Advanced Machine Learning

CSC 722 Spring 2014

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Support Vector Machines

SVMs for regression

In simple regression, the objective is to minimize a regularized error function

$$\frac{1}{2}\sum_{n=1}^{N}\{y_n - t_n\}^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2 \tag{1}$$

To obtain sparse solutions, the above equation can be replaced by a ϵ - *insensitive error function*

$$E_\epsilon(y(\mathbf{x}) - t) = \begin{cases} 0 & \text{if } |y(\mathbf{x}) - t| < \epsilon \\ |y(\mathbf{x}) - t| - \epsilon & \text{otherwise} \end{cases} \tag{2}$$

Minimizing the error function

To obtain the solution, minimize the regularized error function

$$C \sum_{n=1}^{N} E_\epsilon(y(\mathbf{x}_n) - t_n) + \frac{1}{2}\|\mathbf{w}\|^2 \tag{3}$$

where C is the (inverse) regularization parameter

Error function with slack variables

By introducing slack variables for each data point x_n

- $\xi_n \geq 0$ where $t_n > y(\mathbf{x}_n) + \epsilon$
- $\widehat{\xi}_n \geq 0$ where $t_n < y(\mathbf{x}_n) + \epsilon$

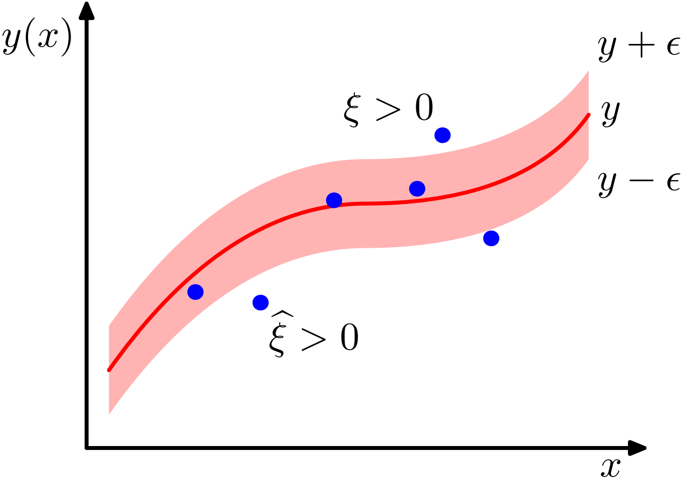
the error function can be written as

$$C \sum_{n=1}^{N} (\xi_n + \widehat{\xi}_n) + \frac{1}{2} \|\mathbf{w}\|^2 \tag{4}$$

This is to be minimized subject to the constraints

- $\widehat{\xi}_n \geq 0$ and $\xi_n \geq 0$
- $t_n \leq y(\mathbf{x}_n) + \epsilon + \xi_n$
- $t_n \geq y(\mathbf{x}_n) - \epsilon - \widehat{\xi}_n$

SVM Regression *tube*



Applying Lagrange multipliers

Plugging in the Lagrange multipliers and simplifying,

$$\widetilde{L}(\mathbf{a}, \widehat{\mathbf{a}}) = -\frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N}(a_n - \widehat{a}_n)(a_m - \widehat{a}_m)k(\mathbf{x}_n, \mathbf{x}_m) - \epsilon\sum_{n=1}^{N}(a_n - \widehat{a}_n) + \sum_{n=1}^{N}(a_n - \widehat{a}_n)t_n \tag{5}$$

where $a_n \geq 0$ and $\widehat{a_n} \geq 0$ are the Lagrange multipliers; and
$k(\mathbf{x}, \mathbf{x}') = \phi(\mathbf{x})^T\phi(\mathbf{x}')$ is the kernel.

Predicting new inputs

The prediction can be made for new inputs using

$$y(\mathbf{x}) = \sum_{n=1}^{N} (a_n - \widehat{a}_n) k(\mathbf{x}, \mathbf{x}_n) + b \tag{6}$$

ν-SVMs

- An alternative for of SVM for regression
- Use a parameter ν that bounds the fraction of points lying *outside* the tube instead of fixing the width ϵ of the *insensitive* region

Maximizing the dual

$$\widetilde{L}(\mathbf{a}, \widehat{\mathbf{a}}) = -\frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N}(a_n - \widehat{a}_n)(a_m - \widehat{a}_m)k(\mathbf{x}_n, \mathbf{x}_m) + \sum_{n=1}^{N}(a_n - \widehat{a}_n)t_n \tag{7}$$

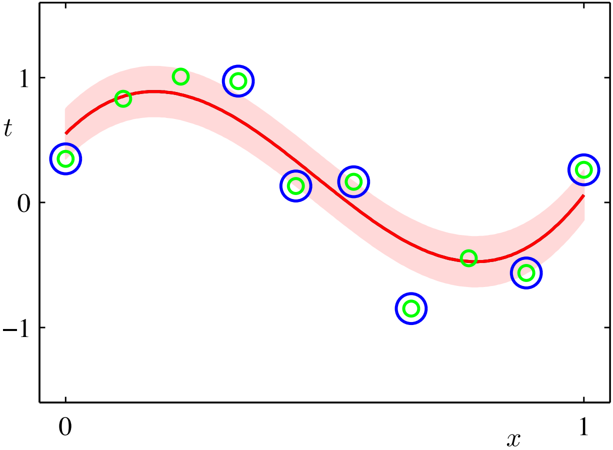
subject to the constraints

- $0 \leq a_n \leq C/N$
- $0 \leq \widehat{a}_n \leq C/N$
- $\sum_{n=1}^{N}(a_n - \widehat{a}_n) = 0$
- $\sum_{n=1}^{N}(a_n + \widehat{a}_n) \leq \nu C$

Observations

- At most νN data points fall outside the insensitive tube, while at least νN data points are the support vectors that lie on or outside the tube
- Parameters ν and C are determined by cross-validation

ν-SVM regression



Relevance Vector Machines

- Bayesian sparse kernel technique similar to SVM
- Leads to much sparser models resulting in faster performance on test data while maintaining the same generalization error

Limitations of SVM

- Outputs of SVM represent decisions rather than posterior probabilities
- Extension to $K > 2$ classes is problematic
- Complexity parameter C or ν to be found out using cross validation
- Kernels used are centered on training data points and are required to be *positive definite* (Mercer kernels)

RVM for regression

Consider the model defining a conditional distribution for a real-valued target variable t, given an input vector $\mathbf{x}$

$$p(t|\mathbf{x}, \mathbf{w}, \beta) = \mathcal{N}(t|y(\mathbf{x}), \beta^{-1}) \tag{8}$$

where $\beta = \sigma^{-2}$ is the noise precision and mean is of the form

$$y(\mathbf{x}) = \sum_{i=1}^{M} w_i \phi_i(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x}) \tag{9}$$

