Support Vector Machines and kernelization

```
[1]: # Global imports and settings
     from preamble import *
     %matplotlib inline
     plt.rcParams['savefig.dpi'] = 120 # Use 300 for PDF, 100 for slides
     #InteractiveShell.ast_node_interactivity = "all"
     HTML('''<style>html, body{overflow-y: visible !important} .CodeMirror{min-w
```

```
<IPython.core.display.HTML object>
```

Linear SVMs

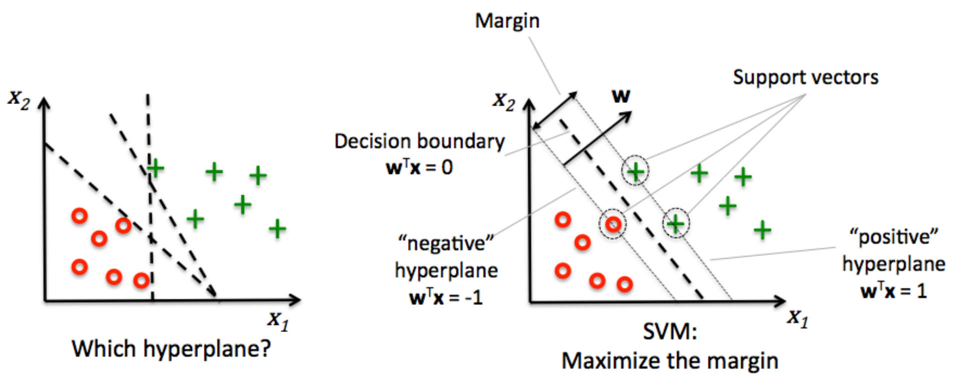
Revisited

Linear models for Classification (recap)

Aims to find a (hyper)plane that separates the examples of each class.
For binary classification (2 classes), we aim to fit the following function:
$\hat{y} = w_0 * x_0 + w_1 * x_1 + ... + w_p * x_p + b > 0$
When $\hat{y} < 0$, predict class -1, otherwise predict class +1

Support vector machines

- In several other linear models, we minimized (misclassification) error
- In SVMs, the optimization objective is to maximize the *margin*
- The **margin** is the distance between the separating hyperplane and the *support vectors*
- The **support vectors** are the training samples closest to the hyperplane
- Intuition: large margins generalize better, small margins may be prone to overfitting



SVC Image

Maximum margin For now, we assume that the data is linearly separable.
The *positive hyperplanes* is defined as:
$b + \mathbf{w^T x_+} = 1$
with $\mathbf{x_+}$ the positive support vectors.
Likewise, the *negative hyperplanes* is defined as:
$b + \mathbf{w^T x_-} = -1$

Substracting them yields:
$\mathbf{w^T}(\mathbf{x_+} - \mathbf{x_-}) = 2$
We can normalize by the length of vector w, defined as
$||w|| = \sqrt{\sum_{j=1}^{m} w_j^2}$
Yielding
$\frac{\mathbf{w^T}(\mathbf{x_+} - \mathbf{x_-})}{||w||} = \frac{2}{||w||}$
The left side can be interpreted as the distance between to positive and negative hyperplane, which is the *margin* that we want to maximize.
Hence, we want to maximize $\frac{2}{||w||}$ under the constraint that all samples are classified correctly:
$b + \mathbf{w^T x^{(i)}} \geq 1 \;\; if \;\; y^{(i)} = 1$
$b + \mathbf{w^T x^{(i)}} \leq -1 \;\; if \;\; y^{(i)} = -1$
i.e. all negative examples should fall on one side of the negative hyperplane and vice versa. Or:
$y^{(i)}(b + \mathbf{w^T x^{(i)}}) \geq 1 \;\; \forall i$
Maximizing $\frac{2}{||w||}$ can be done by minimizing $\frac{||w||^2}{2}$
This is a quadratic objective with linear constraints, and can hence be solved using quadratic programming, and more specifically with the *Lagrangian multipler method*.

Primal and Dual formulations The Primal formulation of the Lagrangian objective function is:

$$minL_P = \frac{1}{2}||\mathbf{w}||^2 - \sum_{i=1}^{l} a_i y_i (\mathbf{x_i} * \mathbf{w} + b) + \sum_{i=1}^{l} a_i$$

so that

$$a_i \geq 0$$
$$\mathbf{w} = \sum_{i=1}^{l} a_i y_i \mathbf{x_i}$$
$$\sum_{i=1}^{l} a_i y_i = 0$$

with l the number of training examples and a the *dual variable*, which acts like a weight for each training example.
It has a Dual formulation as follows:
min

$$L_D(a_i) = \sum_{i=1}^{l} a_i - \frac{1}{2}\sum_{i=1}^{l} a_i a_j y_i y_j (\mathbf{x_i} . \mathbf{x_j})$$

so that

$$a_i \geq 0$$

$$\sum_{i=1}^{l} a_i y_i = 0$$

See ‘Elements of Statistical Learning’ for more detail.
Why are we doing this?

- Because now we can solve the problem by just computing the inner products of $\mathbf{x_i}, \mathbf{x_j}$, which will be important when we want to solve non-linearly separable cases.

Ok, what now?

- Knowing the dual coefficients a_i we can find the weights w for the maximal margin separating hyperplane:

$$\mathbf{w} = \sum_{i=1}^{l} a_i y_i \mathbf{x_i}$$

- Hence, we can classify a new sample $\mathbf{u}$ by looking at the sign of $\mathbf{w} * \mathbf{u} + b$
- Most of the a_i will turn out to be *0*
- The training samples for which a_i is not 0 are the *support vectors*
- Hence, the SVM model is completely defined by the support vectors and their coefficients

SVMs and kNN

Remember, we will classify a new sample u by looking at the sign of:
$f(x) = \mathbf{w} * \mathbf{u} + b = \sum_{i=1}^{l} a_i y_i \mathbf{x_i} * \mathbf{u} + b$
Weighted k-nearest neighbor is a generalization of the k-nearest neighbor classifier would classify by looking at the sign of:
$f(x) = \sum_{i=1}^{k} a_i y_i dist(x_i, u)$
Hence: SVM's predict exactly the same way as k-NN, only: - They only consider the truly important points (the support vectors) - Thus *much* faster - The number of neighbors is the number of support vectors - The distance function can be different

