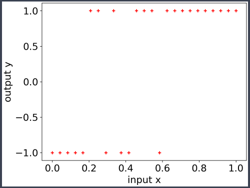
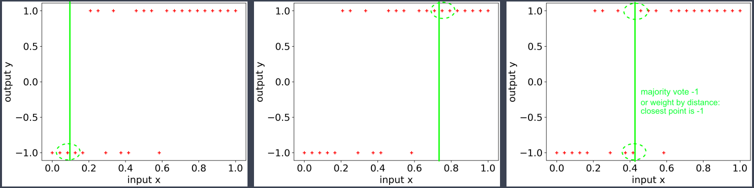
» Kernalising Linear Models: Using Training Data As Features

- Training data $(x^{(i)}, y^{(i)})$, $i = 1, 2, \ldots, m$
- Idea: associate a feature with each training data point and then use linear model ...
- Feature i: function $y^{(i)}K(x^{(i)}, x)$ outputting a real number for input x. $K(x^{(i)}, x)$ measures the distance between input x and training point $x^{(i)}$. $K(x^{(i)}, x)$ is referred to as a *kernel*
- Model: $\hat{y} =$ $sign\left(\theta_0 + \theta_1 y^{(1)}K(x^{(1)}, x) + \theta_2 y^{(2)}K(x^{(2)}, x) + \cdots + \theta_m y^{(m)}K(x^{(m)}, x)\right)$
- Now can learn parameters θ_0, $\theta_1, \ldots$ by selecting them to minimise a cost function e.g. logistic regression or SVM cost function.
- Can do same thing for regression problems, model is then $\hat{y} = \theta_0 + \theta_1 y^{(1)}K(x^{(1)}, x) + \theta_2 y^{(2)}K(x^{(2)}, x) + \cdots + \theta_m y^{(m)}K(x^{(m)}, x)$

» Using Training Data As Features



training data

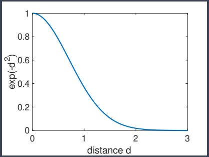


Remind you of a *k*NN Model? I hope so ...

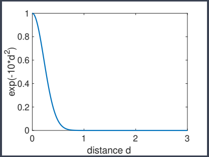
- We want to attach more weight to training data points that are close to input x and less weight to far away training points.
- So $K(x^{(i)}, x)$ should be about 1 when distance between $x^{(i)}$ and x is small, falling to 0 as distance grows.

» Using Training Data As Features

- Model: $\hat{y} = sign(\theta_0 + \theta_1 y^{(1)} K(x^{(1)}, x) + \theta_2 y^{(2)} K(x^{(2)}, x) + \cdots + \theta_m y^{(m)} K(x^{(m)}, x)$
- *Gaussian* kernel $K(x^{(i)}, x) = e^{-\gamma d(x^{(i)}, x)^2}$
- Parameter γ controls how quickly $K(x^{(i)}, x)$ decreases as distance between $x^{(i)}$ and x grows.



$\gamma = 1$

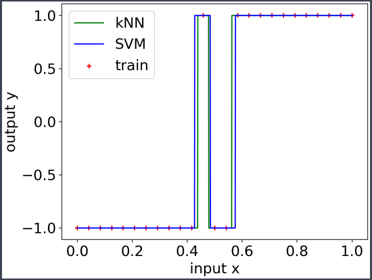


$\gamma = 10$

Choose γ using cross-validation.

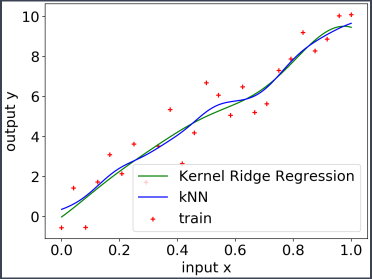
- Now train parameters θ to improve on basic fit to training data provided by kernel.
  - This is like a kNN with $k = m$ (all of training data) and enhanced by addition of parameters θ that provide extra flexibility to tune model.
  - Another way to think about it is that in kNN model the parameters θ change with the input x, i.e. $\theta_i = 1$ for training points $i \in N_k$ and $\theta_i = 0$ for $i \notin N_k$ (N_k is the set of k points closest to x)

» Classification example



- Kernalised SVM: 1) $\gamma = 50$, L_2 penalty weight $C = 1$
- kNN model: 1) Euclidean distance, 2) (i) $k = m$, 3) gaussian weights, 4) sign(weighted average)
- SVM and kNN predictions are not identical, but much the same.
- *Note: No kernalised version of logistic regression available in sklearn currently. Its certainly possible to implement one but SVM lends itself to more efficient kernelised implementation than logistic regression.*

» Regression example



- Kernalised Ridge Regression: 1) $\gamma = 10$, L_2 penalty weight $C = 10$
- kNN model: 1) Euclidean distance, 2) $k = m$, 3) gaussian weights, 4) weighted average
- kernel and kNN predictions are not identical, but much the same.

