Lab 4: Support Vector Machines

In this lab you will:

- train a support vector machine (SVM) for classification, on synthetic and real data;
- observe that SVMs are sensitive to the relative scale of input features;
- compute the "accuracy" of an SVM on held-out test data.

Run the code cell below to import the required packages.

In [1]:

1. Fitting an SVM to synthetic data

Exercises 1.1–1.7 ask you to apply scikit-learn's support vector classifier (sklearn.svm.SVC (https://scikit-learn.svm.SVC (https://scikit-learn.svm.svc.html (https://scikit-learn.svm.svc.html (https://scikit-learn.svm.svc.html (https://scikit-learn.svm.svc.html (https://scikit-learn.svm.svc.html (https://scikit-learn.svc.html (https://scikit-learn.svc.html (https://sci

The SVC object is a binary classifier, so it is used much the same way as sklearn.linear_model.LogisticRegression (https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html). The goal of Exercise 1 is to connect mathematical concepts from lecture to the SVC object's basic parameters (C, kernel, gamma, degree, coef0) and attributes (support_, supportvectors, dualcoef, nsupport).

Exercise 1.1 — Build the 1D training data from lecture

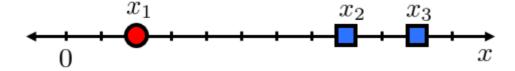
Read the documentation for the SVC fit (https://scikit-

<u>learn.org/stable/modules/generated/sklearn.svm.SVC.html#sklearn.svm.SVC.fit)</u> method, specifically arguments X (the training features) and y (the training targets). In lecture we called the targets t_i (like the Bishop book) rather than y_i (scikit-learn) so we'll continue using t_i below.

You are asked to build the small training set shown below (same as from lecture). Each pair (x_i,t_i) comprises an *feature* input $x_i\in\mathbb{R}$ and a corresponding *class label* target $t_i\in\{-1,+1\}$:

$$\mathcal{D} = \{(2, -1), (8, +1), (10, +1)\}$$

This training set can be depicted as below, where red indicates negative class and blue indicates positive class:



Write a few lines of code to define a variable X that refers to a 3×1 matrix of features (dtype *float64*), and a variable t that refers to a length-3 array of targets (dtype int32). The features and targets should correspond to \mathcal{D} above.

In [2]:

```
X = np.array([2, 8, 10],dtype=np.float64).reshape(3,1)
t = np.array([-1, +1, +1],dtype=np.int32)
```

Check your answer by running the code cell below.

In [3]:

```
assert 'X' in globals(), "No X variable!"
assert 't' in globals(), "No t variable!"
assert isinstance(X, np.ndarray)
assert isinstance(t, np.ndarray)
assert X.shape == (3, 1)
assert t.shape == (3,)
assert X.dtype == np.float64
assert t.dtype in (np.int32, np.int64)
assert np.array_equal(X.ravel()[[-1,0,-2]], [10,2,8]), "Hmm features look wrong"
assert np.array_equal(t.ravel()[[-1,0,-2]], [1,-1,1]), "Hmm targets look wrong"
print("Correct!")
```

Correct!

Exercise 1.2 — Train an SVM on the 1D data and inspect the support vectors

Read the first few lines of documentation for sklearn.svm.SVC (https://scikit-learn.org/stable/modules/generated/sklearn.svm.SVC. It least create an SVC object. You only have to worry about the kernel parameter for now, not the rest. You are asked to create an SVC object that uses a linear kernel and fit it to training data.

Write a few line of code to create a variable called *svm* that refers to a new *SVC* object. Fit the SVM to the training data from Exercise 1.1.

```
In [4]:
svm = sklearn.svm.SVC(kernel='linear').fit(X, t)
```

Check your answer by running the code cell below.

```
In [5]:
```

```
assert 'svm' in globals(), "No variable called 'svm' was found!"
assert isinstance(svm, sklearn.svm.SVC), "Expected svm to be an SVC instance!"
assert svm.kernel == 'linear', "Expected linear kernel!"
assert svm.fit_status_ == 0, "Forgot to train the SVM!"
assert hasattr(svm, 'dual_coef_'), "Forgot to train the SVM!"
assert np.array_equal(X[svm.support_], [[2.], [8.]]), "Hmm the support vectors don't lo ok right!"
print("Looks good!")
```

Looks good!

