Mudcard

- **Is there EDA or other exploration that you can do to determine whether the l1 or l2 norms would be more helpful in the error calculation?**
  - Nope, you have to try both and let the validation scores decide which one is more predictive.
- **How about with the various algorithms that have tradeoffs?**
  - Sometimes you can exclude some ML algorithms based on their cons, we will talk about that this week
  - But there is no EDA step that can tell you in advance which ML algo will be the best, you have to try all of them
- **"I am a bit muddle on the connection of this lecture to the last lecture. Is it correct that the methods used in the last lecture are for linear relationships and todays methods are for non linear relationships?**
  - Nope, regularization does not change the model relationships. Linear regression with regularuzation still gives you linear models.
  - Regularization changes the model weights and tends to train less complex models, less prone for overfitting.
- **What is the difference between Lasso and Ridge regularization and how would you know which one is appropriate to use?**
  - You need to use both.
  - There is no way to determine in advance which model will perform best on your dataset so you need to rely on validation scores.
  - Here is a stackexcange entry on the topic.

The supervised ML pipeline

The goal: Use the training data (X and y) to develop a model which can accurately predict the target variable (y_new') for previously unseen data (X_new).

1. Exploratory Data Analysis (EDA): you need to understand your data and verify that it doesn't contain errors

- do as much EDA as you can!

2. Split the data into different sets: most often the sets are train, validation, and test (or holdout)

- practitioners often make errors in this step!
- you can split the data randomly, based on groups, based on time, or any other non-standard way if necessary to answer your ML question

3. Preprocess the data: ML models only work if X and Y are numbers! Some ML models additionally require each feature to have 0 mean and 1 standard deviation (standardized features)

- often the original features you get contain strings (for example a gender feature would contain 'male', 'female', 'non-binary', 'unknown') which needs to transformed into numbers
- often the features are not standardized (e.g., age is between 0 and 100) but it needs to be standardized

4. Choose an evaluation metric: depends on the priorities of the stakeholders

- often requires quite a bit of thinking and ethical considerations

5. Choose one or more ML techniques: it is highly recommended that you try multiple models

- start with simple models like linear or logistic regression
- try also more complex models like nearest neighbors, support vector machines, random forest, etc.

6. Tune the hyperparameters of your ML models (aka cross-validation)

- ML techniques have hyperparameters that you need to optimize to achieve best performance
- for each ML model, decide which parameters to tune and what values to try
- loop through each parameter combination
  - train one model for each parameter combination
  - evaluate how well the model performs on the validation set
- take the parameter combo that gives the best validation score
- evaluate that model on the test set to report how well the model is expected to perform on previously unseen data

7. Interpret your model: black boxes are often not useful

- check if your model uses features that make sense (excellent tool for debugging)

- often model predictions are not enough, you need to be able to explain how the model arrived to a particular prediction (e.g., in health care)

Supervised ML algorithms

By the end of this **week**, you will be able to

- Summarize how decision trees, random forests, and support vector machines work
- Describe how the predictions of these techniques behave in classification and regression
- Describe which hyper-parameters should be tuned

Which ML algorithm to try on your dataset?

- there is no algo that performs well under all conditions! - no free lunch theorem
- you need to try as many as you can to find the one that performs best
- other than predictive power, what else is important for you?
    - how the model behaves with respect to outliers?
    - does the prediction varies smoothly with the feature values?
    - can the model capture non-linear dependencies?
    - is the model easy to interpret for a human?

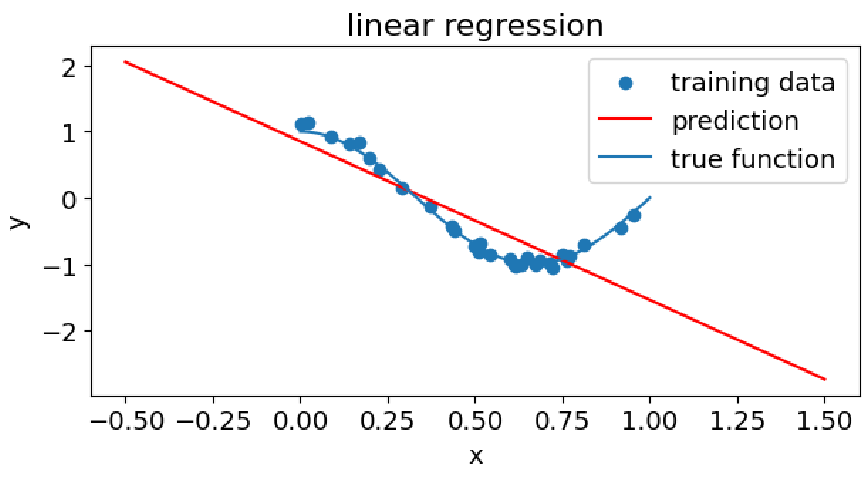
Goal for this week: fill out the table:

