Supervised ML algorithms

By the end of this lecture, 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!
- you need to try a few to find the one that performs best
- but you might be able to exclude some algos in advance
 - large dataset (>1e6 points)
 - more features than points
- · 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 today: fill out this 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	I1 and/or I2 reg	yes	yes
logistic regression	yes	tbd	no	I1 and/or I2 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
        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()
```

<Figure size 640x480 with 1 Axes>

plt.savefig('figures/lin_reg.png',dpi=300)

Logistic regression

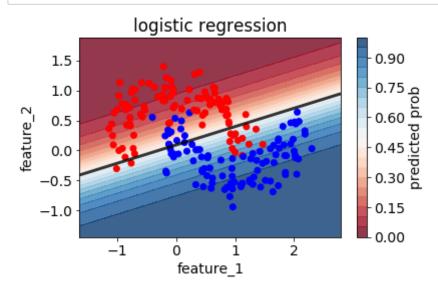
plt.show()

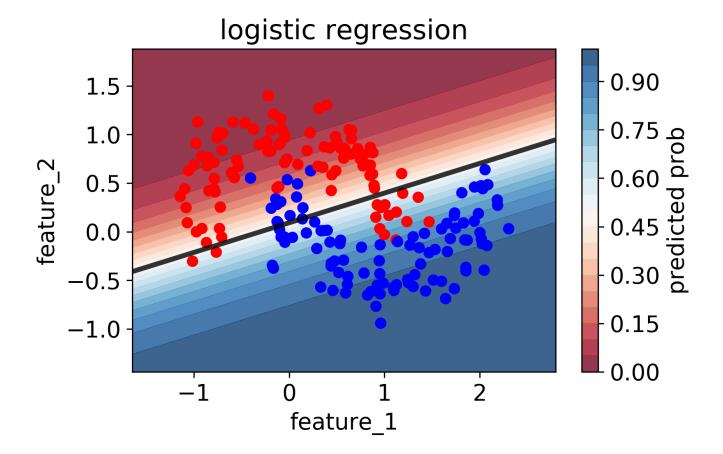
```
In [3]: from sklearn.datasets import make_moons
    import numpy as np
    from sklearn.linear_model import LogisticRegression
    # create the data
    X,y = make_moons(noise=0.2, random_state=1,n_samples=200)
    # set the hyperparameters
    clf = LogisticRegression()
    # fit the model
    clf.fit(X,y)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

/anaconda3/envs/datasci_v0.0.2_local4.yml/lib/python3.6/site-packages/s klearn/linear_model/logistic.py:432: FutureWarning: Default solver will be changed to 'lbfgs' in 0.22. Specify a solver to silence this warnin g.

FutureWarning)

```
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_{x \in X} y \max_{x \in X} = 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.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()
```



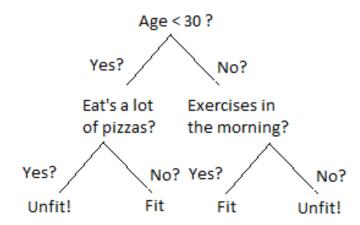


ML algo	suitable for large datasets?	behaviour wrt outliers	non- linear?	params to tune	smooth predictions	easy to interpret?
linear regression	yes	linear extrapolation	no	I1 and/or I2 reg	yes	yes
logistic regression	yes	scales with distance from the decision boundary	no	I1 and/or I2 reg	yes	yes
random 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

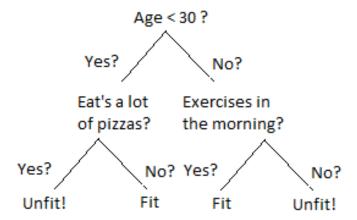
Decision trees and random forests

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

Is a Person Fit?

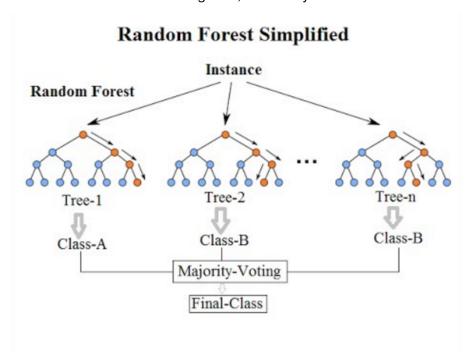


Is a Person Fit?



- · 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.