Inspect the SVM parameters by running the code cell below. How do they compare to the values from lecture?

```
In [6]:
```

```
print("Support vector indices:")
print(svm.support_)

print("Support vectors:")
print(svm.support_vectors_)

print()
print("Dual coefficients (t_i * alpha_i) for the support vectors:")
print(svm.dual_coef_)

Support vector indices:
[0 1]

Support vectors:
[[2.]
[8.]]

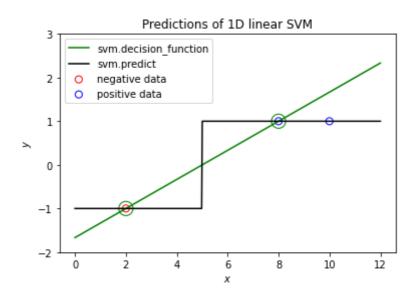
Dual coefficients (t_i * alpha_i) for the support vectors:
[[-0.05555556 0.05555556]]
```

Exercise 1.3 — Plot the decision function and class predictions

Here you are asked to plot the SVM "decision function" y(x) and the SVM classification sign(y(x)). These are provided by the SVC decision function (https://scikit-

<u>learn.org/stable/modules/generated/sklearn.svm.SVC.html#sklearn.svm.SVC.decision_function)</u> and <u>predict (https://scikit-</u>

<u>learn.org/stable/modules/generated/sklearn.svm.SVC.html#sklearn.svm.SVC.predict)</u> methods respectively. Evaluate both across the range $x \in [0, 12]$. Your final plot should look like this:

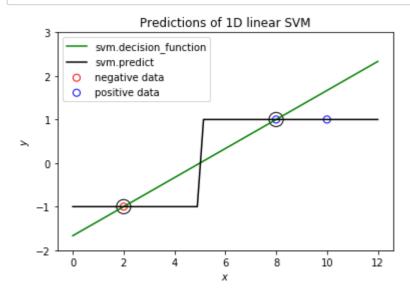


Write code to generate the plot above, using np.linspace

(https://numpy.org/devdocs/reference/generated/numpy.linspace.html) to create a vector of values spanning the range [0,12]. To highlight the support vectors, use the support attribute of your SVC object. Your code should be completely vectorized, with no for-loops.

In [7]:

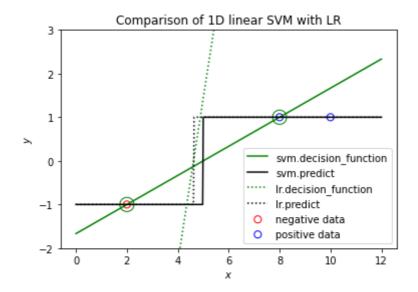
```
def plot toy 1d data(X, t, title, support=None): # You can use this function throughou
t the Lab
    Plots 1-dimensional data X with targets t.
    If 'support' is given, it specifies the indices of data points in X that
    are the support vectors of an SVM. Those points will be circled to highlight them.
    plt.scatter(X[t==-1], t[t==-1], s=50, edgecolors='r', facecolors='none', label='neg
ative data')
    plt.scatter(X[t==+1], t[t==+1], s=50, edgecolors='b', facecolors='none', label='pos
itive data')
    if support is not None:
        plt.scatter(X[support], t[support], s=200, edgecolors='g', facecolors='none')
    plt.xlabel('$x$')
    plt.ylabel('$y$')
    plt.ylim(-2, 3)
    plt.title(title)
    plt.legend()
plt.plot(np.linspace(0, 12).reshape(-1, 1), (svm.coef_)*np.linspace(0, 12).reshape(-1,
1) + svm.intercept_, 'green')
plt.plot(np.linspace(0, 12).reshape(-1, 1), svm.predict(np.linspace(0, 12).reshape(-1,
1)), 'black')
plot_toy_1d_data(X, t, 'Predictions of 1D linear SVM')
plt.scatter(svm.support_vectors_[0], svm.classes_[0],s=200, linewidth=1, facecolors='no
ne',edgecolors='black')
plt.scatter(svm.support vectors [1], svm.classes [1],s=200, linewidth=1, facecolors='no
ne',edgecolors='black')
plt.legend(['svm.decision_function','svm.predict','negative data','positive data'])
plt.show()
```