ML algo	suitable for large datasets?	behaviour wrt outliers	non-linear?	params to tune	smooth predictions	easy to interpret?
linear regression	yes	tbd	no	l1 and/or l2 reg	yes	yes
logistic regression	yes	tbd	no	l1 and/or l2 reg	yes	yes
random forest regression	tbd	tbd	tbd	tbd	tbd	tbd
random forest classification	tbd	tbd	tbd	tbd	tbd	tbd
SVM rbf regression	tbd	tbd	tbd	tbd	tbd	tbd
SVM rbf classification	tbd	tbd	tbd	tbd	tbd	tbd

Linear regression

In [1]:
```
import numpy as np
from sklearn.linear_model import LinearRegression
np.random.seed(10)
def true_fun(X):
    return np.cos(1.5 * np.pi * X)

n_samples = 30

X = np.random.rand(n_samples)
y = true_fun(X) + np.random.randn(n_samples) * 0.1

X_new = np.linspace(-0.5, 1.5, 2000)

reg = LinearRegression()
reg.fit(X[:, np.newaxis],y)
y_new = reg.predict(X_new[:, np.newaxis])
```

In [2]:
```
import matplotlib.pyplot as plt
import matplotlib
matplotlib.rcParams.update({'font.size': 13})


plt.figure(figsize=(6.4,3.6))
plt.scatter(X,y,label='training data')
plt.plot(X_new,y_new,'r',label='prediction')
plt.plot(np.linspace(0, 1, 100),true_fun(np.linspace(0, 1, 100)),label='true function')
plt.xlabel('x')
plt.ylabel('y')
plt.title('linear regression')
plt.legend()
plt.tight_layout()
plt.savefig('figures/lin_reg.png',dpi=300)
plt.show()
```

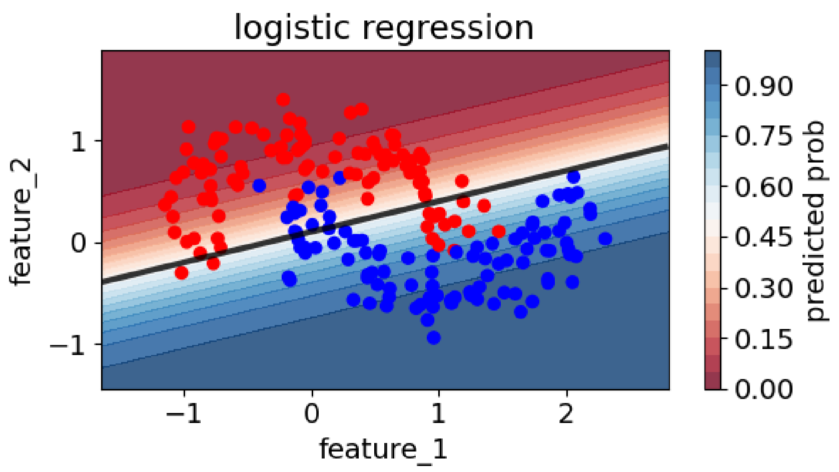


Logistic regression

In [3]:
```
from sklearn.datasets import make_moons
import numpy as np
from sklearn.linear_model import LogisticRegression
# create the data
X,y = make_moons(noise=0.2, random_state=1,n_samples=200)
# set the hyperparameters
clf = LogisticRegression()
# fit the model
clf.fit(X,y)
# predict new data
#y_new = clf.predict(X_new)
# predict probabilities
#y_new = clf.predict_proba(X_new)
```

Out[3]:
```
▾ LogisticRegression
LogisticRegression()
```

In [4]:
```
from matplotlib.colors import ListedColormap
from sklearn.preprocessing import StandardScaler
matplotlib.rcParams.update({'font.size': 14})

h = .02  # step size in the mesh

x_min, x_max = X[:, 0].min() - .5, X[:, 0].max() + .5
y_min, y_max = X[:, 1].min() - .5, X[:, 1].max() + .5
xx, yy = np.meshgrid(np.arange(x_min, x_max, h),
                     np.arange(y_min, y_max, h))

cm_bright = ListedColormap(['#FF0000', '#0000FF'])
cm = plt.cm.RdBu

Z = clf.predict_proba(np.c_[xx.ravel(), yy.ravel()])[:, 1]
# Put the result into a color plot
Z = Z.reshape(xx.shape)
plt.figure(figsize=(6.4,3.6))
plt.contourf(xx, yy, Z, cmap=cm, alpha=.8,vmin=0,vmax=1,levels=np.arange(0,1.05,0.05))
plt.colorbar(label='predicted prob')
plt.contour(xx, yy, Z, alpha=.8,vmin=0,vmax=1,levels=[0.5],colors=['k'],linewidths=3)
plt.scatter(X[:, 0], X[:, 1], c=y,cmap=cm_bright)
plt.xlabel('feature_1')
plt.ylabel('feature_2')
plt.title('logistic regression')
plt.tight_layout()
plt.savefig('figures/logistic_reg.png',dpi=300)
plt.show()
```