SVMs in scikit-learn

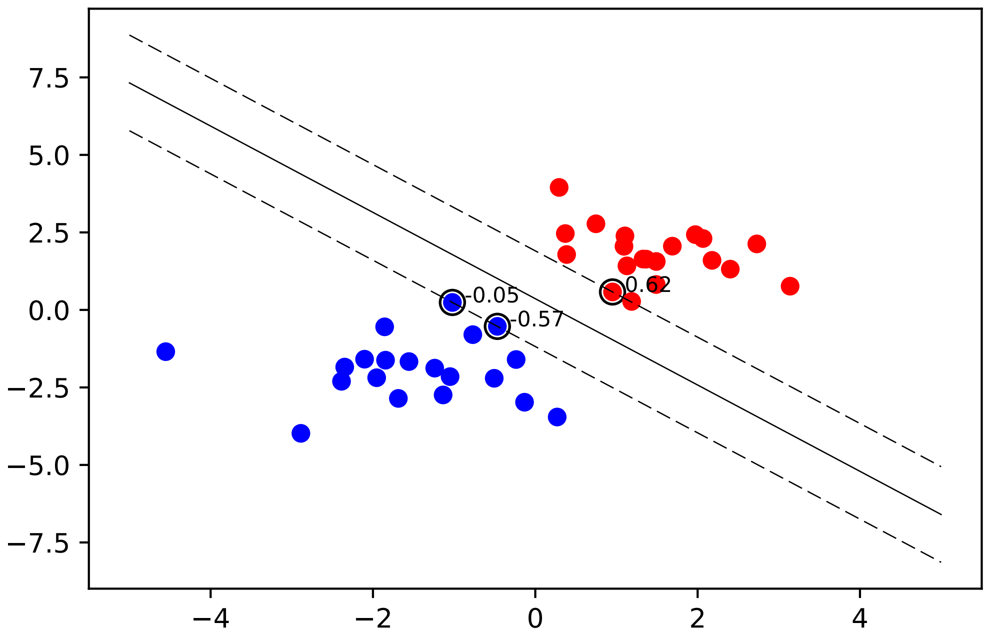
- We can use the `svm.SVC` classifier
  - or `svm.SVR` for regression
- To build a linear SVM use `kernel=linear`
- It returns the following:
  - support_vectors_: the support vectors
  - dual_coef_: the dual coefficients a, i.e. the `weigths` of the support vectors
  - coef_: only for linear SVMs, the feature weights w

```
[3]: from sklearn import svm

     # Linearly separable data
     X = np.r_[np.random.randn(20, 2) - [2, 2], np.random.randn(20, 2) + [2, 2]]
     Y = [0] * 20 + [1] * 20

     # Fit the model
     clf = svm.SVC(kernel='linear')
     clf.fit(X, Y)

     # Get the support vectors and weights
     print("Support vectors:")
     print(clf.support_vectors_[:])
     print("Coefficients:")
     print(clf.dual_coef_[:])
```

```
Support vectors:
[[-1.702 -0.71 ]
 [-0.665 -1.856]
 [ 1.168 -0.113]]
Coefficients:
[[-0.012 -0.301  0.313]]
```

SVM result. The circled samples are support vectors, together with their coefficients.

```
[2]: mglearn.plots.plot_svm_linear()
```



Dealing with nonlinearly separable data

- If the data is not linearly separable, (hard) margin maximization becomes meaningless
  - The constraints would contradict
- We can allow for violatings of the margin constraint by introducing *slack variables* $\xi^{(i)}$

$$b + \mathbf{w^T x^{(i)}} \geq 1 - \xi^{(i)} \;\; if \;\; y^{(i)} = 1$$
$$b + \mathbf{w^T x^{(i)}} \leq -1 + \xi^{(i)} \;\; if \;\; y^{(i)} = -1$$

- The new objective (to be minimized) becomes:

$$\frac{||w||^2}{2} + C(\sum_i \xi^{(i)})$$

- C is a penalty for misclassification
  - Large C: large error penalties
  - Small C: less strict about violations (more regularization)

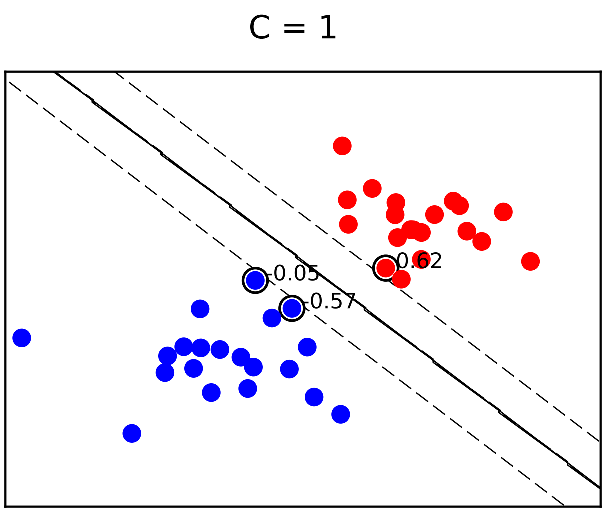
- This is known as the *soft margin* SVM (or *large margin* SVM)
  - Some support vectors are exactly on the margin hyperplane, with margin = 1
  - Others are margin violators, with margin < 1 and a positive slack variable: $\xi^{(i)} > 0$
    * If $\xi^{(i)} \geq 1$, they are misclassified

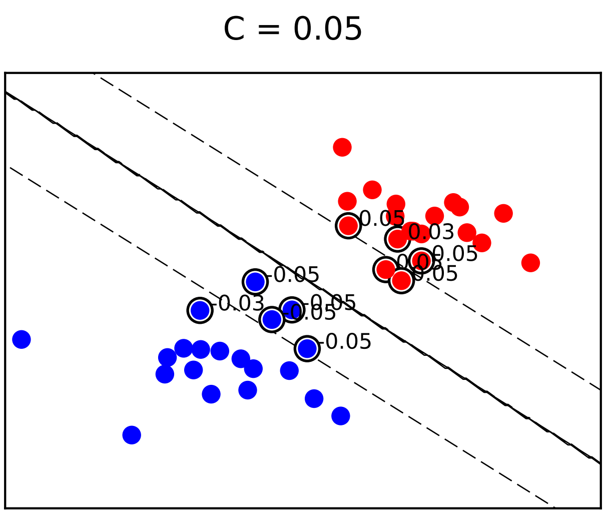
C and regularization

- Hence, we can use C to control the size of the margin and tune the bias-variance trade-off
  - Large C: Increases bias, reduces variance, more underfitting
  - Small C: Reduces bias, increases variance, more overfitting
- The penalty term $C(\sum_i \xi^{(i)})$ acts as an L1 regularizer on the dual coefficients
  - Also known as hinge loss
  - This induces sparsity: large C values will set many dual coefficients to 0, hence fewer support vectors
  - Small C values will typically lead to more support vectors
  - Again, it depends on the data how flexible or strict you need to be
- The *least squares SVM* is a variant that does L2 regularization
  - Will have many more support vectors (with low weights)
  - In scikit-learn, this is only available for the `LinearSVC` classifier (`loss='squared_hinge'`)