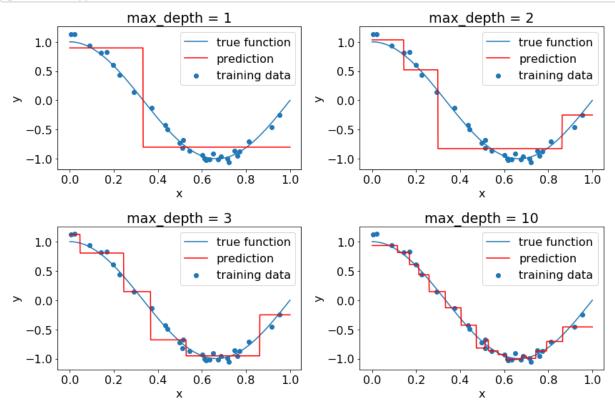


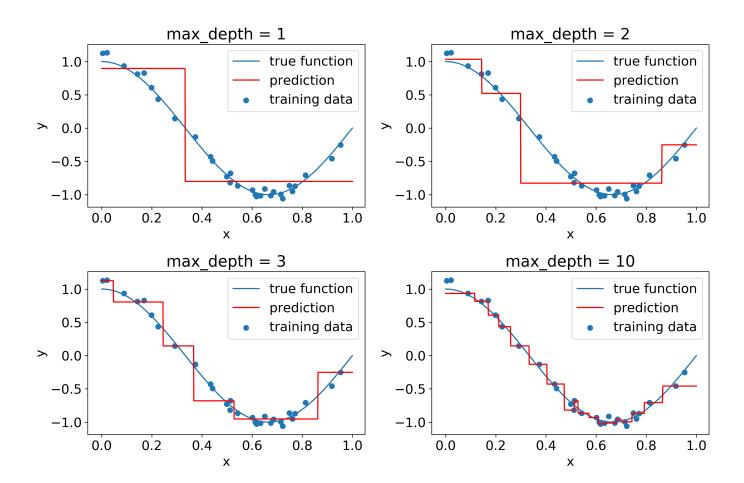
A decision tree in regression

```
In [6]: import matplotlib.pyplot as plt
        import matplotlib
        matplotlib.rcParams.update({'font.size': 16})
        plt.figure(figsize=(12,8))
        plt.subplot(2,2,1)
        plt.scatter(X,y,label='training data')
        plt.plot(np.linspace(0, 1, 100),true_fun(np.linspace(0, 1, 100)),label=
        'true function')
        reg = RandomForestRegressor(n estimators=1, max depth=1)
        reg.fit(X[:, np.newaxis],y)
        y new = reg.predict(X new[:, np.newaxis])
        plt.plot(X_new,y_new,'r',label='prediction')
        plt.xlabel('x')
        plt.ylabel('y')
        plt.title('max depth = 1')
        plt.legend()
        plt.subplot(2,2,2)
        plt.scatter(X,y,label='training data')
        plt.plot(np.linspace(0, 1, 100),true_fun(np.linspace(0, 1, 100)),label=
        'true function')
        reg = RandomForestRegressor(n estimators=1, max depth=2)
        reg.fit(X[:, np.newaxis],y)
        y new = reg.predict(X new[:, np.newaxis])
        plt.plot(X_new,y_new,'r',label='prediction')
        plt.xlabel('x')
        plt.ylabel('y')
        plt.title('max depth = 2')
        plt.legend()
        plt.subplot(2,2,3)
        plt.scatter(X,y,label='training data')
        plt.plot(np.linspace(0, 1, 100), true fun(np.linspace(0, 1, 100)), label=
        'true function')
        reg = RandomForestRegressor(n estimators=1, max depth=3)
        reg.fit(X[:, np.newaxis],y)
        y new = reg.predict(X new[:, np.newaxis])
        plt.plot(X_new,y_new,'r',label='prediction')
        plt.xlabel('x')
        plt.ylabel('y')
        plt.title('max depth = 3')
        plt.legend()
        plt.subplot(2,2,4)
        plt.scatter(X,y,label='training data')
        plt.plot(np.linspace(0, 1, 100), true fun(np.linspace(0, 1, 100)), label=
        'true function')
        reg = RandomForestRegressor(n estimators=1, max depth=10)
        reg.fit(X[:, np.newaxis],y)
        y_new = reg.predict(X_new[:, np.newaxis])
        plt.plot(X new, y new, 'r', label='prediction')
        plt.xlabel('x')
```

```
plt.ylabel('y')
plt.title('max_depth = 10')
plt.legend()

plt.tight_layout()
plt.savefig('figures/tree_reg.png',dpi=300)
plt.show()
```





How to avoid overfitting with random forests?