» Classification Example Python Code

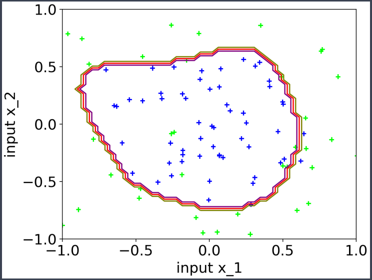
```
import numpy as np
m = 25
Xtrain = np.linspace(0.0,1.0,num=m)
ytrain = np.sign(Xtrain−0.5+np.random.normal(0,0.2,m))
Xtrain = Xtrain.reshape(−1, 1)

def gaussian_kernel(distances):
        weights = np.exp(−100∗(distances∗∗2))
        return weights

from sklearn.neighbors import KNeighborsClassifier
model = KNeighborsClassifier(n_neighbors=25,weights=gaussian_kernel).fit(Xtrain, ytrain)

Xtest=np.linspace(0.0,1.0,num=1000).reshape(−1, 1)
ypred = model.predict(Xtest)
import matplotlib.pyplot as plt
plt.rc('font', size=18); plt.rcParams['figure.constrained_layout.use'] = True
plt.scatter(Xtrain, ytrain, color='red', marker='+')
plt.plot(Xtest, ypred, color='green')

from sklearn.svm import SVC
model = SVC(C=1000, kernel='rbf', gamma=50).fit(Xtrain, ytrain)
ypred = model.predict(Xtest)
plt.plot(Xtest, ypred, color='blue')

plt.xlabel("input x"); plt.ylabel("output y")
plt.legend(["kNN","SVM","train"])
plt.show()
```

» Regression Example Python Code

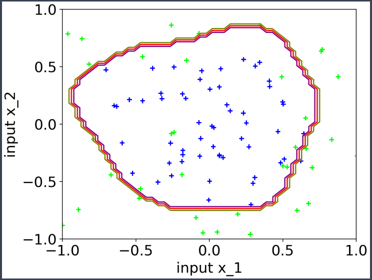
```
import numpy as np
m = 25
Xtrain = np.linspace(0.0,1.0,num=m)
ytrain = 10∗Xtrain + np.random.normal(0.0,1.0,m)
Xtrain = Xtrain.reshape(−1, 1)
from sklearn.kernel_ridge import KernelRidge
C=10;
model = KernelRidge(alpha=1.0/C, kernel='rbf', gamma=10).fit(Xtrain, ytrain)

Xtest=np.linspace(0.0,1.0,num=1000).reshape(−1, 1)
ypred = model.predict(Xtest)

def gaussian_kernel(distances):
        weights = np.exp(−100∗(distances∗∗2))
        return weights

from sklearn.neighbors import KNeighborsRegressor
model2 = KNeighborsRegressor(n_neighbors=m,weights=gaussian_kernel).fit(Xtrain, ytrain)
ypred2 = model2.predict(Xtest)

import matplotlib.pyplot as plt
plt.rc('font', size=18); plt.rcParams['figure.constrained_layout.use'] = True
plt.scatter(Xtrain, ytrain, color='red', marker='+')
plt.plot(Xtest, ypred, color='green')
plt.plot(Xtest, ypred2, color='blue')
plt.xlabel("input x"); plt.ylabel("output y")
plt.legend(["Kernel Ridge Regression","kNN","train"])
plt.show()
```

» Another Classification example

When points from one class are clumped together then using training data as features can work nicely:



SVM

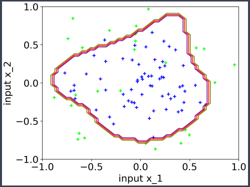


*k*NN

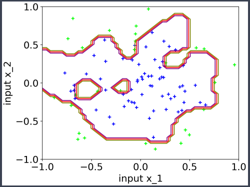
- Kernalised SVM: 1) $\gamma = 1$, L_2 penalty weight $C = 1$
- *k*NN model: 1) Euclidean distance, 2) (i) $k = m$, 3) gaussian weights, 4) sign(weighted average)

» Another Classification example (cont)