Effect on linearly separable data

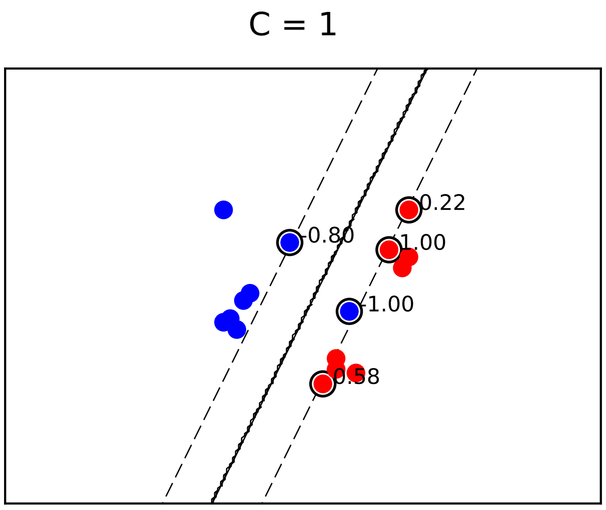
```
[5]: mglearn.plots.plot_svm_margins()
```

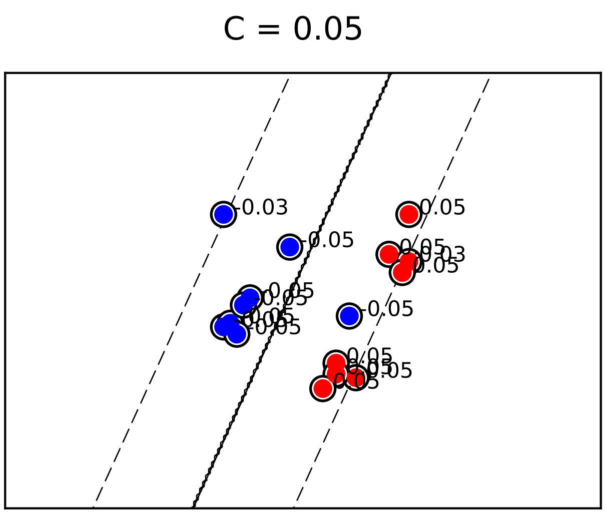




Effect on non-linearly separable data

```
[2]: mglearn.plots.plot_svm_margins_nonlin()
```

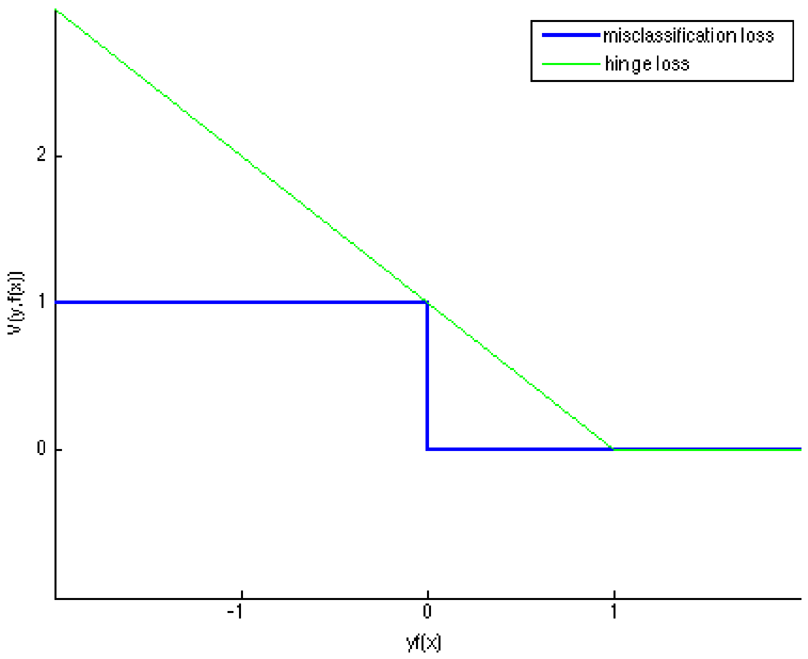




Hinge loss We are trying to: - Maximize the margin - Minimize the sum of margin violations

We could also try to maximize the margin and minimize the number of misclassifications - Turns out that the corresponding objective function is not convex, NP-hard

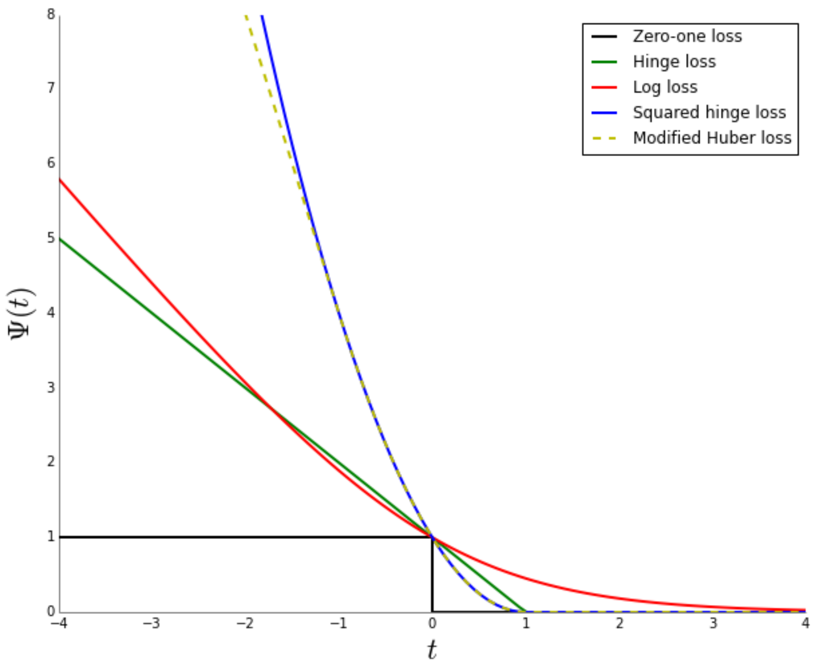
The best convex relation is hinge loss: L(γ) = max{0, 1 $-$ γ}
It measures the margin violation ξ_i.