Using kernel for each data point in place of the the bias function $\phi_i(\mathbf{x})$

$$y(\mathbf{x}) = \sum_{n=1}^{N} w_n k(\mathbf{x}, \mathbf{x}_n) + b \tag{10}$$

Given a set of set of N observations of the input vector $\mathbf{x}$, which can be denote collectively by data matrix $\mathbf{X}$ whose n^{th} row is $\mathbf{x}_n^T$ with $n = 1, \ldots, N$ and corresponding target values $\mathbf{t} = (t_1, \ldots, t_N)^T$, the *likelihood* function is

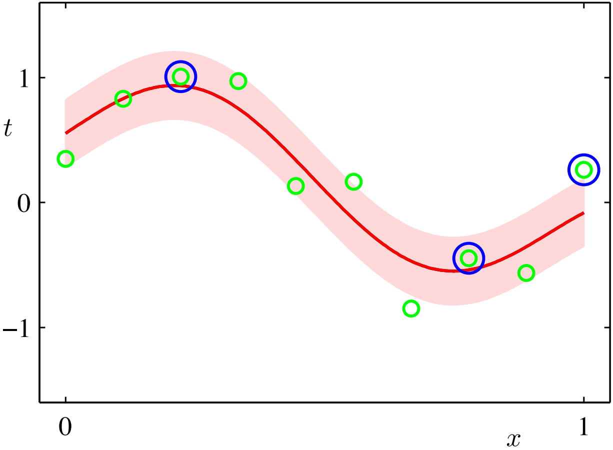
$$p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = \prod_{n=1}^{N} p(t_n|\mathbf{x}_n, \mathbf{w}, \beta^{-1}) \tag{11}$$

Simplifying, the predictive distribution over t for a new input x is

$$p(t|\mathrm{x}, \mathbf{X}, \mathbf{t}, \alpha^*, \beta^*) = \mathcal{N}(t|\mathbf{m}^T\phi(\mathrm{x}), \sigma^2(\mathrm{x})) \qquad (12)$$

where $\alpha^* and \beta^*$ are hyperparameters that maximize the marginal likelihood and
m is the posterior mean and variance of the predictive distribution is $\sigma^2(\mathrm{x})$

RVM vs ν-SVM regression



RVM vs SVM

- Training involves optimizing a non convex function $\Rightarrow$ longer training time $O(N^3)$ as compared to SVM $O(N^2)$
- Parameters governing the complexity and noise variance are determined automatically from a single run, as compared to SVM which requires multiple training runs (cross validation) for determining C and ϵ (or ν)

SVM vs Logistic regression

Given the number of features n and the number of training samples m

- n is large relative to m: Logistic regression or SVM with linear kernel
- n is small and m is intermediate: SVM with Gaussian kernel
- n is small and m is large: Create/add more features, then use logistic regression or SVM with linear kernel

SVM vs ANN

- ANNs can be used when there is a large number of training sample available
- SVMs have a better generalization than ANNs due to Structural Risk Minimization (SRM) principle

