correct.float().mean().item()
            print(f"Epoch {epoch:3}: Loss {loss_value.item():.2f},
Err {error * 100:.2f}%")
```


In [5]:
```
def plot_prediction_grid(x_range, y_range, model, samples=100):
    x, y = torch.meshgrid(torch.linspace(*x_range, samples), torch.
linspace(*y_range, samples))
    positions = torch.stack((x.reshape(-1), y.reshape(-1)), axis=1)
.reshape(-1, 2)
    prediction = model(positions)[:, 0].exp().detach().reshape(samp
les, samples).numpy()
    plt.imshow(prediction.T, origin="lower", extent=(*x_range, *y_r
ange),
               cmap="coolwarm_r", vmin=0, vmax=1, alpha=0.3)
    plt.colorbar(label="Predicted Probability class 0")
    plt.contour(x, y, prediction.reshape(samples, samples), [0.5])
```

Linear network (no hidden layer)

In [6]:
```
torch.manual_seed(2398)
model = build_model(0, 0)
train_model(model, features, labels, 150, 0.3)

plt.title("Prediction by NN")
plot_prediction(features, labels, predict_label(model, features).nu
mpy())
plot_prediction_grid(x_range, y_range, model)
```

```
Epoch   0: Loss 0.70, Err 70.00%
Epoch  25: Loss 0.69, Err 47.00%
Epoch  50: Loss 0.69, Err 49.00%
Epoch  75: Loss 0.69, Err 48.00%
Epoch 100: Loss 0.69, Err 49.00%
Epoch 125: Loss 0.69, Err 49.00%
```



One hidden layer

In [7]:
```
torch.manual_seed(2398)
model = build_model(1, 5)
train_model(model, features, labels, 150, 1.)

plt.title("Prediction by NN")
plot_prediction(features, labels, predict_label(model, features).nu
mpy())
plot_prediction_grid(x_range, y_range, model)
```

```
Epoch   0: Loss 0.67, Err 38.00%
Epoch  25: Loss 0.38, Err 8.00%
Epoch  50: Loss 0.08, Err 0.00%
Epoch  75: Loss 0.03, Err 0.00%
Epoch 100: Loss 0.02, Err 0.00%
Epoch 125: Loss 0.01, Err 0.00%
```