Hinge

Other loss functions It is possible to use generalize SVMs by training them with other loss functions and gradient descent as the optimizer

See the `SGDCLassifier` - `SGDCLassifier(loss='hinge')` will act like an SVM



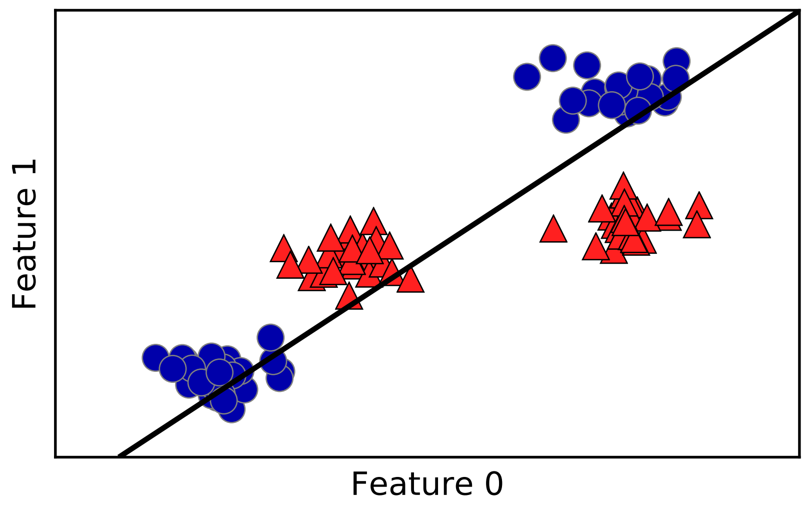
Hinge

Kernelized Support Vector Machines

- Linear models work well in high dimensional spaces.
- You can *create* additional dimensions yourself.
- Let's start with an example.

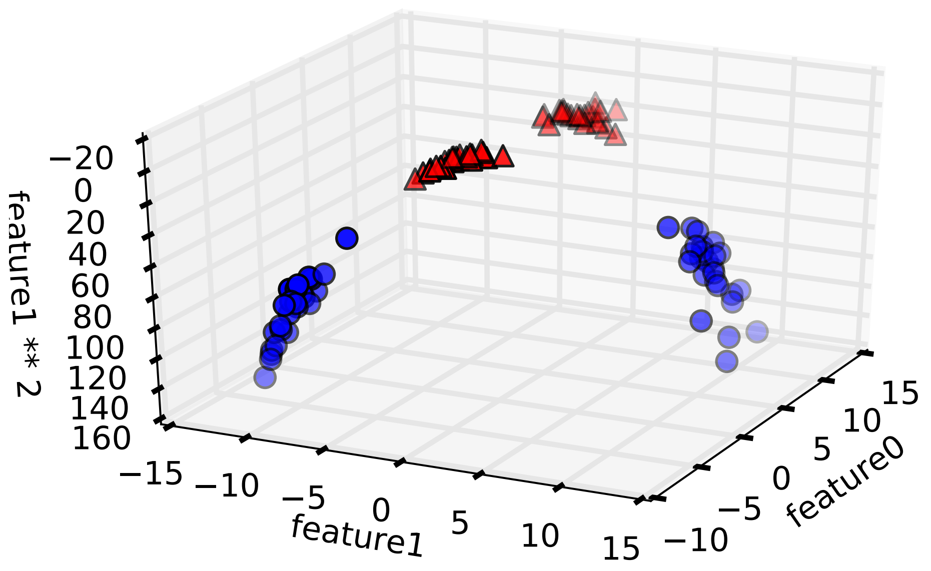
Our linear model doesn't fit the data well

```
[60]: from sklearn.svm import LinearSVC
      X, y = make_blobs(centers=4, random_state=8)
      y = y % 2
      linear_svm = LinearSVC().fit(X, y)

      mglearn.plots.plot_2d_separator(linear_svm, X)
      mglearn.discrete_scatter(X[:, 0], X[:, 1], y)
      plt.xlabel("Feature 0")
      plt.ylabel("Feature 1");
```



We can add a new feature by taking the squares of feature1 values

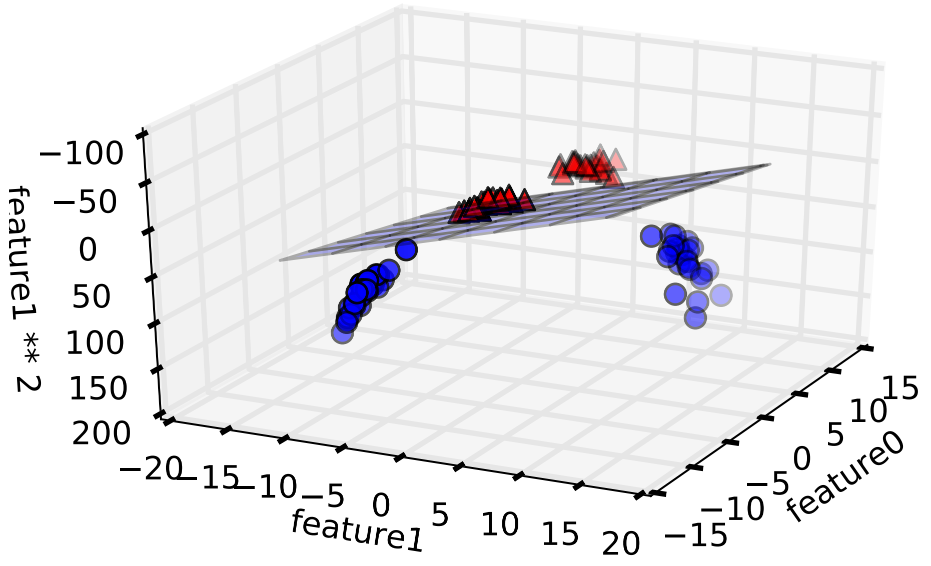
```
[61]: # add the squared first feature
      X_new = np.hstack([X, X[:, 1:] ** 2])


      from mpl_toolkits.mplot3d import Axes3D, axes3d
      figure = plt.figure()
      # visualize in 3D
      ax = Axes3D(figure, elev=-152, azim=-26)
      # plot first all the points with y==0, then all with y == 1
      mask = y == 0
      ax.scatter(X_new[mask, 0], X_new[mask, 1], X_new[mask, 2], c='b',
                 cmap=mglearn.cm2, s=60)
      ax.scatter(X_new[~mask, 0], X_new[~mask, 1], X_new[~mask, 2], c='r', marke
                 cmap=mglearn.cm2, s=60)
      ax.set_xlabel("feature0")
      ax.set_ylabel("feature1")
      ax.set_zlabel("feature1 ** 2");
```