Demo of SVM in Mathematica

Prelims

Linearly Seperable Data

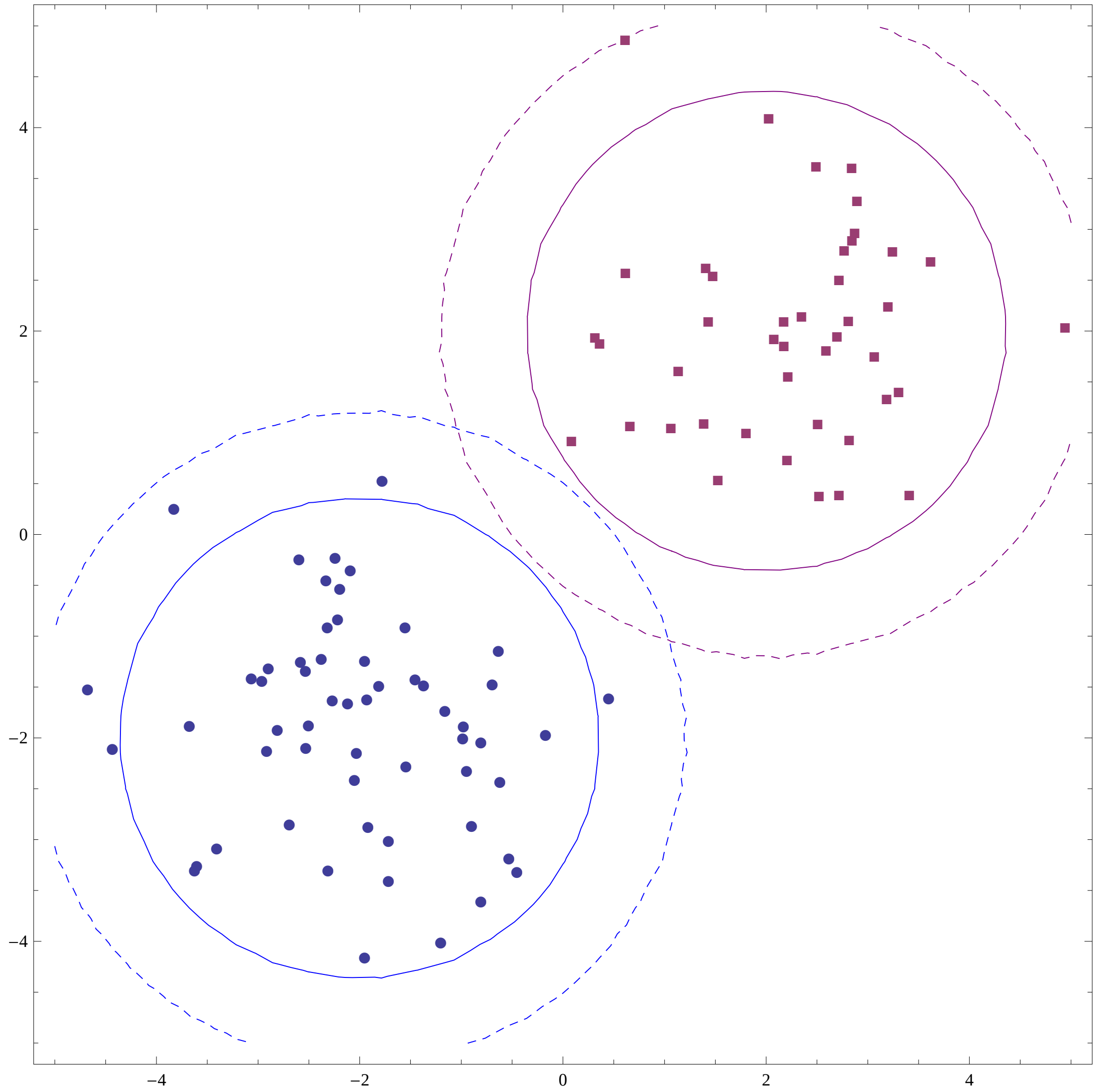
```
GenData[n_] := Module[{X, y, pos, neg, npos, nneg},
   {npos} = Ceiling[n RandomVariate[NormalDistribution[0.5, 0.25], 1]];
   nneg = n - npos;
   X = Join[
     RandomVariate[NormalDistribution[-2, 1], {npos, 2}],
     RandomVariate[NormalDistribution[2, 1], {nneg, 2}]];
   y = Join[Table[1, {npos}], Table[-1, {nneg}]];
   pos = Take[X, npos];
   neg = Take[X, -nneg];
   {X, y, pos, neg}];

dlen = 100;
{X, y, pos, neg} = GenData[dlen];

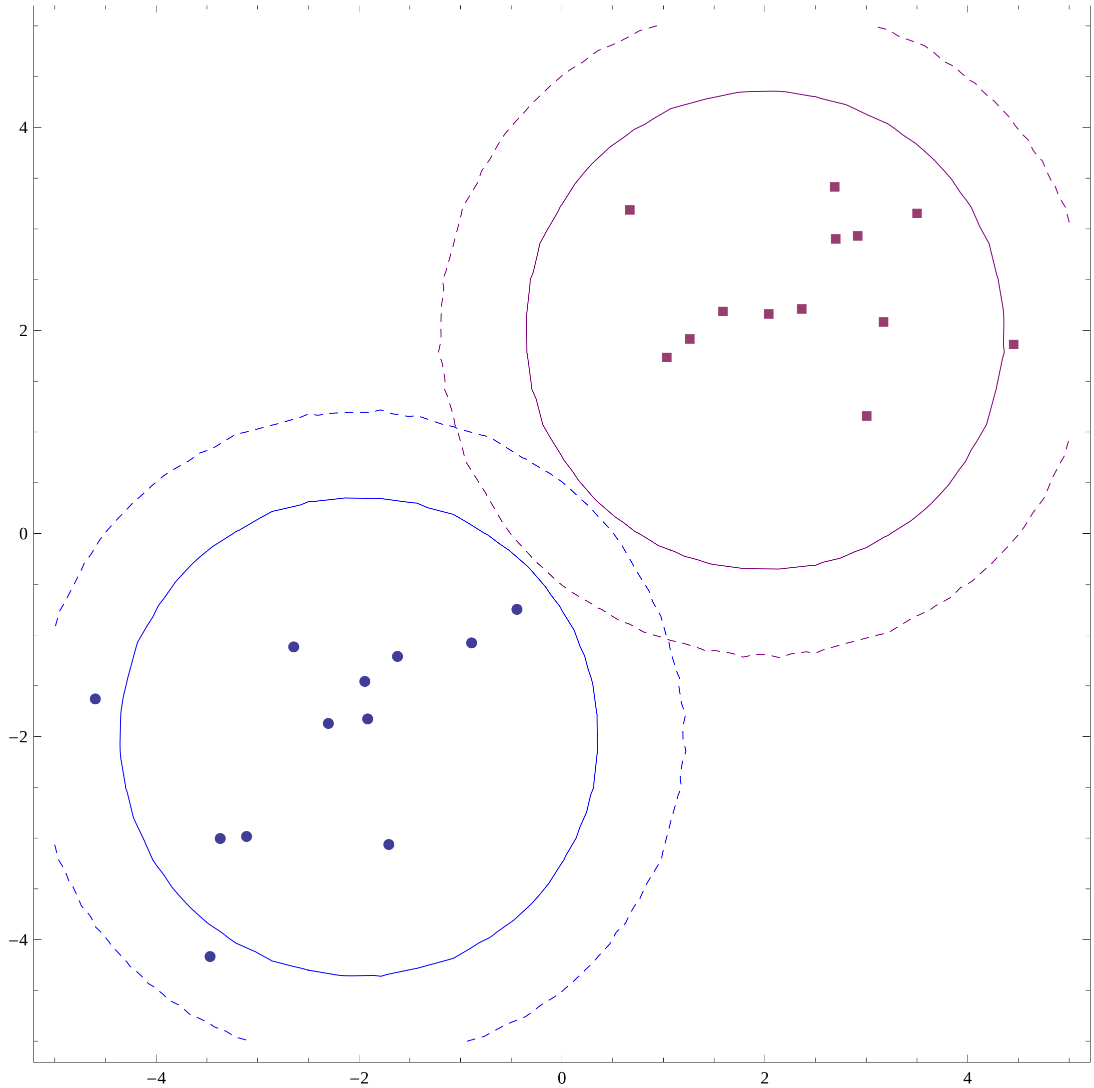
tlen = 25;
{tpos, tneg} = Take[GenData[tlen], -2];

distro = ContourPlot[
   {PDF[NormalDistribution[-2, 1], x] PDF[NormalDistribution[-2, 1], y] == 0.001,
    PDF[NormalDistribution[2, 1], x] PDF[NormalDistribution[2, 1], y] == 0.001,
    PDF[NormalDistribution[-2, 1], x] PDF[NormalDistribution[-2, 1], y] == 0.01,
    PDF[NormalDistribution[2, 1], x] PDF[NormalDistribution[2, 1], y] == 0.01},
   {x, -5, 5}, {y, -5, 5}, ContourStyle →
    {Directive[Dashed, Blue], Directive[Dashed, Purple], Blue, Purple}];
```

```
Show[distro, dataPlot = ListPlot[{pos, neg}, PlotMarkers → Automatic]]
```



```
Show[distro, testPlot = ListPlot[{tpos, tneg}, PlotMarkers → Automatic]]
```




```
τ = 0.01;
α = SeparableSVM[X, y, τ]
```

```
{0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0.530622, 0, 0,
 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0.281524, 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, 0, 0, 0, 0, 0, 0, 0,
 0, 0, 0.812146, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0}
```

```
w = {WeightVector[α, X, y]}
```

```
{{-0.884729, -0.921494}}
```

```
b = Bias[α, X, y]
```