Exercise 1.4 — Compare SVM to Logistic Regression

A 1-dimensional logistic regression classifier predicts class probabilities using the form $\sigma(w_1x+w_0)$. The quantity $\hat{y}(x)=w_1x+w_0$ used as input to the sigmoid is the classifier's "decision function," and it plays the same role as the decision function of an SVM: the actual class prediction for x can be written $\mathrm{sign}(\hat{y}(x))\in\{-1,+1\}$.

Here you are asked to train a sklearn.linear_model.LogisticRegression (https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html) object on the same data, and compare is decision function and predictions to that of the SVM. You should end up with the following plot:



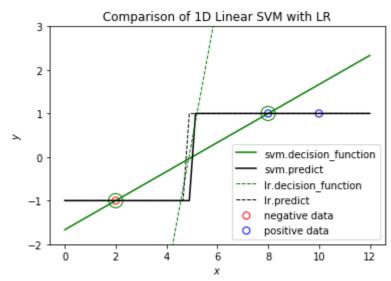
Write code to train a *LogisticRegression* object with no regularization (*penalty='none'*). Then write code to plot the result of the **decision function** (https://scikit-

<u>learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html#sklearn.linear_model.add</u>

<u>learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html#sklearn.linear_model.togisticRegression.html#sklear.html#sklear.html#sklear</u>

In [8]:

```
lr = sklearn.linear model.LogisticRegression(C = 1e10)
lr.fit(X, t)
plt.plot(np.linspace(0, 12).reshape(-1, 1), (svm.coef_)*np.linspace(0, 12).reshape(-1,
1) + svm.intercept , 'green')
plt.plot(np.linspace(0, 12).reshape(-1, 1), svm.predict(np.linspace(0, 12).reshape(-1,
1)), 'black')
plt.plot(np.linspace(0, 12).reshape(-1, 1),(lr.coef_)*np.linspace(0, 12).reshape(-1, 1)
+ lr.intercept_,'--g', linewidth=1)
plt.plot(np.linspace(0, 12).reshape(-1, 1),lr.predict(np.linspace(0, 12).reshape(-1, 1
)),'--k', linewidth=1)
plot_toy_1d_data(X, t, 'Comparison of 1D Linear SVM with LR')
plt.scatter(svm.support_vectors_[0], svm.classes_[0],s=200, linewidth=1, facecolors='no
ne',edgecolors='green')
plt.scatter(svm.support_vectors_[1], svm.classes_[1],s=200, linewidth=1, facecolors='no
ne',edgecolors='green')
plt.legend(['svm.decision_function','svm.predict','lr.decision_function',
            'lr.predict','negative data','positive data'])
plt.show()
```



For fun, you can see an animation of logistic regression "training" if you use *LogisticRegression* object's *max_iter* parameter to stop training early and plot the resulting decision function. To do this, re-run your code cell with *max_iter=4*, then with *max_iter=5*, and so on. (Don't worry about the *ConvergenceWarning* — everything is fine!)

Exercise 1.4 — Build a non-separable 1D data set

Update your X matrix and t vector to include a new $4^{\rm th}$ point $(x_4,t_4)=(11,-1)$. This will make the data non-separable in one dimension.

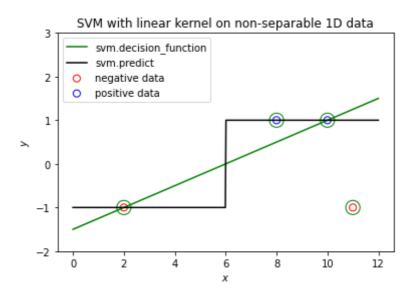
Write code to define new *X* and *t* variables with the same data as Exercise 1.1 but this time with the 4th data point. Easy!