- tune some (or all) of following hyperparameters:
 - max_depth
 - min_samples_split
- With sklearn random forests, do not tune n_estimators!
 - the larger this value is, the better the forest will be
 - set n_estimators to maybe a 100 while tuning hyperparameters
 - increase it if necessary once the best hyperparameters are found

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	I1 and/or I2 reg	yes	yes
logistic regression	yes	scales with distance from the decision boundary	no	I1 and/or I2 reg	yes	yes
random forest regression	so so	constant	yes	max_features, max_depth	no	so so
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

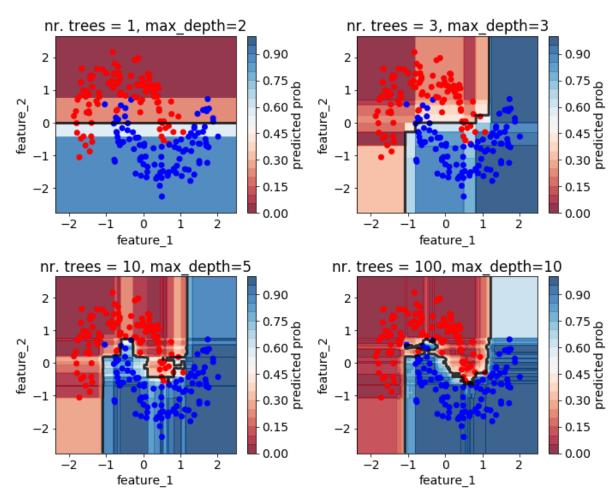
A random forest in classification

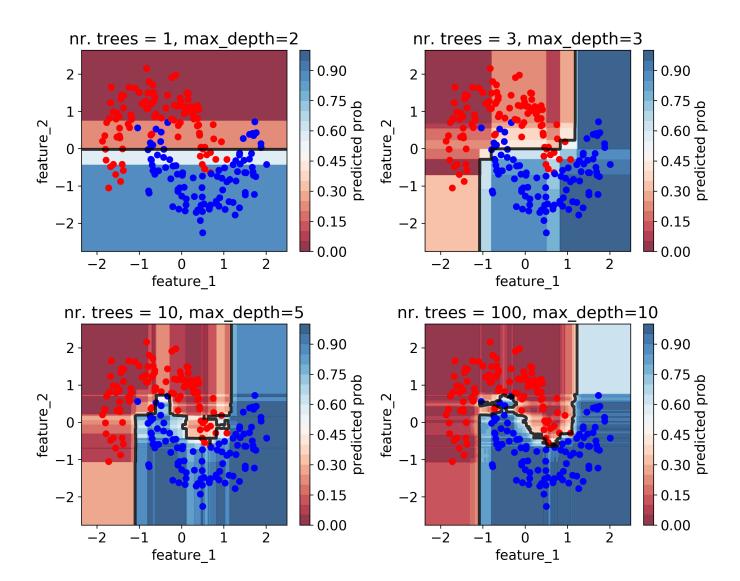
```
In [7]: from sklearn.datasets import make_moons
   import numpy as np
   from sklearn.ensemble import RandomForestClassifier

# create the data
X,y = make_moons(noise=0.2, random_state=1,n_samples=200)
# set the hyperparameters
clf = RandomForestClassifier(n_estimators=1,max_depth=3,random_state=0)
# 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)
```

```
In [8]: from sklearn.datasets import make moons
        import numpy as np
        import matplotlib.pyplot as plt
        import matplotlib
        from matplotlib.colors import ListedColormap
        from sklearn.ensemble import RandomForestClassifier
        from sklearn.preprocessing import StandardScaler
        from sklearn.linear model import LogisticRegression
        matplotlib.rcParams.update({'font.size': 14})
        X = StandardScaler().fit transform(X)
        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))
        plt.figure(figsize=(10,8))
        cm bright = ListedColormap(['#FF0000', '#0000FF'])
        cm = plt.cm.RdBu
        plt.subplot(2,2,1)
        clf = RandomForestClassifier(n_estimators=1, max_depth=2, random_state=1)
        clf.fit(X,y)
        Z = clf.predict proba(np.c_[xx.ravel(), yy.ravel()])[:, 1]
        # Put the result into a color plot
        Z = Z.reshape(xx.shape)
        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('nr. trees = 1, max depth=2')
        plt.subplot(2,2,2)
        clf = RandomForestClassifier(n estimators=3, max depth=3, random state=4)
        clf.fit(X,y)
        Z = clf.predict proba(np.c [xx.ravel(), yy.ravel()])[:, 1]
        # Put the result into a color plot
        Z = Z.reshape(xx.shape)
        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('nr. trees = 3, max depth=3')
```

```
plt.subplot(2,2,3)
clf = RandomForestClassifier(n estimators=10, max depth=5, random state=3)
clf.fit(X,y)
Z = clf.predict proba(np.c [xx.ravel(), yy.ravel()])[:, 1]
# Put the result into a color plot
Z = Z.reshape(xx.shape)
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('nr. trees = 10, max depth=5')
plt.subplot(2,2,4)
clf = RandomForestClassifier(n_estimators=100,max_depth=10,random_state=
3)
clf.fit(X,y)
Z = clf.predict_proba(np.c_[xx.ravel(), yy.ravel()])[:, 1]
# Put the result into a color plot
Z = Z.reshape(xx.shape)
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('nr. trees = 100, max depth=10')
plt.tight_layout()
plt.savefig('figures/forest clf.png',dpi=300)
plt.show()
```