Now we can fit a linear model

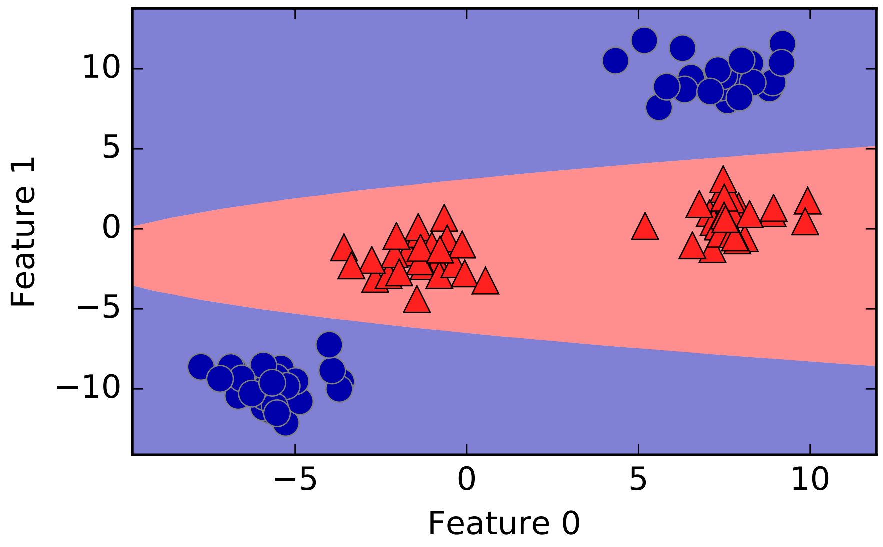
```
[62]: linear_svm_3d = LinearSVC().fit(X_new, y)
      coef, intercept = linear_svm_3d.coef_.ravel(), linear_svm_3d.intercept_

      # show linear decision boundary
      figure = plt.figure()
      ax = Axes3D(figure, elev=-152, azim=-26)
      xx = np.linspace(X_new[:, 0].min() - 2, X_new[:, 0].max() + 2, 50)
      yy = np.linspace(X_new[:, 1].min() - 2, X_new[:, 1].max() + 2, 50)

      XX, YY = np.meshgrid(xx, yy)
      ZZ = (coef[0] * XX + coef[1] * YY + intercept) / -coef[2]
      ax.plot_surface(XX, YY, ZZ, rstride=8, cstride=8, alpha=0.3)
      ax.scatter(X_new[mask, 0], X_new[mask, 1], X_new[mask, 2], c='b',
                 cmap=mglearn.cm2, s=60)
      ax.scatter(X_new[~mask, 0], X_new[~mask, 1], X_new[~mask, 2], c='r', marke
                 cmap=mglearn.cm2, s=60)

      ax.set_xlabel("feature0")
      ax.set_ylabel("feature1")
      ax.set_zlabel("feature1 ** 2")
```

```
<matplotlib.text.Text at 0x114af5c50>
```



As a function of the original features, the linear SVM model is not actually linear anymore, but more of an ellipse

```
[63]: ZZ = YY ** 2
      dec = linear_svm_3d.decision_function(np.c_[XX.ravel(), YY.ravel(), ZZ.rav
      plt.contourf(XX, YY, dec.reshape(XX.shape), levels=[dec.min(), 0, dec.max(
                   cmap=mglearn.cm2, alpha=0.5)
      mglearn.discrete_scatter(X[:, 0], X[:, 1], y)
      plt.xlabel("Feature 0")
      plt.ylabel("Feature 1");
```



Kernels

A (Mercer) Kernel on a space X is a (similarity) function

$k : X \times X \rightarrow \mathbb{R}$

Of two arguments with the properties:

- Symmetry: $k(x_1, x_2) = k(x_2, x_1) \;\; \forall x_1, x_2 \in X$
- Positive definite: for each finite subset of data points $x_1, ..., x_n$, the kernel Gram matrix is positive semi-definite

Kernel matrix = $K \in \mathbb{R}^{n \times n}$ with $K_{ij} = k(x_i, x_j)$

What is this good for?

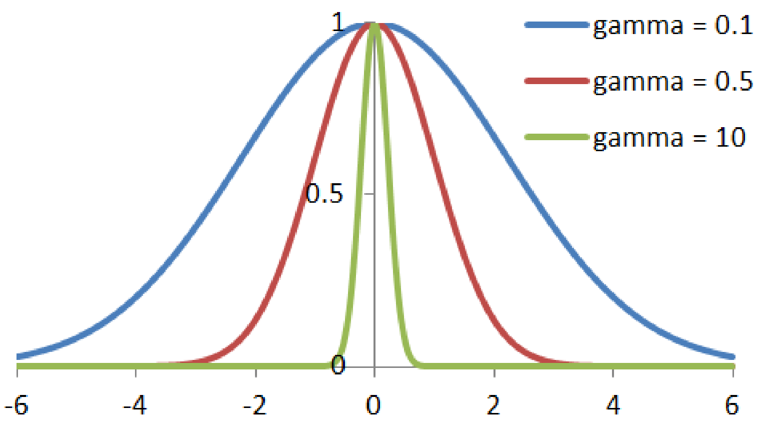
Mercer's Theorem states that

- there exists a Hilbert space $\mathcal{H}$ of continuous functions $X \rightarrow \mathbb{R}$ - basically, a possibly infinite-dimensional vector space with inner product where all operations are meaningful - and a continuous "feature map" $\phi : X \rightarrow \mathcal{H}$ - so that the kernel computes the inner product of the features $k(x_1, x_2) = \langle \phi(x_1), \phi(x_2) \rangle$

Hence, a kernel can be thought of as a 'shortcut' computation for the 2-step procedure feature map + inner product

Kernels: examples

- The inner product is a kernel. The standard inner product is the **linear kernel**: $k(x_1, x_2) = x_1^T x_2$
- Kernels can be constructed from other kernels k_1 and k_2:
  - For $\lambda \geq 0$, $\lambda.k_1$ is a kernel
  - $k_1 + k_2$ is a kernel
  - $k_1.k_2$ is a kernel (thus also k_1^n)
- This allows to construct the **polynomial kernel**: $k(x_1, x_2) = (x_1^T x_2 + b)^d$, for $b \geq 0$ and $d \in \mathbb{N}$
- The 'radial' **Gaussian kernel** is defined as: $k(x_1, x_2) = exp(-\gamma ||x_1 - x_2||^2)$, for $\gamma \geq 0$