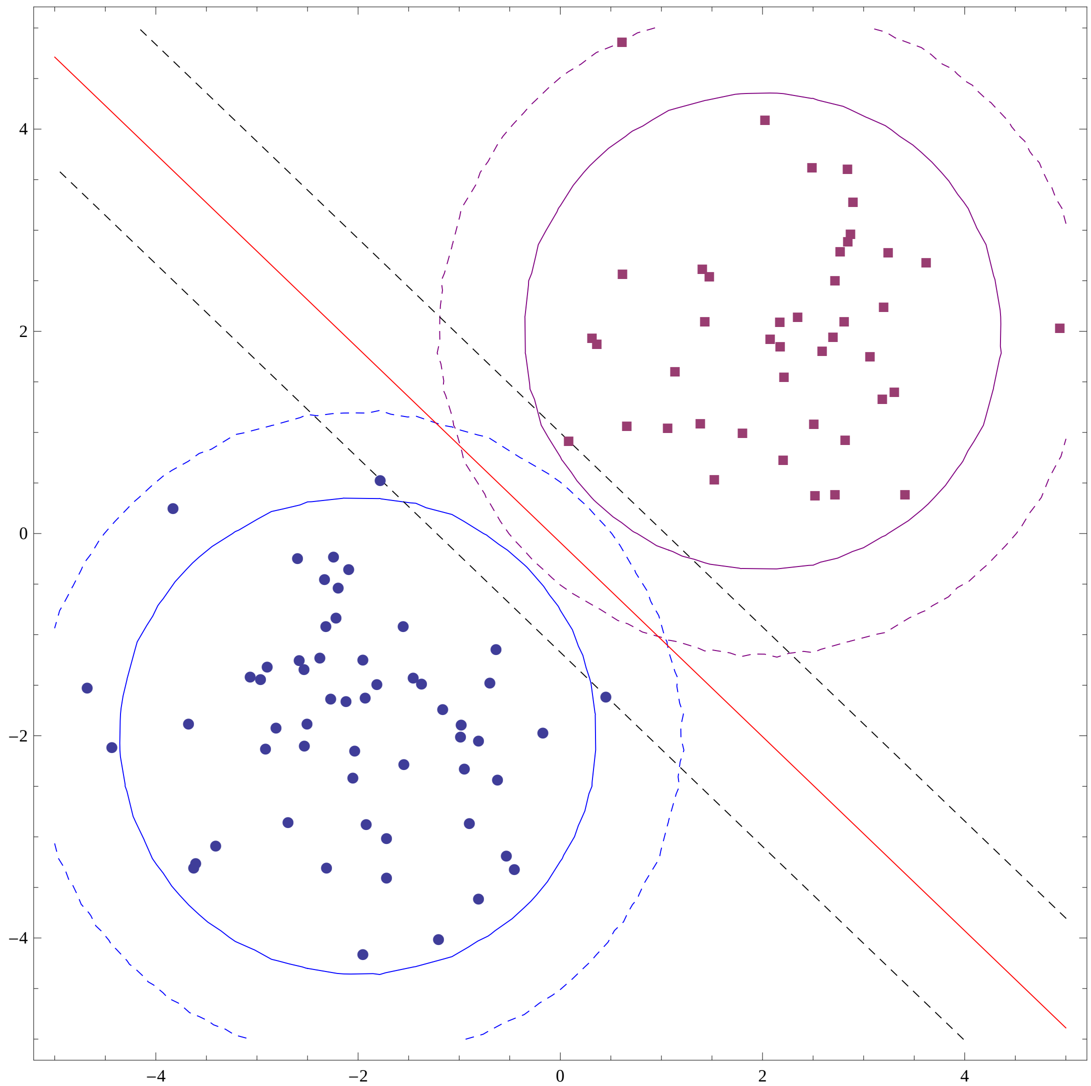
```
-0.0816545
```

```
g[x_, y_] := w.{{x}, {y}} + b
```

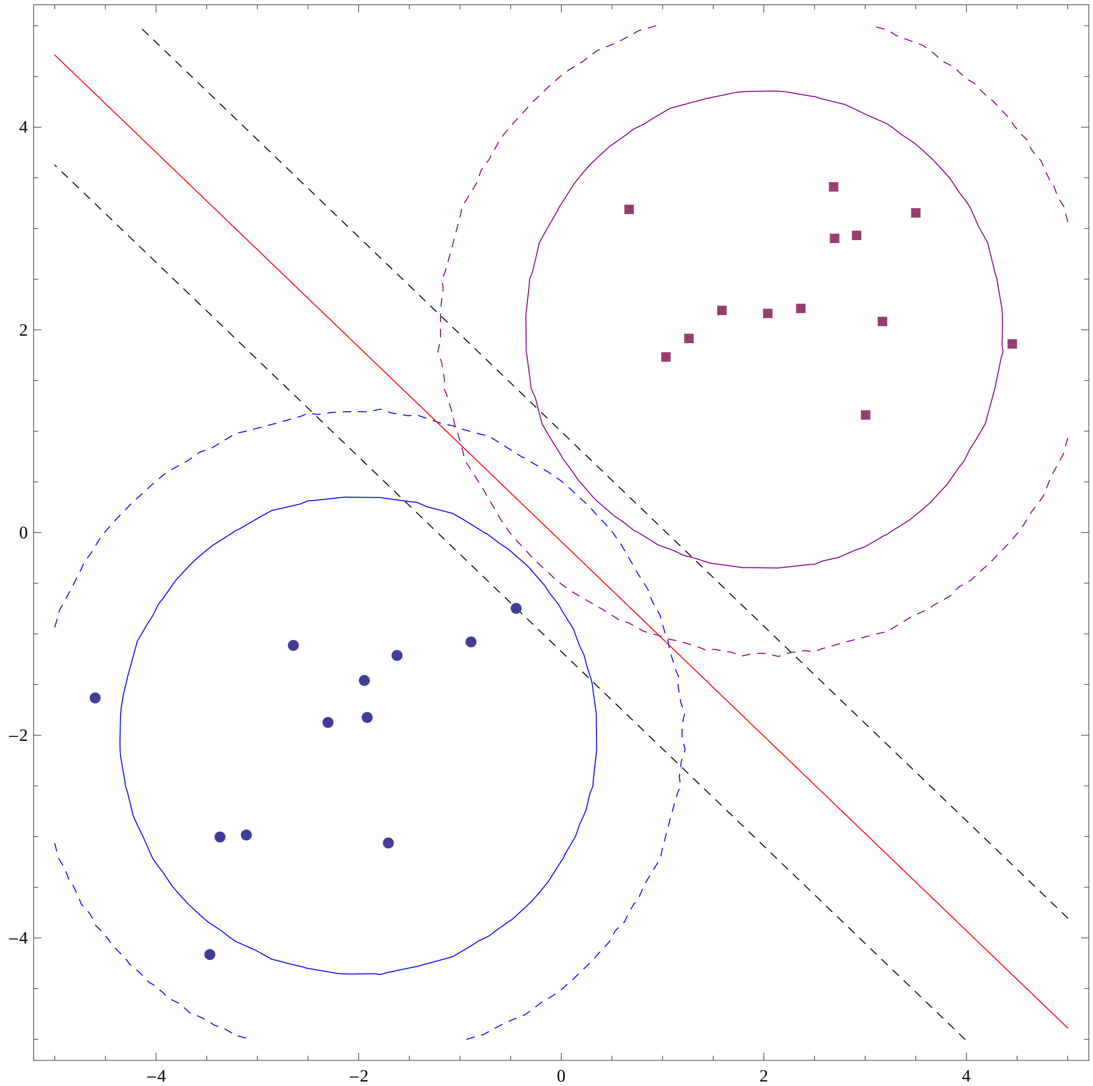
```
contour = ContourPlot[{g[x, y] == -1, g[x, y] == 0, g[x, y] == 1},
   {x, -5, 5}, {y, -5, 5}, ContourStyle → {Dashed, Red, Dashed}];
PDF[NormalDistribution[2, 1], x]
```

$$\frac{e^{-\frac{1}{2}(-2+x)^2}}{\sqrt{2\pi}}$$

```
Show[distro, contour, dataPlot]
```



```
Show[distro, contour, testPlot]
```