ML algo	suitable for large datasets?	behaviour wrt outliers	non-linear?	params to tune	smooth predictions	easy to interpret?
linear regression	yes	linear extrapolation	no	l1 and/or l2 reg	yes	yes
logistic regression	yes	scales with distance from the decision boundary	no	l1 and/or l2 reg	yes	yes
random forest regression	tbd	tbd	tbd	tbd	tbd	tbd
random forest classification	tbd	tbd	tbd	tbd	tbd	tbd
SVM rbf regression	tbd	tbd	tbd	tbd	tbd	tbd
SVM rbf classification	tbd	tbd	tbd	tbd	tbd	tbd

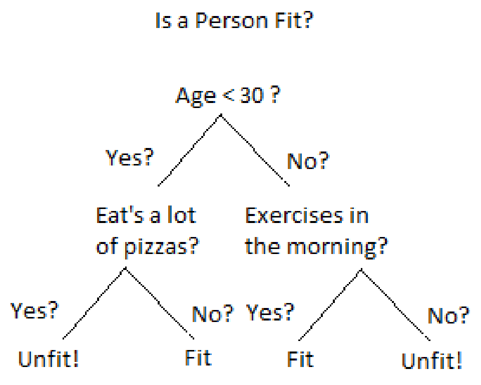
Quiz 1

Calculate the predicted probabilities on X for the logistic regression model and determine what critical probability gives the best f1 score. Round to the second significant digit!

In [5]:
```
# add your code below
```

Decision trees and random forests

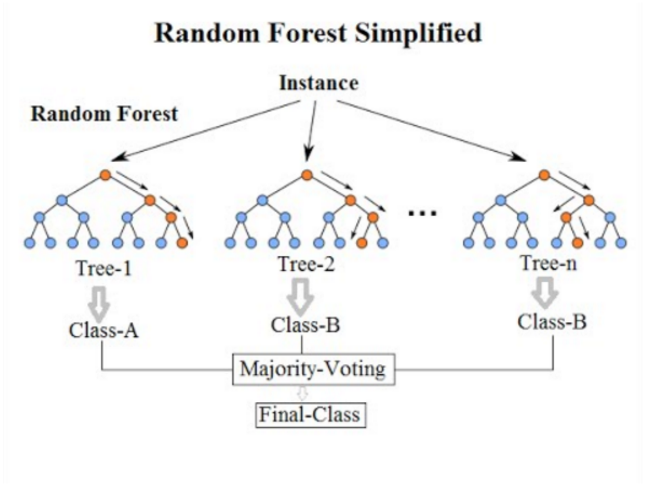
- Decision tree: the data is split according to certain features
- Here is an example tree fitted to data:



- Trees have nodes and leaves.

- The critical values and features in the nodes are determined automatically by minimizing a cost function.

- Random forest: ensemble of random decision trees
- Each tree sees a random subset of the training data, that's why the forest is random.



Quiz 2

- Use the dataset below and create a decision tree with max_depth = 2 to predict the target variable! What is your tree's prediction for each person?
- Remember, your tree does not need to predict everyone perfectly.
- It just needs to get as many people as possible right.

In [6]:
```
# how many features should your team use?
nr_ftrs = np.random.randint(1,4)
# which features should your team use?
ftrs_to_use = np.random.randint(0,6,size=nr_ftrs)
print('use columns with indices', sorted(ftrs_to_use), 'to create your decision tree.')
```

```
use columns with indices [0, 1] to create your decision tree.
```

X	age	gender (M=0, F=1)	is student?	is parent?	uses computer for work?	nr. of hours on c.	Like computer games?
person 0	5	0	1	0	0	0.0	1
person 1	48	1	0	1	0	1.8	1
person 2	62	0	0	1	0	0.2	0
person 3	10	1	1	0	0	2.4	1
person 4	23	1	1	0	1	4.2	0
person 5	36	0	0	0	1	3.1	1
person 6	12	0	1	0	0	3.1	1
person 7	85	0	0	0	1	1.0	0
person 8	33	1	1	1	0	1.5	0
person 9	56	0	0	0	1	0.1	1

Mud card

In [ ]:
```
```