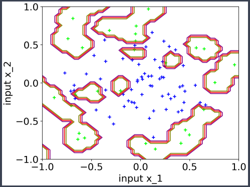
Impact of Gaussian kernel parameter γ:



$\gamma = 2$

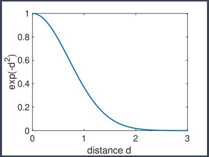


$\gamma = 10$

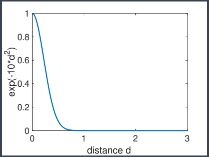


$\gamma = 100$

* As γ increases the kernel decreases more quickly with distance. This makes the predictions tend to be less smooth and to just snap to the nearest training point



$\gamma = 1$



$\gamma = 10$

* Use γ to manage trade-off between under-fitting and over-fitting

» Circle Example Python Code

```
import numpy as np
m = 100
Xtrain = 0.5*np.random.randn(m,2)
ytrain = np.sign((Xtrain[:,0]**2+Xtrain[:,1]**2)-0.5+np.random.normal(0,0.2,m))

import matplotlib.pyplot as plt
plt.rc('font', size=18); plt.rcParams['figure.constrained_layout.use'] = True

xx,yy = np.meshgrid(np.linspace(-1, 1, 50),np.linspace(-1, 1, 50))
Xtest = np.c_[xx.ravel(), yy.ravel()]
ytest = np.sign((xx**2+yy**2)-0.5)

from sklearn.svm import SVC
model = SVC(C=1000, kernel='rbf', gamma=1).fit(Xtrain, ytrain)
ypred = model.predict(Xtest)
plt.contour(xx,yy, ypred.reshape(xx.shape), c=ypred,cmap=plt.cm.brg, levels=2)
#plt.scatter(xx,yy,marker='.',c=ypred.reshape(xx.shape),cmap=plt.cm.brg)
plt.scatter(Xtrain[:,0],Xtrain[:,1],marker='+',c=ytrain,cmap=plt.cm.brg)
plt.xlim((-1,1)); plt.ylim((-1,1))
plt.xlabel("input x_1"); plt.ylabel("input x_2")
plt.show()

def gaussian_kernel(distances):
        weights = np.exp(-10*(distances**2))
        return weights

from sklearn.neighbors import KNeighborsClassifier
model = KNeighborsClassifier(n_neighbors=m,weights=gaussian_kernel).fit(Xtrain, ytrain)
ypred = model.predict(Xtest)
plt.contour(xx,yy, ypred.reshape(xx.shape), c=ypred,cmap=plt.cm.brg, levels=2)
plt.scatter(Xtrain[:,0],Xtrain[:,1],marker='+',c=ytrain,cmap=plt.cm.brg)
plt.xlim((-1,1)); plt.ylim((-1,1))
plt.xlabel("input x_1"); plt.ylabel("input x_2")
plt.show()
```

» Some More Details

- So far we used predictions of the form:

  $$\hat{y} = \theta_0 + \theta_1 y^{(1)} K(x^{(1)}, x) + \theta_2 y^{(2)} K(x^{(2)}, x) + \cdots + \theta_m y^{(m)} K(x^{(m)}, x)$$

- Can also consider predictions of the form:

  $$\hat{y} = \theta_0 + w_1 K(x^{(1)}, x) + w_2 K(x^{(2)}, x) + \cdots + w_m K(x^{(m)}, x)$$

  where parameters $w_1, w_2, \ldots, w_m$ are learned. Choosing $w_i = \theta_i y^{(i)}$ gives our previous setup.
- Kernalised SVM predictions are always of the first form (with $\theta_i y^{(i)}$'s)
- Kernalised ridge regression and kernalised logistic regression actually use the second form (with w_i's) but when the weight $1/C$ given to the regularisation penalty is large enough then the w_i's learned are of the form $w_i \approx \theta_i y^{(i)}$
  $\rightarrow$ needs a bit of maths to show this, beyond this module but if interested see e.g.
  - www.cs.cornell.edu/courses/cs4780/2018fa/lectures/lecturenote14.html
  - www.ics.uci.edu/~welling/classnotes/papers_class/Kernel-Ridge.pdf

» Some More Details

* L_2 regularisation $\sum_{i=1}^{m} \theta_m^2 = \theta^T\theta$
* With kernelised models number of parameters θ is same as size of training data, so often quite large
* SVM implementation used weighted penalty $\theta^T M\theta$ where M is a weighting matrix $\rightarrow$ improves computational performance