Spiral Data

$$\texttt{func[t\_, y\_] := } \frac{2}{17\,\mathrm{Pi}} \texttt{\{y t Sin[t], y t Cos[t]\}}$$

```
Clear[next];
```

$$\texttt{next[a\_, n\_] := next[a, n] = a + NArgMin}\left[\left\{\frac{1}{n}\,\texttt{Sum}\left[\texttt{Norm}\left[\texttt{D}\left[\texttt{func}\left[\texttt{a + i}\,\frac{b}{n}\texttt{, 1}\right]\right]\right]\texttt{, \{i, 0, n\}}\right]\texttt{,}\right.\right.$$
$$\left.\left.\frac{1}{n}\,\texttt{Sum}\left[\texttt{Norm}\left[\texttt{D}\left[\texttt{func}\left[\texttt{a + i}\,\frac{b}{n}\texttt{, 1}\right]\right]\right]\texttt{, \{i, 0, n\}}\right] > \frac{1}{20}\texttt{, b > 0}\right\}\texttt{, \{b\}}\right]\texttt{[[1]];}$$

```
Clear[next];
next[a_, n_] := next[a, n] = a + NArgMin[{Norm[func[a, 1] - func[a + b, 1]],
    Norm[func[a, 1] - func[a + b, 1]] > 1 / 20, b > 0}, {b}][[1]];
```

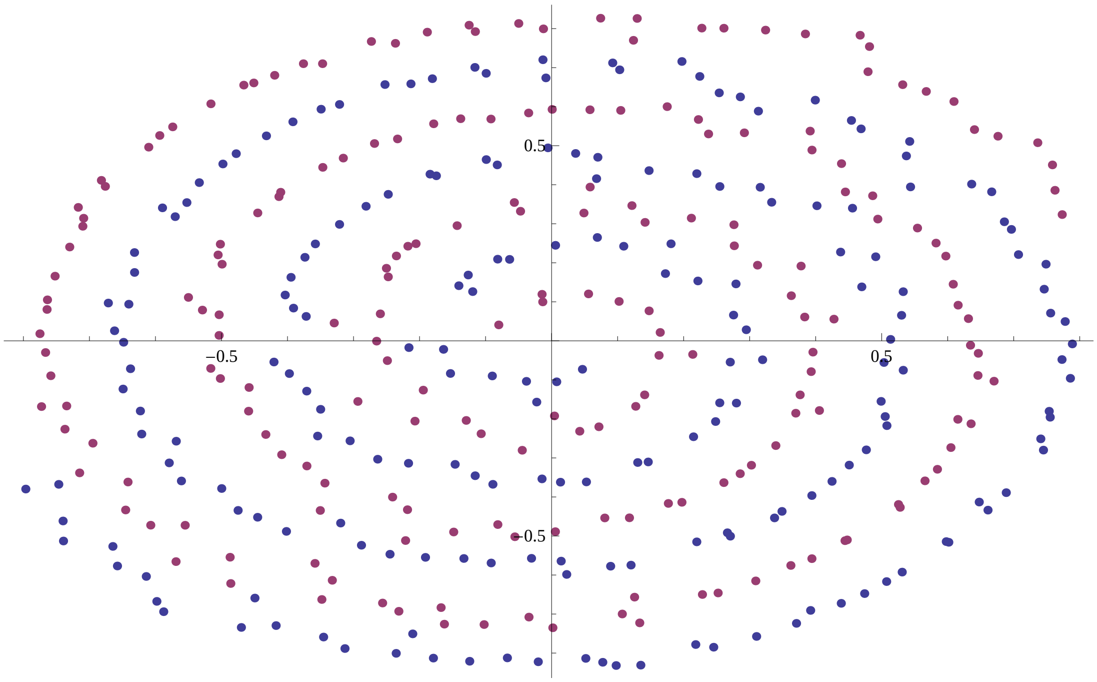
```
indices = Table[Nest[next[#, 10] &, 13 / 25 Pi, i], {i, 1, 200}]
```

```
{2.25815, 2.75919, 3.18869, 3.57022, 3.91676, 4.23637, 4.53442, 4.81472, 5.08008,
 5.33265, 5.57409, 5.80576, 6.02873, 6.24392, 6.45208, 6.65386, 6.8498, 7.04039,
 7.22603, 7.40709, 7.5839, 7.75673, 7.92584, 8.09147, 8.25382, 8.41307, 8.56939,
 8.72295, 8.87388, 9.02231, 9.16836, 9.31214, 9.45376, 9.59331, 9.73087, 9.86653,
 10.0004, 10.1325, 10.2629, 10.3916, 10.5188, 10.6445, 10.7688, 10.8916, 11.0131,
 11.1333, 11.2522, 11.3698, 11.4863, 11.6016, 11.7157, 11.8288, 11.9408, 12.0518,
 12.1617, 12.2707, 12.3788, 12.4859, 12.5921, 12.6974, 12.8018, 12.9054, 13.0082,
 13.1102, 13.2114, 13.3118, 13.4115, 13.5105, 13.6087, 13.7063, 13.8031, 13.8993,
 13.9948, 14.0897, 14.184, 14.2776, 14.3706, 14.463, 14.5549, 14.6461, 14.7368, 14.827,
 14.9166, 15.0057, 15.0942, 15.1822, 15.2698, 15.3568, 15.4434, 15.5294, 15.615,
 15.7001, 15.7848, 15.869, 15.9528, 16.0361, 16.119, 16.2015, 16.2836, 16.3653,
 16.4465, 16.5274, 16.6078, 16.6879, 16.7676, 16.8469, 16.9259, 17.0045, 17.0827,
 17.1606, 17.2381, 17.3153, 17.3921, 17.4686, 17.5447, 17.6206, 17.6961, 17.7713,
 17.8461, 17.9207, 17.995, 18.0689, 18.1426, 18.2159, 18.289, 18.3617, 18.4342,
 18.5064, 18.5783, 18.65, 18.7213, 18.7924, 18.8633, 18.9338, 19.0041, 19.0742,
 19.144, 19.2135, 19.2828, 19.3518, 19.4206, 19.4892, 19.5575, 19.6256, 19.6934,
 19.761, 19.8284, 19.8955, 19.9625, 20.0292, 20.0957, 20.1619, 20.228, 20.2938,
 20.3594, 20.4248, 20.49, 20.555, 20.6198, 20.6844, 20.7488, 20.813, 20.877, 20.9407,
 21.0044, 21.0678, 21.131, 21.194, 21.2569, 21.3195, 21.382, 21.4443, 21.5064,
 21.5683, 21.6301, 21.6917, 21.7531, 21.8143, 21.8754, 21.9363, 21.997, 22.0576,
 22.118, 22.1782, 22.2383, 22.2982, 22.3579, 22.4175, 22.477, 22.5362, 22.5953,
 22.6543, 22.7131, 22.7718, 22.8303, 22.8887, 22.9469, 23.0049, 23.0629, 23.1206}
```