Exercise 1

- 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 predict everyone perfectly.
- It just needs to get as many people as possible right.

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

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	I1 and/or I2 reg	yes	yes
logistic regression	yes	scales with distance from the decision boundary	no	l1 and/or l2 reg	yes	yes
random forest regression	so so	constant	yes	max_features, max_depth	no	so so
random forest classification	so so	step-like, difficult to tell	yes	max_features, max_depth	no	SO SO
SVM rbf regression	tbd	tbd	tbd	tbd	tbd	tbd
SVM rbf classification	tbd	tbd	tbd	tbd	tbd	tbd

Support Vector Machine

- very versatile technique, it comes in lots of flavors/types, read moree about it here (https://scikit-learn.org/stable/modules/svm.html)
- · SVM classifier motivation
 - points in n dimensional space with class 0 and 1
 - we want to find the (n-1) dimensional hyperplane that best separates the points
 - this hyperplane is our (linear) decision boundary
- · we cover SVMs with radial basis functions (rbf)
 - we apply a kernel function (a non-linear transformation) to the data points
 - the kernel function basically "smears" the points
 - gaussian rbf kernel: $\exp(-\gamma(|x-x'|)^2)$ where $\gamma > 0$

SVR

```
In [9]: import numpy as np
    from sklearn.svm import SVR
    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

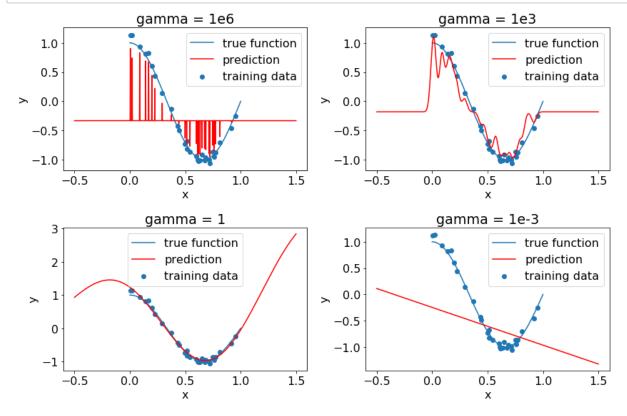
        X_new = np.linspace(-0.5, 1.5, 2000)

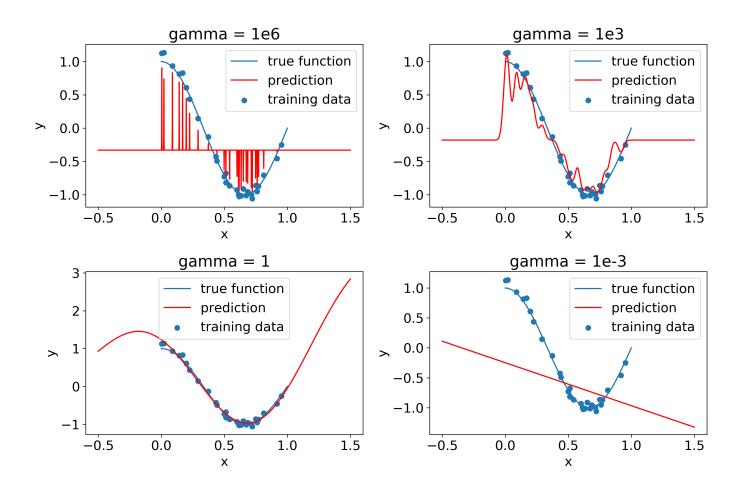
        reg = SVR(gamma = 1, C = 1)
        reg.fit(X[:, np.newaxis],y)
        y_new = reg.predict(X_new[:, np.newaxis])
```

```
In [10]:
         import matplotlib.pyplot as plt
         import matplotlib
         matplotlib.rcParams.update({'font.size': 16})
         plt.figure(figsize=(12,8))
         plt.subplot(2,2,1)
         plt.scatter(X,y,label='training data')