» Kernel SVMs[1] [Optional]

Linear model: $sign(\theta^T x)$. First try at kernalising:

* We'll refer to parameters in kernelised model as α_i rather than θ_i.
* Replace $\theta^T x$ with $\sum_{j=1}^{m} \alpha_j y^{(j)} K(x, x^{(j)})$
* Hypothesis: $sign(\sum_{j=1}^{m} \alpha_j y^{(j)} K(x, x^{(j)}))$
* Cost: $\frac{1}{m} \sum_{i=1}^{m} \max(0, 1 - y^{(i)} \sum_{j=1}^{m} \alpha_j y^{(j)} K(x^{(i)}, x^{(j)})) + \lambda \theta^T \theta$
* What about $\theta^T \theta$ term ? We'd like cost to be only in terms of α

[1] Training a Support Vector Machine in the Primal. Olivier Chapelle, Neural Computation 2007

» Kernel SVMs [Optional]

Second try at kernalising:

* Write $K(x, x^{(j)}) = \phi(x^{(j)})^T\phi(x) \rightarrow$ can't do this for all weight functions K, need to restrict ourselves to ones where we can.
* Replace x by $\phi(x)$ and define $\theta = \sum_{j=1}^{m} \alpha_j y^{(j)} \phi(x^{(j)})$
* Then

$$\theta^T\phi(x) = \sum_{j=1}^{m} \alpha_j y^{(j)} \phi(x^{(j)})^T\phi(x) = \sum_{j=1}^{m} \alpha_j y^{(j)} K(x, x^{(j)})$$

$$\begin{aligned}\theta^T\theta &= \sum_{j=1}^{m} \alpha_j y^{(j)} \phi(x^{(j)})^T \sum_{i=1}^{m} \alpha_i y^{(i)} \phi(x^{(i)}) \\ &= \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_j y^{(j)} K(x^{(j)}, x^{(i)}) y^{(i)} \alpha_i = \alpha^T M \alpha\end{aligned}$$

  where M is matrix with $M_{ij} = y^{(j)} K(x^{(j)}, x^{(i)}) y^{(i)}$ and α is parameter vector.
* Cost: $\frac{1}{m}\sum_{i=1}^{m} \max(0, 1 - y^{(i)} \sum_{j=1}^{m} \alpha_j y^{(j)} K(x^{(i)}, x^{(j)})) + \lambda \alpha^T M \alpha$
* Now everything is in terms of the new parameters α.

» Kernel Logistic Regression [Optional]

- Replace $\theta^T x$ with $\sum_{j=1}^{m} \alpha_j y^{(j)} K(x, x^{(j)})$
- Hypothesis: $sign(\sum_{j=1}^{m} \alpha_j y^{(j)} K(x, x^{(j)}))$
- Cost: $\frac{1}{m} \sum_{i=1}^{m} \log(1 + e^{-y^{(i)} \sum_{j=1}^{m} \alpha_j y^{(j)} K(x^{(i)}, x^{(j)})})$

» Kernalised Ridge Regression [Optional]

* Replace $\theta^T x$ with $\sum_{j=1}^{m} \alpha_j y^{(i)} K(x, x^{(j)})$
* Use $\theta^T\theta = \alpha^T M \alpha$ where M is matrix with $M_{ij} = y^{(j)} K(x^{(j)}, x^{(i)}) y^{(i)}$ and α is parameter vector.
* Hypothesis: $\sum_{j=1}^{m} \alpha_j y^{(i)} K(x, x^{(j)})$
* Cost: $\frac{1}{m} \sum_{i=1}^{m} (y^{(i)} - \sum_{j=1}^{m} \alpha_j y^{(i)} K(x^{(i)}, x^{(j)}))^2 + \lambda \alpha^T M \alpha$

» Kernel Summary

- Easy to use $\rightarrow$ hyperparameters are kernel parameter γ and L_2 penalty weight C. Also need to choose kernel, but Gaussian usually works well.
- Essentially an enhanced form of kNN model, so shares many of the same characteristics
- Small data only $\rightarrow$ as training data increases kernel approaches tend to become expensive/slow.
- Efficient kernel SVM implementations:
  - Often online "SVM" is used to mean "kernel SVM", so can get confusing. Often you'll also be told that SVM is better than logistic regression etc without further explanation
  - Its important to keep clearly in mind that *two* tools are usually being conflated here: (i) use of kernels and (ii) use of SVMs. Its use of kernels that's key – its a powerful approach but kernels can be applied with any linear model not just SVMs