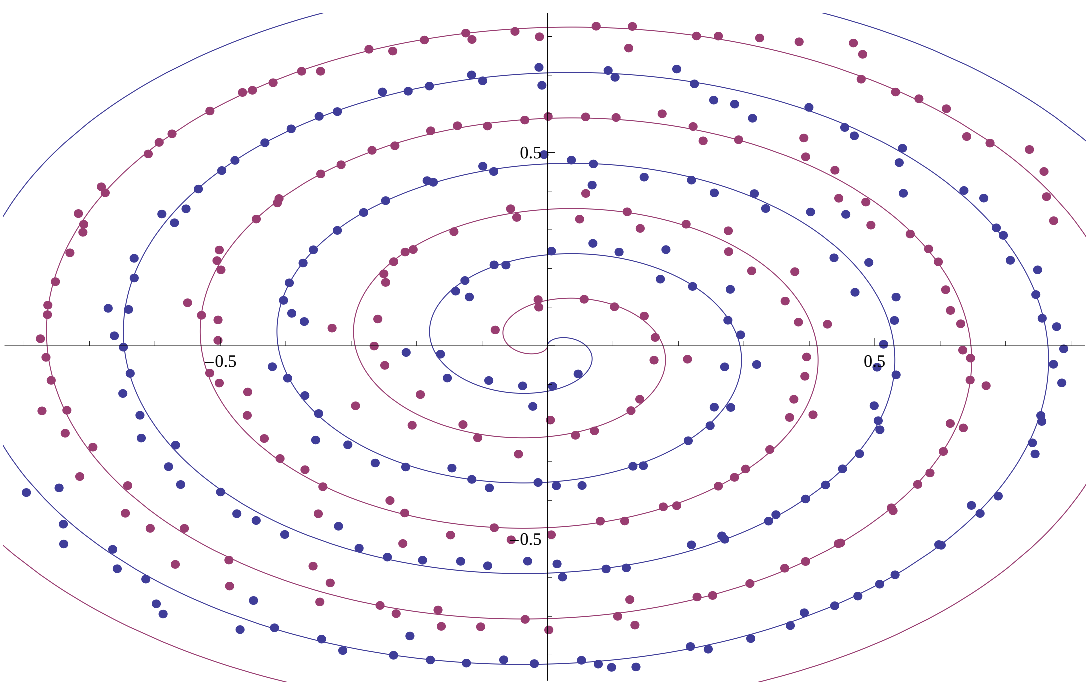
```
funcPlot = ParametricPlot[{func[t, 1], func[t, -1]}, {t, 0, (8 + 1 / 2) Pi}];
```

```
Nd = 200;
(*data=Table[Join[func[(i+12)/25Pi,(-1)^i+RandomReal[]/25]
     (*+{RandomReal[],RandomReal[]}/15*),{(-1)^i}],{i,1,Nd}]//N;*)
(*data=Import["spiral-data.csv"];*)
dist = NormalDistribution[0, 0.02];
RandomIndices[n_, k_] := Intersection[Round /@ Table[RandomReal[] * n, {k}]];
genPoint[t_, c_] :=
  Join[func[t + RandomReal[] / 25, c] + RandomVariate[dist] {1, 1}, {c}];
data = Join[Table[genPoint[indices[[i]], 1], {i, 1, Length[indices]}],
   Table[genPoint[indices[[i]], -1], {i, 1, Length[indices]}]];
test = Join[Table[genPoint[indices[[i]], 1],
     {i, RandomIndices[Length[indices], Ceiling[0.2 Length[indices]]]}],
   Table[genPoint[indices[[i]], -1],
     {i, RandomIndices[Length[indices], Ceiling[0.2 Length[indices]]]}]];
Nd = Length[data];
xdata = Table[{data[[i, 1]], data[[i, 2]]}, {i, 1, Nd}];
ydata = Table[data[[i, 3]], {i, 1, Nd}];
pos = Table[{item[[1]], item[[2]]}, {item, Select[data, #[[3]] > 0 &]}];
neg = Table[{item[[1]], item[[2]]}, {item, Select[data, #[[3]] < 0 &]}];
tpos = Table[{item[[1]], item[[2]]}, {item, Select[test, #[[3]] > 0 &]}];
tneg = Table[{item[[1]], item[[2]]}, {item, Select[test, #[[3]] < 0 &]}];
```

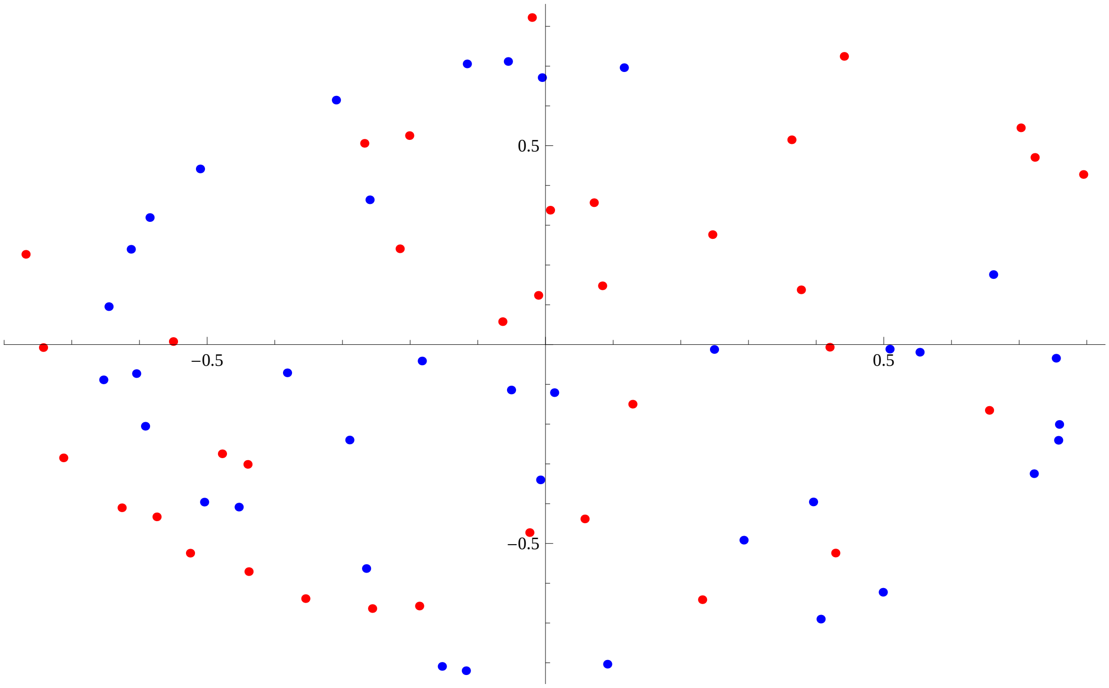
```
dPlot = ListPlot[{pos, neg}, PlotStyle → PointSize[Medium]]
```




```
Show[dPlot, funcPlot]
```



```
tPlot = ListPlot[{tpos, tneg},
  PlotStyle → {Directive[PointSize[Medium], Blue], Directive[PointSize[Medium], Red]}]
```