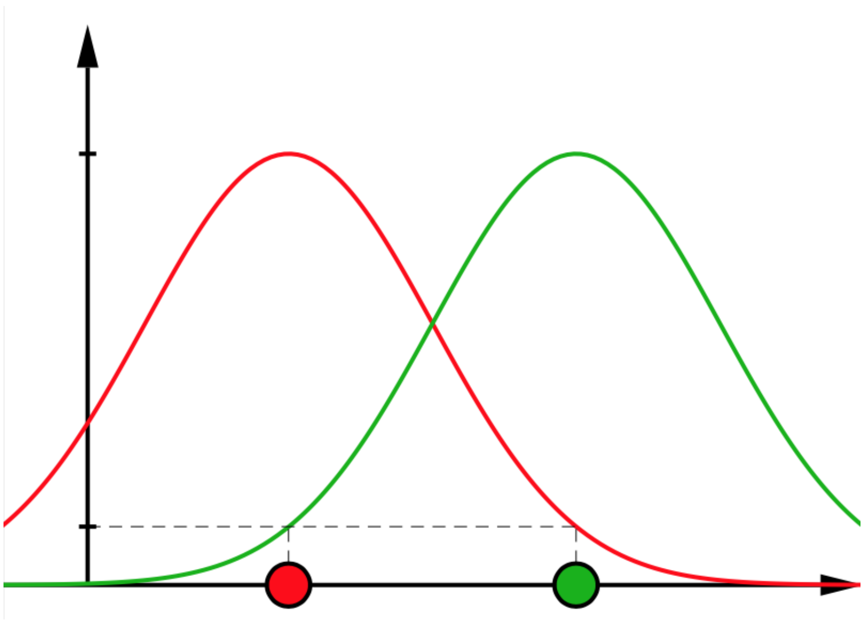
gamma

The Kernel Trick

- Adding nonlinear features can make linear models much more powerful
- Often we don't know which features to add, and adding many features might make computation very expensive
- Mathematical trick (*kernel trick*) allows us to directly compute distances (scalar products) in the high dimensional space
  - We can search for the nearest support vector in the high dimensional space
- A *kernel function* is a distance (similarity) function with special properties for which this trick is possible
  - Polynomial kernel: computes all polynomials up to a certain degree of the original features
  - Gaussian kernel, or radial basis function (RBF): considers all possible polynomials of all degrees
    - Infinite high dimensional space (Hilbert space), where the importance of the features decreases for higher degrees

The kernel trick: intuition

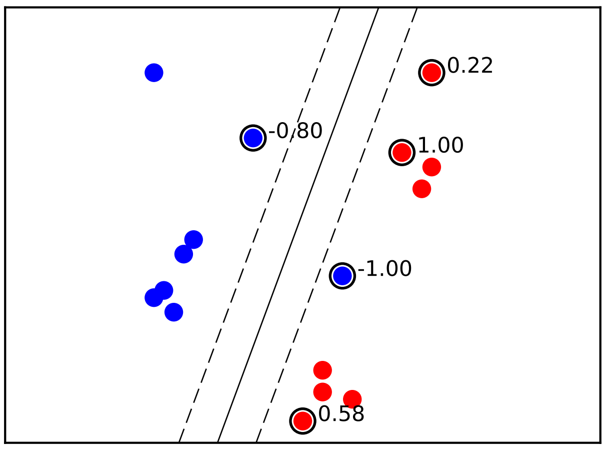
- There exists many feature map (and hence Hilbert space) for the same kernel, but they are all equivalent
- The Reproducing Kernel Hilbert Space (RKHS) has feature map $\phi : X \to C(X); x \to k(x,)$ Where C is the space of continuous functions $X \to \mathbb{R}$
- Thus, an input $x \in X$ is mapped to the basis function $\phi(x) = k(x,)$
  - For every point, the mappings are continuous functions $k(x,)$
- Kernel computes ⟨k(x1,·),k(x2,·)⟩=k(x1,x2)



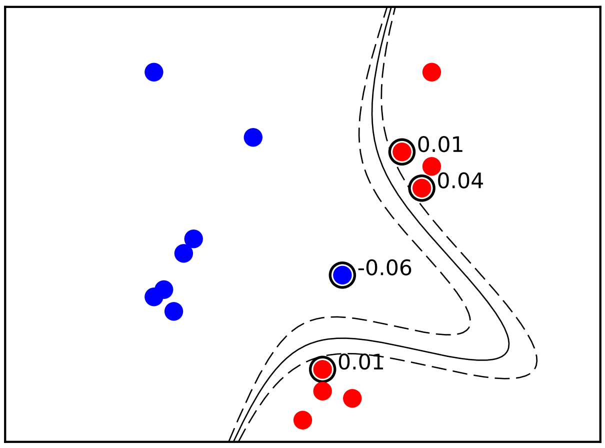
gamma

```
[4]: mglearn.plots.plot_svm_kernels()
```