In [9]:

```
X = np.array([2, 8, 10, 11],dtype=np.float64).reshape(4,1)
t = np.array([-1, +1, +1, -1],dtype=np.int32)
```

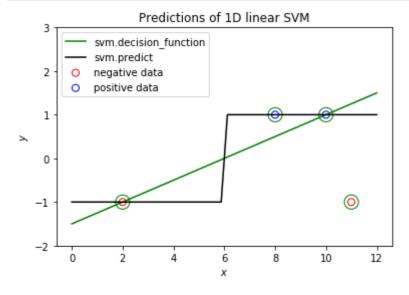
Exercise 1.5 — Fit a linear SVM to the non-separable data

Write code to fit an *SVC* object with linear kernel to this new data and plot the decision function just as before. You should get the plot below. What changed in terms of the decision function and decision boundary? What changed in terms of the support vectors?



In [10]:

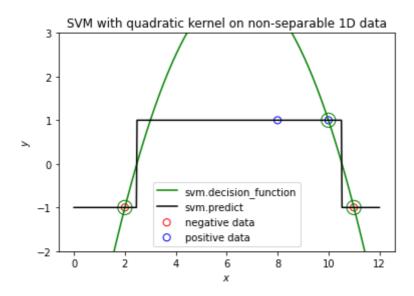
```
svm = sklearn.svm.SVC(kernel='linear').fit(X, t)
c = svm.predict(X)
plt.plot(np.linspace(0, 12).reshape(-1, 1), (svm.coef_)*np.linspace(0, 12).reshape(-1,
1) + svm.intercept_, 'green')
plt.plot(np.linspace(0, 12).reshape(-1, 1), svm.predict(np.linspace(0, 12).reshape(-1,
1)),'black')
plot_toy_ld_data(X, t, 'Predictions of 1D linear SVM')
plt.scatter(X, t,s=200,linewidth=1, facecolors='none',edgecolors='green')
plt.legend(['svm.decision_function','svm.predict','negative data','positive data'])
plt.show()
```



Exercise 1.6 — Fit a polynomial SVM to the non-separable data

Repeat Exercise 1.5 using an *SVC* object with a "polynomial kernel", which in one dimension is $k(x,x')=(xx'+c)^d$.

See the sklearn.svm.SVC (https://scikit-learn.org/stable/modules/generated/sklearn.svm.SVC.html) documentation for how to specify the kernel and related parameters. Use polynomial degree d=2 and try different coefficients for the constant different c such as $\{0,0.1,1,2,3\}$ until you get a plot similar to the one below. Note that these parameters are called degree and coef0 on the SVC object. (Scikit-learn's polynomial kernel also has a gamma scaling factor; just set gamma=1 for this exercise.)



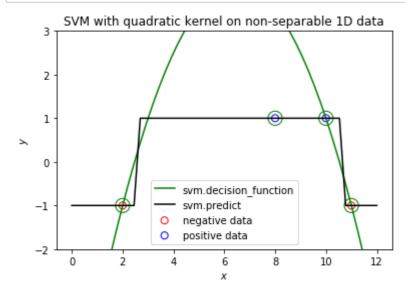
Ask yourself:

- Would this fit be possible if we tried to fit a regular polynomial to this data, rather than an SVM?
- Does the first decision threshold seem like its maximizing the margin in the original 1-dimensional feature space?

In [11]:

```
coef0 = [0,0.1,1,2,3]
svm = sklearn.svm.SVC(kernel='poly',degree=2, coef0=coef0[4]).fit(X, t)

plt.plot(np.linspace(0, 12).reshape(-1, 1), svm.decision_function(np.linspace(0, 12).reshape(-1, 1)), 'green')
plt.plot(np.linspace(0, 12).reshape(-1, 1), svm.predict(np.linspace(0, 12).reshape(-1, 1)),'black')
plot_toy_1d_data(X, t, 'SVM with quadratic kernel on non-separable 1D data')
plt.scatter(X, svm.predict(X),s=200,linewidth=1, facecolors='none',edgecolors='green')
plt.legend(['svm.decision_function','svm.predict','negative data','positive data'])
plt.show()
# Your training code here. Aim for 1-2 lines.
# Your prediction and plotting code here. Aim for 3-5 lines.
```