■ As a separable dataset

```
? SeparableSVM
```

SeparableSVM[X,y,τ] trains a separable SVM on data X, labels y, and solution tolerance τ (see QPSolve). Returns the multiplier vector α. Option KernelFunction determines the kernel to use; default is IdentityKernel (i.e., no kernel).

```
krbf[x_, y_] := RBFKernel[x, y, 100];

α = SeparableSVM[xdata, ydata, 0.01, KernelFunction → krbf];

ynew[α_, X_, y_, k_] := Sum[α[[i]] y[[i]] k[#, X[[i]]], {i, 1, Length[X]}] &

rbfY = ynew[α, xdata, ydata, krbf];

rbfPlot = ContourPlot[rbfY[{x, y}], {x, -1, 1}, {y, -1, 1}, Contours → {-1, 0, 1},
   ContourStyle → {Dashed, Black, Dashed}, ContourShading → None];

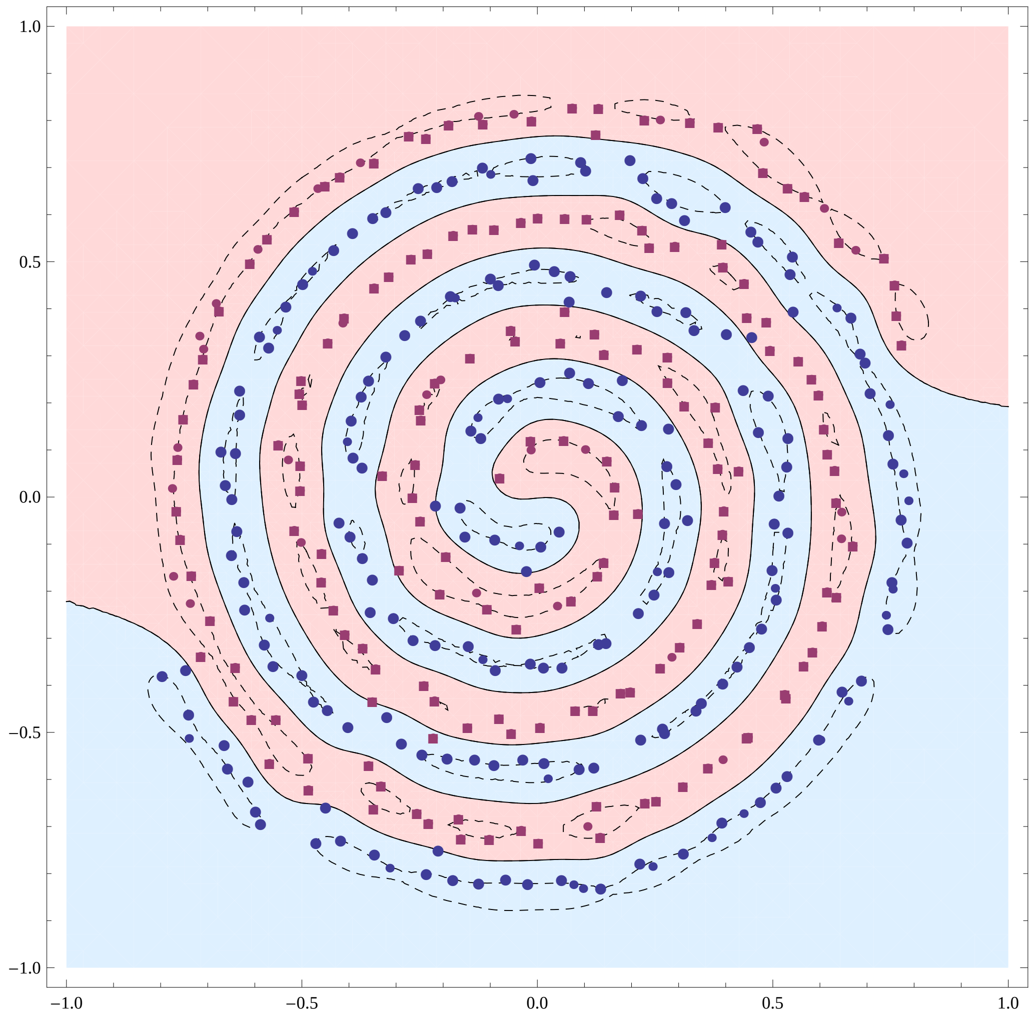
rbfPlotShading = ContourPlot[rbfY[{x, y}], {x, -1, 1}, {y, -1, 1}, Contours → {0},
   ContourStyle → {Dashed, Black, Dashed}, ContourShading → {LightRed, LightBlue}];

SVs = ListPlot[{({#[[1]], #[[2]]}) & /@ #1[[1]], ({#[[1]], #[[2]]}) & /@ #2[[1]]} & @@
    SplitBy[Table[data[[i]], {i, SupportVectors[α, ydata]}], #[[3]] &],
   PlotMarkers → Automatic];
```