         plt.plot(np.linspace(0, 1, 100),true_fun(np.linspace(0, 1, 100)),label=
         'true function')
         reg = SVR(gamma = 1000000, C = 100)
         reg.fit(X[:, np.newaxis],y)
         y new = reg.predict(X new[:, np.newaxis])
         plt.plot(X_new,y_new,'r',label='prediction')
         plt.xlabel('x')
         plt.ylabel('y')
         plt.title('gamma = 1e6')
         plt.legend()
         plt.subplot(2,2,2)
         plt.scatter(X,y,label='training data')
         plt.plot(np.linspace(0, 1, 100),true_fun(np.linspace(0, 1, 100)),label=
         'true function')
         reg = SVR(gamma = 1000, C = 100)
         reg.fit(X[:, np.newaxis],y)
         y new = reg.predict(X new[:, np.newaxis])
         plt.plot(X_new,y_new,'r',label='prediction')
         plt.xlabel('x')
         plt.ylabel('y')
         plt.title('gamma = 1e3')
         plt.legend()
         plt.subplot(2,2,3)
         plt.scatter(X,y,label='training data')
         plt.plot(np.linspace(0, 1, 100), true fun(np.linspace(0, 1, 100)), label=
         'true function')
         reg = SVR(gamma = 1, C = 100)
         reg.fit(X[:, np.newaxis],y)
         y new = reg.predict(X new[:, np.newaxis])
         plt.plot(X_new,y_new,'r',label='prediction')
         plt.xlabel('x')
         plt.ylabel('y')
         plt.title('gamma = 1')
         plt.legend()
         plt.subplot(2,2,4)
         plt.scatter(X,y,label='training data')
         plt.plot(np.linspace(0, 1, 100), true fun(np.linspace(0, 1, 100)), label=
          'true function')
         reg = SVR(gamma = 0.001, C = 100)
         reg.fit(X[:, np.newaxis],y)
         y_new = reg.predict(X_new[:, np.newaxis])
         plt.plot(X new, y new, 'r', label='prediction')
         plt.xlabel('x')
```

```
plt.ylabel('y')
plt.title('gamma = 1e-3')
plt.legend()

plt.tight_layout()
plt.savefig('figures/SVM_reg.png',dpi=300)
plt.show()
```