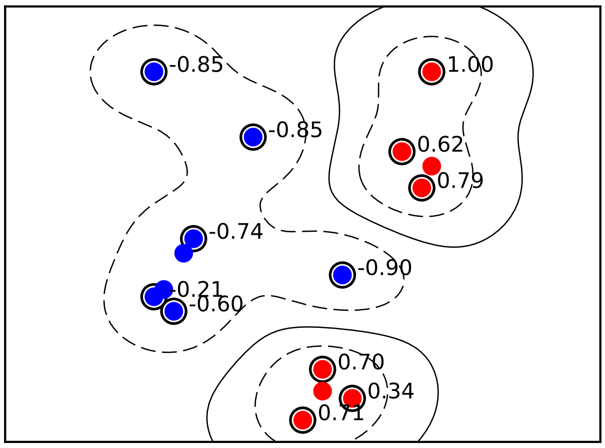
kernel = linear



kernel = poly



kernel = rbf



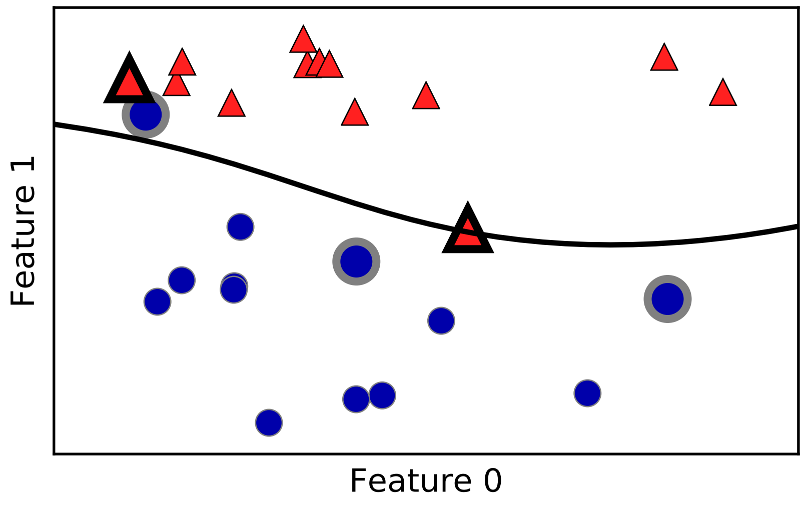
Understanding SVMs

To make a prediction for a new point, the distance to each of the support vectors is measured.

- The weight of each support vector is stored in the `dual_coef_` attribute of SVC
- The distance between data points is measured by the kernel
  - Gaussian kernel: $krbf(x_1, x_2) = \exp(\gamma||x_1 - x_2||^2)$
    * γ controls the width of the kernel and can be tuned

Given the support vectors, their weigths, and the kernel, we can plot the decision boundary

[64]:
```
from sklearn.svm import SVC

X, y = mglearn.tools.make_handcrafted_dataset()
svm = SVC(kernel='rbf', C=10, gamma=0.1).fit(X, y)
mglearn.plots.plot_2d_separator(svm, X, eps=.5)
# plot data
mglearn.discrete_scatter(X[:, 0], X[:, 1], y)
# plot support vectors
sv = svm.support_vectors_
# class labels of support vectors are given by the sign of the dual coeffi
sv_labels = svm.dual_coef_.ravel() > 0
mglearn.discrete_scatter(sv[:, 0], sv[:, 1], sv_labels, s=15, markeredgewi
plt.xlabel("Feature 0")
plt.ylabel("Feature 1");
```



Tuning SVM parameters

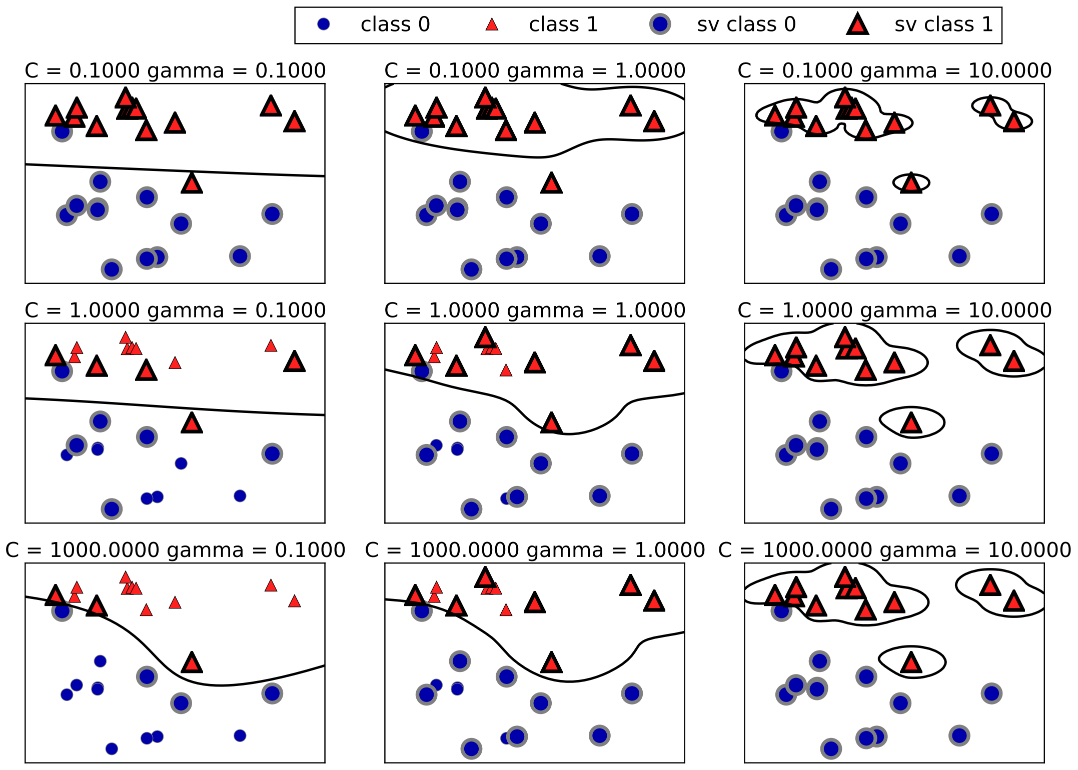
Several important parameters:

- gamma (kernel width): high values means that points are further apart

- Leads to many support vectors, narrow Gaussians, overfitting
- Low values lead to underfitting

- C (our linear regularizer): limits the weights of the support vectors
  - Higher values: more regularization, less overfitting
- For polynomial kernels, the *degree* (exponent) defines the complexity of the models

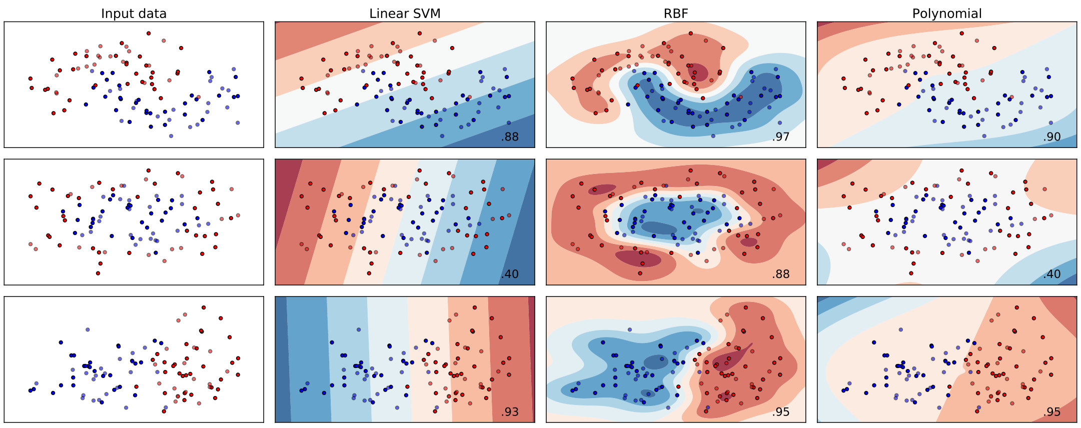
```
[65]: plt.rcParams.update({'font.size': 14})
      fig, axes = plt.subplots(3, 3, figsize=(15, 10))

      for ax, C in zip(axes, [-1, 0, 3]):
          for a, gamma in zip(ax, range(-1, 2)):
              mglearn.plots.plot_svm(log_C=C, log_gamma=gamma, ax=a)

      axes[0, 0].legend(["class 0", "class 1", "sv class 0", "sv class 1"],
                        ncol=4, loc=(.9, 1.2));
```