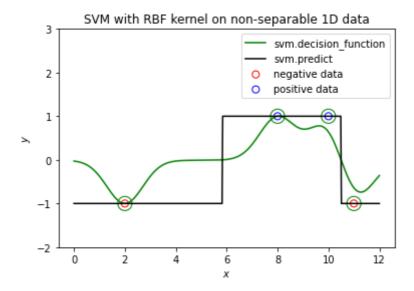
Try setting coefficient c=0 and degree d=4 (or higher) and re-run your code cell above. Notice how the training time suddenly gets noticeably longer, despite the ridiculously small training set and state-of-the-art SVM implementation (LIBSVM). In real-life, wildly varying training times can be a big problem with SVMs.

Exercise 1.7 — Fit an RBF SVM (Gaussian kernel) to the non-separable data

Repeat Exercise 1.5 using an SVC object with a "radial basis function (RBF) kernel," which in one dimension is $k(x,x')=\exp\left(-\gamma|x-x'|^2\right)$ where γ is the 'spread' coefficient.

See the <u>sklearn.svm.SVC (https://scikit-learn.org/stable/modules/generated/sklearn.svm.SVC.html)</u> documentation for how to specify the RBF kernel, and see the SVM lecture slides on "Gaussian kernel" for description of how it is influenced by the *gamma* (γ) coefficient. The *degree* and *coef0* parameters are not used for RBF kernels.

Use $\gamma = 1$ to get a plot similar to the one below.

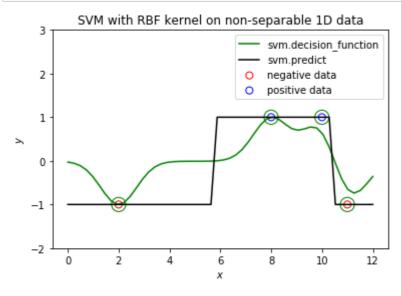


In [12]:

```
svm = sklearn.svm.SVC(kernel='rbf',gamma=1).fit(X, t)

plt.plot(np.linspace(0, 12).reshape(-1, 1), svm.decision_function(np.linspace(0, 12).reshape(-1, 1)), 'green')
plt.plot(np.linspace(0, 12).reshape(-1, 1), svm.predict(np.linspace(0, 12).reshape(-1, 1)), 'black')
plot_toy_1d_data(X, t, 'SVM with RBF kernel on non-separable 1D data')
plt.scatter(X, svm.predict(X),s=200,linewidth=1, facecolors='none',edgecolors='green')
plt.legend(['svm.decision_function','svm.predict','negative data','positive data'])
plt.show()
# Your training code here. Aim for 1-2 lines.

# Your prediction and plotting code here. Aim for 3-5 lines.
```



Modify the spread coefficient to be a large value like $\gamma=10$ and re-run your code cell above. What happens to the decision function? Does anything happen to the actual decision boundary? What happens to the rightmost decision threshold when you make $\gamma=0.1$, and why?

2. Loading real data and fitting an SVM to it

Exercises 2.1–2.3 ask you to load a real data set, train an SVM on it, and make predictions on new test data.

Run the code cell below to define some utility functions you will need.