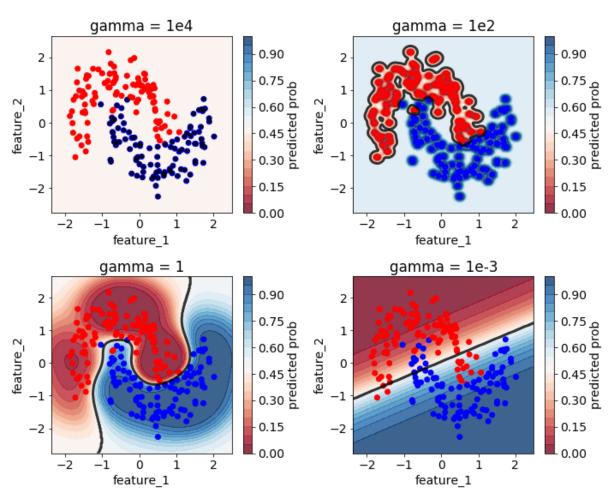


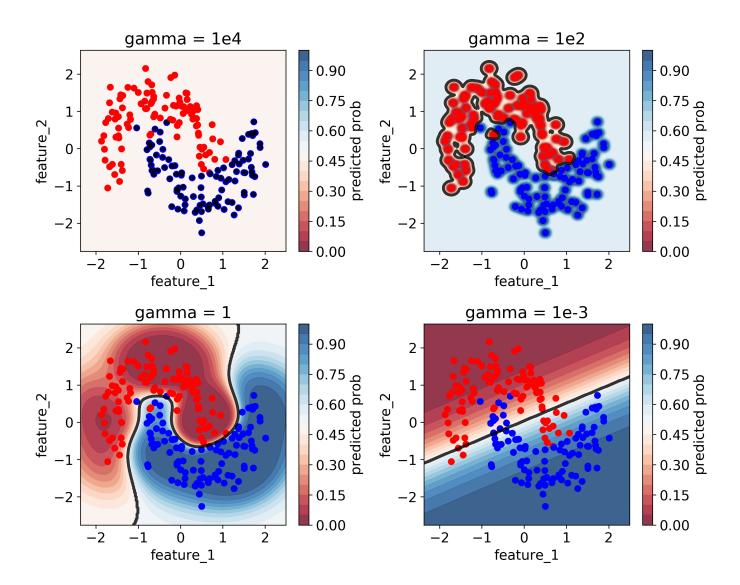
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logistic regression	yes	scales with distance from the decision boundary	no	I1 and/or I2 reg	yes	yes
random forest regression	so so	constant	yes	max_features, max_depth	no	so so
random forest classification	so so	step-like, difficult to tell	yes	max_features, max_depth	no	so so
SVM rbf regression	no	non-linear extrapolation	yes	C, gamma	yes	SO SO
SVM rbf classification	tbd	tbd	tbd	tbd	tbd	tbd

SVC

```
In [12]: from sklearn.datasets import make moons
         import numpy as np
         import matplotlib.pyplot as plt
         import matplotlib
         from matplotlib.colors import ListedColormap
         from sklearn.svm import SVC
         from sklearn.preprocessing import StandardScaler
         matplotlib.rcParams.update({'font.size': 14})
         X = StandardScaler().fit transform(X)
         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))
         plt.figure(figsize=(10,8))
         cm bright = ListedColormap(['#FF0000', '#0000FF'])
         cm = plt.cm.RdBu
         plt.subplot(2,2,1)
         clf = SVC(gamma = 1e4, C = 100, probability=True)
         clf.fit(X,y)
         Z = clf.predict proba(np.c [xx.ravel(), yy.ravel()])[:, 1]
         # Put the result into a color plot
         Z = Z.reshape(xx.shape)
         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('gamma = 1e4')
         plt.subplot(2,2,2)
         clf = SVC(gamma = 1e2, C = 100, probability=True)
         clf.fit(X,y)
         Z = clf.predict proba(np.c [xx.ravel(), yy.ravel()])[:, 1]
         # Put the result into a color plot
         Z = Z.reshape(xx.shape)
         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('gamma = 1e2')
         plt.subplot(2,2,3)
```

```
clf = SVC(gamma = 1e0, C = 100, probability=True)
clf.fit(X,y)
Z = clf.predict_proba(np.c_[xx.ravel(), yy.ravel()])[:, 1]
# Put the result into a color plot
Z = Z.reshape(xx.shape)
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('gamma = 1')
plt.subplot(2,2,4)
clf = SVC(gamma = 1e-3, C = 100, probability=True)
clf.fit(X,y)
Z = clf.predict_proba(np.c_[xx.ravel(), yy.ravel()])[:, 1]
# Put the result into a color plot
Z = Z.reshape(xx.shape)
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('gamma = 1e-3')
plt.tight layout()
plt.savefig('figures/SVM clf.png',dpi=300)
plt.show()
```





Exercise 2

Identify high bias and high variance models!

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	I1 and/or I2 reg	yes	yes
logistic regression	yes	scales with distance from the decision boundary	no	I1 and/or I2 reg	yes	yes
random forest regression	so so	constant	yes	max_features, max_depth	no	so so
random forest classification	so so	step-like, difficult to tell	yes	max_features, max_depth	no	so so
SVM rbf regression	no	non-linear extrapolation	yes	C, gamma	yes	so so
SVM rbf classification	no	50-50	yes	C, gamma	yes	SO SO