- Low gamma (left): wide Gaussians, very smooth decision boundaries
- High gamma (right): narrow Gaussians, boundaries focus on single points (high complexity)
- Low C (top): each support vector has very limited influence: many support vectores, almost linear decision boundary
- High C (bottom): Stronger influence, decision boundary bends to every support vector

```
[72]: names = ["Linear SVM", "RBF", "Polynomial"]
```

```
classifiers = [
    SVC(kernel="linear", C=0.025),
    SVC(gamma=2, C=1),
    SVC(kernel="poly", degree=3, C=0.1)
    ]

pc.plot_classifiers(names, classifiers, figuresize=(20,8))
```



Preprocessing Data for SVMs

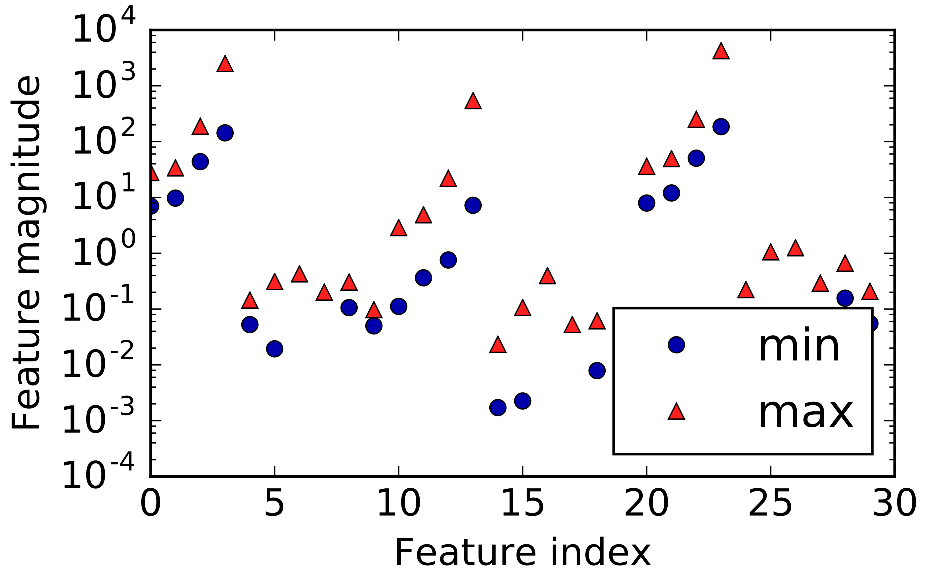
- SVMs are very sensitive to hyperparameter settings
- They expect all features to be approximately on the same scale
    - If not, they overfit easily

```
[66]: X_train, X_test, y_train, y_test = train_test_split(
          cancer.data, cancer.target, random_state=0)

      svc = SVC()
      svc.fit(X_train, y_train)

      print("Accuracy on training set: {:.2f}".format(svc.score(X_train, y_train
      print("Accuracy on test set: {:.2f}".format(svc.score(X_test, y_test)))
```

```
Accuracy on training set: 1.00
Accuracy on test set: 0.63
```

We can plot the scales of the features by plotting their min and max value

```
[67]: plt.plot(X_train.min(axis=0), 'o', label="min")
      plt.plot(X_train.max(axis=0), '^', label="max")
      plt.legend(loc=4)
      plt.xlabel("Feature index")
      plt.ylabel("Feature magnitude")
      plt.yscale("log")
```



We can scale all features between 0 and 1 Note: the sklearn.prepr ocessing package supports many preprocessing techniques, including the ‘MinMaxScaler‘

```
[68]:  # Compute the minimum value per feature on the training set
      min_on_training = X_train.min(axis=0)
      # Compute the range of each feature (max - min) on the training set
      range_on_training = (X_train - min_on_training).max(axis=0)

      # subtract the min, divide by range
      # afterwards min=0 and max=1 for each feature
      X_train_scaled = (X_train - min_on_training) / range_on_training
      print("Minimum for each feature\n{}".format(X_train_scaled.min(axis=0)))
      print("Maximum for each feature\n {}".format(X_train_scaled.max(axis=0)))
```

```
Minimum for each feature
[ 0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.]
Maximum for each feature
 [ 1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.
  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.]
```

- We must now apply the SAME transformation on the test set
  - Don’t rescale the test set separately
  - Don’t apply rescaling before making train test spits
- sklearn offers `pipelines` which make this easier
  - Wrapper around series of operators

```
[69]: # use THE SAME transformation on the test set,
      # using min and range of the training set.
      X_test_scaled = (X_test - min_on_training) / range_on_training
```

Much better results, but they can still be tuned further

```
[70]: svc = SVC()
      svc.fit(X_train_scaled, y_train)

      print("Accuracy on training set: {:.3f}".format(
              svc.score(X_train_scaled, y_train)))
      print("Accuracy on test set: {:.3f}".format(svc.score(X_test_scaled, y_tes
```

```
Accuracy on training set: 0.948
Accuracy on test set: 0.951
```

```
[71]: svc = SVC(C=1000)
      svc.fit(X_train_scaled, y_train)

      print("Accuracy on training set: {:.3f}".format(
              svc.score(X_train_scaled, y_train)))
      print("Accuracy on test set: {:.3f}".format(svc.score(X_test_scaled, y_tes
```

```
Accuracy on training set: 0.988
Accuracy on test set: 0.972
```

Strengths, weaknesses and parameters

- SVMs allow complex decision boundaries, even with few features.
- Work well on both low- and high-dimensional data
- Don't scale very well to large datasets (>100000)
- Require careful preprocessing of the data and tuning of the parameters.
- SVM models are hard to inspect

Important parameters: * regularization parameter C * choice of the kernel and kernel-specific parameters * Typically string correlation with C