In [13]:

```
def get_data_extent(X):
    Given an Nx2 matrix X, returns a good range of values for plotting
    the data, in the form (x1min, x1max, x2min, x2max).
    dilation = 1.2
    x1min, x2min = X.min(axis=0)
    x1max, x2max = X.max(axis=0)
    x1mid = (x1max + x1min)/2
    x2mid = (x2max + x2min)/2
    x1min = x1mid - (x1mid - x1min)*dilation
    x1max = x1mid + (x1max - x1mid)*dilation
    x2min = x2mid - (x2mid - x2min)*dilation
    x2max = x2mid + (x2max - x2mid)*dilation
    return (x1min, x1max, x2min, x2max)
def plot_2d_decision_function(model, extent):
    Plots the decision function of a model as a red-blue heatmap.
    The region evaluated, along with x and y axis limits, are determined by 'extent'.
    x1min, x1max, x2min, x2max = extent
    x1, x2 = np.meshgrid(np.linspace(x1min, x1max, 200),
                         np.linspace(x2min, x2max, 200))
    X = np.column_stack([x1.ravel(), x2.ravel()])
    y = model.decision_function(X).reshape(x1.shape)
    plt.imshow(-y, extent=extent, origin='lower', vmin=-1, vmax=1, cmap='bwr', alpha=0.
5)
    plt.contour(x1, x2, y, levels=[0], colors='k') # Decision boundary
    plt.xlim([x1min, x1max])
    plt.ylim([x2min, x2max])
    plt.gca().set_aspect('auto')
```

Exercise 2.1 — Load data from a CSV file and plot it

CSV files contain comma-separated data, sometimes with a header line to hint at what the numbers mean. In this exercise you'll be loading <u>data_train.csv</u> (<u>data_train.csv</u>), a file accompanying this lab. Here's a preview of its contents:

```
mean_texture,mean_compactness,label
19.59,0.08,0
17.88,0.16,1
17.60,0.17,1
10.91,0.05,0
13.16,0.09,0
...
```

The first two comman-separated columns are features. They encode characteristics of cell nuclei in breast cancer samples. The labels are binary: 0 for benign, 1 for malignant.

Write a few lines of code to:

- 1. load this CSV file from disk into a single array,
- 2. split the columns into feature matrix X and target vector t, and
- 3. rescale the targets t from $\{0,1\}$ to integers $\{-1,+1\}$.

Use the np.loadtxt (https://numpy.org/devdocs/reference/generated/numpy.loadtxt.html) function to load the data for you. Use the delimiter parameter to tell Numpy how to separate each line (by comma) and use the skiprows argument to tell Numpy to skip the header line that contains the feature names (since the header line contains text, not numbers). Use the ndarray astype

(<u>https://numpy.org/devdocs/reference/generated/numpy.ndarray.astype.html</u>) method to convert the targets from type *np.float64* to type *np.int32*, since they are integer labels.

In [14]:

```
from numpy import genfromtxt
my_data = genfromtxt('data_train.csv', delimiter=',',skip_header=1)
X = my_data[:,0:2]
t = my_data[:,2]
t = np.interp(t, (t.min(), t.max()), (-1, +1)).astype(np.int32)
```

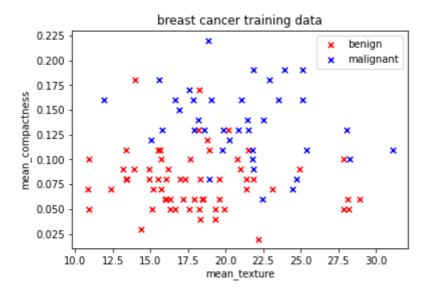
Check your answer by running the code cell below.

In [15]:

```
assert 'X' in globals(), "No X variable!"
assert 't' in globals(), "No t variable!"
assert isinstance(X, np.ndarray)
assert isinstance(t, np.ndarray)
assert X.shape == (100,2), "X was wrong shape!"
assert X.dtype in (np.float32, np.float64), "X was wrong data type!"
assert t.shape == (100,), "t was wrong shape!"
assert t.dtype == np.int32, "t was wrong data type!"
assert np.array_equal(X[0], [19.59, 0.08]), "Wrong features in X!"
assert np.array_equal(X[-1], [16.03, 0.06]), "Wrong features in X!"
assert np.array_equal(t[0:6], [-1,1,1,-1,-1]), "Wrong labels in t!"
print("Correct!")
```

Correct!

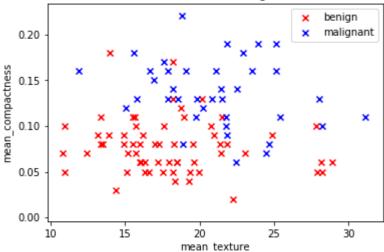
Write plotting code to plot your features data in two dimensions. Your plot should look like this:



In [16]:

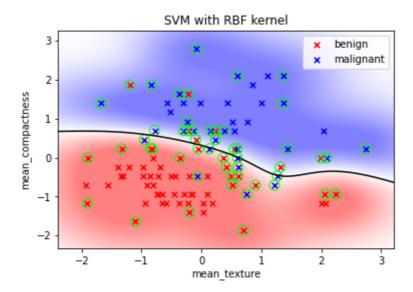
```
def plot_breast_data(X, t, title):
    data = np.array(list(zip(X[:,0],X[:,1],t))) #Create a 2d array combining X and y
lists
    Cgp = {-1:'red', 1:'blue'}
    for i in np.unique(data[:,2]):
        ix = np.where(t==i)
        plt.scatter(data[ix,0], data[ix,1], c = cgp[i], label = f'y = {i}',marker='x')
    plt.legend(['benign','malignant'])
    plt.xlabel('mean_texture')
    plt.ylabel('mean_compactness')
    plt.title('breast cancer training data')
    plt.show()
plot_breast_data(X, t, 'breast cancer training data')
```

breast cancer training data



Exercise 2.2 — Train an RBF SVM on the breast cancer data

You must train an RBF SVM on the breast cancer data. Your final result should look like this:



If your decision function does *not* look like the above, then check the relative scale of the features and consider preprocessing your data. Do you understand why the RBF kernel gave such terrible predictions on the 'raw' features?

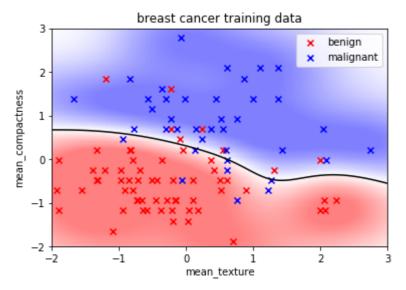
Write a few lines of code to train an SVC object on the data and plot the resulting predictor. Use $\gamma=1$ for the RBF kernel.

Optional: plot the support vectors as little green circles, using Matplotlib's *scatter* function, just like the *plot_toy_1d_data* function did from Exercise 1.3.

In [17]:

```
from sklearn import preprocessing
mm_scaler = preprocessing.StandardScaler()
X = mm_scaler.fit_transform(my_data[:,0:2])

svm = sklearn.svm.SVC(kernel='rbf',gamma=1).fit(X, t)
plot_2d_decision_function(svm,(-2,3,-2,3))
plot_breast_data(X, t, 'breast cancer training data')
```



Try different spread coefficients by setting $\gamma=0.1$ and $\gamma=10$. What do you observe in terms of the decision boundary? What do you observe in terms of the number of support vectors?. When finished, re-train your model with the original $\gamma=1$ and proceed to the final exercise.

Exercise 2.3 — Evaluate your SVM on held-out test data

Here you must use your *SVC* object from Exercise 2.2 to make predictions on data from <u>data_test.csv</u> (<u>data_test.csv</u>), a held-out test set for the breast cancer data.

Write a few lines of code to load the features and labels for the test data (just like you did for the training data in Exercise 2.1). Then make predictions on the test set. To see what fraction of your SVM predictions were correct on the test set, read the documentation for the sklearn.metrics.accuracy_score ((https://scikit-

<u>learn.org/stable/modules/generated/sklearn.metrics.accuracy_score.html#sklearn.metrics.html#sklearn.metrics.html#sklearn.metrics.html#sklearn.metrics.html#sklearn.metrics.html#sklearn.metrics.html#sklearn.metr</u>

In [18]:

```
test_data = genfromtxt('data_test.csv', delimiter=',',skip_header=1)
X_test = test_data[:,0:2]
t = test_data[:,2]
t_test = np.interp(t, (t.min(), t.max()), (-1, +1)).astype(np.int32)
X_test = mm_scaler.transform(X_test)

t_pred = svm.predict(X_test)
print(sklearn.metrics.accuracy_score(t_test, t_pred))
```

0.805

If your accuracy is below 80%, then maybe you likely didn't process your test features correctly.