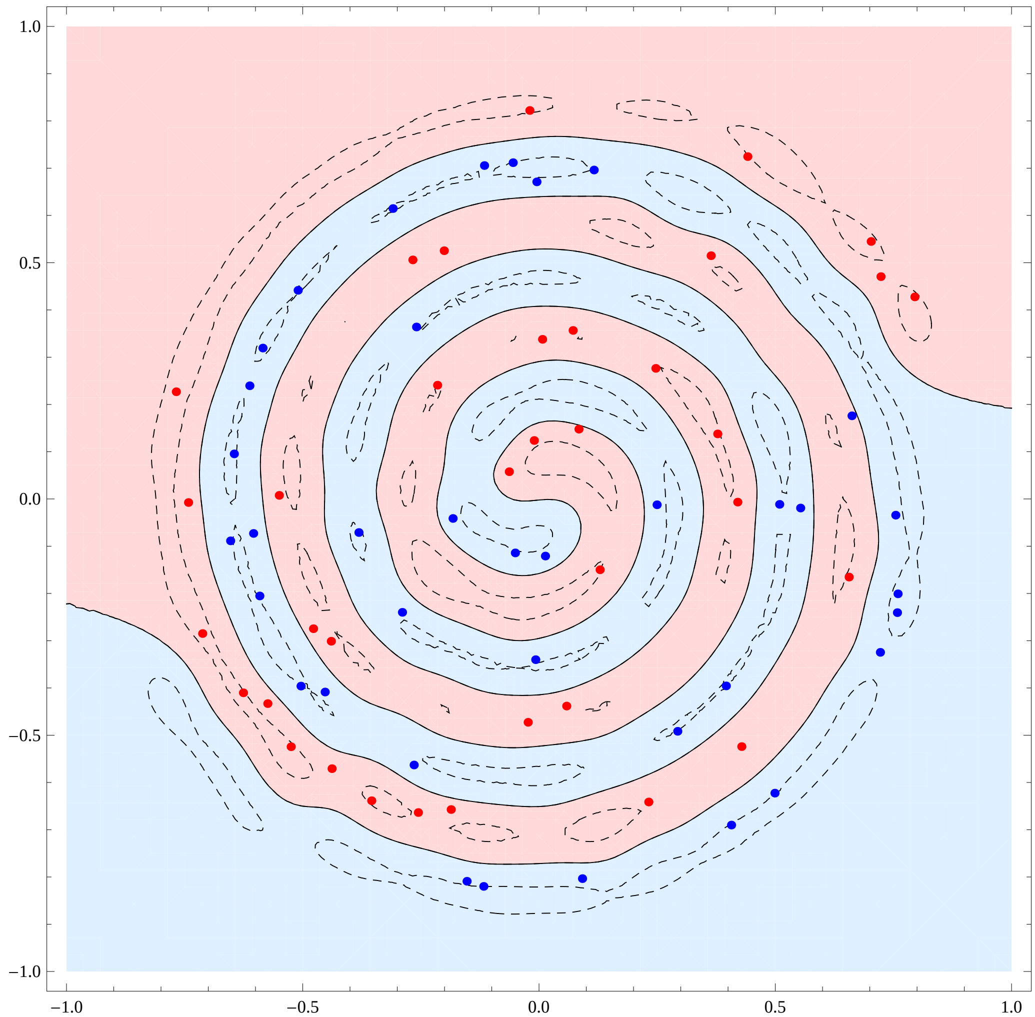
```
SupportVectors[α, ydata]
```

```
{{1, 2, 3, 5, 6, 7, 8, 9, 10, 12, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 26, 27, 28, 29,
  30, 31, 32, 33, 34, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 48, 49, 50, 51, 52,
  53, 54, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74,
  75, 76, 77, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 92, 93, 94, 95, 96, 97,
  98, 99, 100, 101, 102, 103, 104, 105, 107, 108, 109, 110, 111, 112, 113, 114, 115,
  116, 117, 119, 120, 121, 123, 124, 125, 126, 127, 128, 129, 130, 132, 133, 134, 135,
  136, 137, 138, 139, 140, 141, 142, 143, 144, 145, 146, 148, 149, 150, 151, 153, 154,
  157, 158, 159, 162, 163, 164, 166, 168, 169, 170, 173, 174, 176, 177, 180, 181, 182,
  183, 184, 185, 186, 188, 189, 190, 191, 192, 193, 194, 195, 196, 198, 199, 200},
 {201, 202, 204, 206, 207, 208, 209, 210, 211, 212, 214, 215, 216, 218, 219, 220, 221,
  222, 223, 224, 225, 226, 228, 230, 231, 232, 233, 234, 235, 236, 237, 238, 239, 240,
  241, 242, 243, 244, 245, 246, 247, 248, 249, 250, 251, 253, 254, 255, 256, 257, 258,
  259, 260, 261, 262, 263, 264, 265, 266, 267, 268, 269, 270, 271, 273, 274, 275, 277,
  278, 279, 280, 281, 283, 284, 285, 286, 287, 288, 289, 290, 291, 292, 293, 294, 295,
  296, 297, 298, 299, 300, 301, 302, 303, 304, 305, 306, 307, 308, 309, 310, 311, 314,
  315, 316, 317, 318, 319, 320, 321, 322, 323, 325, 326, 327, 328, 329, 331, 332, 333,
  334, 335, 336, 337, 338, 339, 340, 341, 342, 343, 344, 345, 346, 347, 348, 349, 350,
  352, 354, 355, 357, 359, 360, 361, 364, 366, 368, 369, 371, 372, 374, 375, 376, 377,
  379, 381, 382, 383, 384, 385, 387, 388, 389, 391, 392, 393, 395, 397, 398, 399, 400}}
```

```
Show[rbfPlotShading, rbfPlot, dPlot, SVs]
```



```
Show[rbfPlotShading, rbfPlot, tPlot]
```



- **As a nonseparable dataset**

```
? NonseparableSVM
```

NonSeparableSVM[X, y, C, τ] trains a non-separable SVM on data X, labels y, penalty term C and solution tolerance τ (see QPSolve). Returns the multiplier vector α. Option KernelFunction determines the kernel to use; default is IdentityKernel (i.e., no kernel)

```
α2 = NonseparableSVM[xdata, ydata, 1.0, 0.01, KernelFunction → krbf];

rbfY2 = ynew[α, xdata, ydata, krbf];

rbfPlot2 = ContourPlot[rbfY2[{x, y}], {x, -1, 1}, {y, -1, 1}, Contours → {-1, 0, 1},
   ContourStyle → {Dashed, Black, Dashed}, ContourShading → None];

rbfPlotShading2 = ContourPlot[rbfY2[{x, y}], {x, -1, 1}, {y, -1, 1}, Contours → {0},
   ContourStyle → {Dashed, Black, Dashed}, ContourShading → {LightRed, LightBlue}];
```

```
SVs2 = ListPlot[{({#[[1]], #[[2]]}) & /@ #1[[1]], ({#[[1]], #[[2]]}) & /@ #2[[1]]} & @@
    SplitBy[Table[data[[i]], {i, SupportVectors[α2, ydata]}], #[[3]] &],
   PlotMarkers → Automatic];
```

```
SupportVectors[α2, ydata]
```

```
{{1, 2, 3, 5, 6, 7, 8, 9, 10, 12, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 26, 27, 28, 29,
  30, 31, 32, 33, 34, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 48, 49, 50, 51, 52,
  53, 54, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74,
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Show[rbfPlotShading2, rbfPlot2, dPlot, SVs2]
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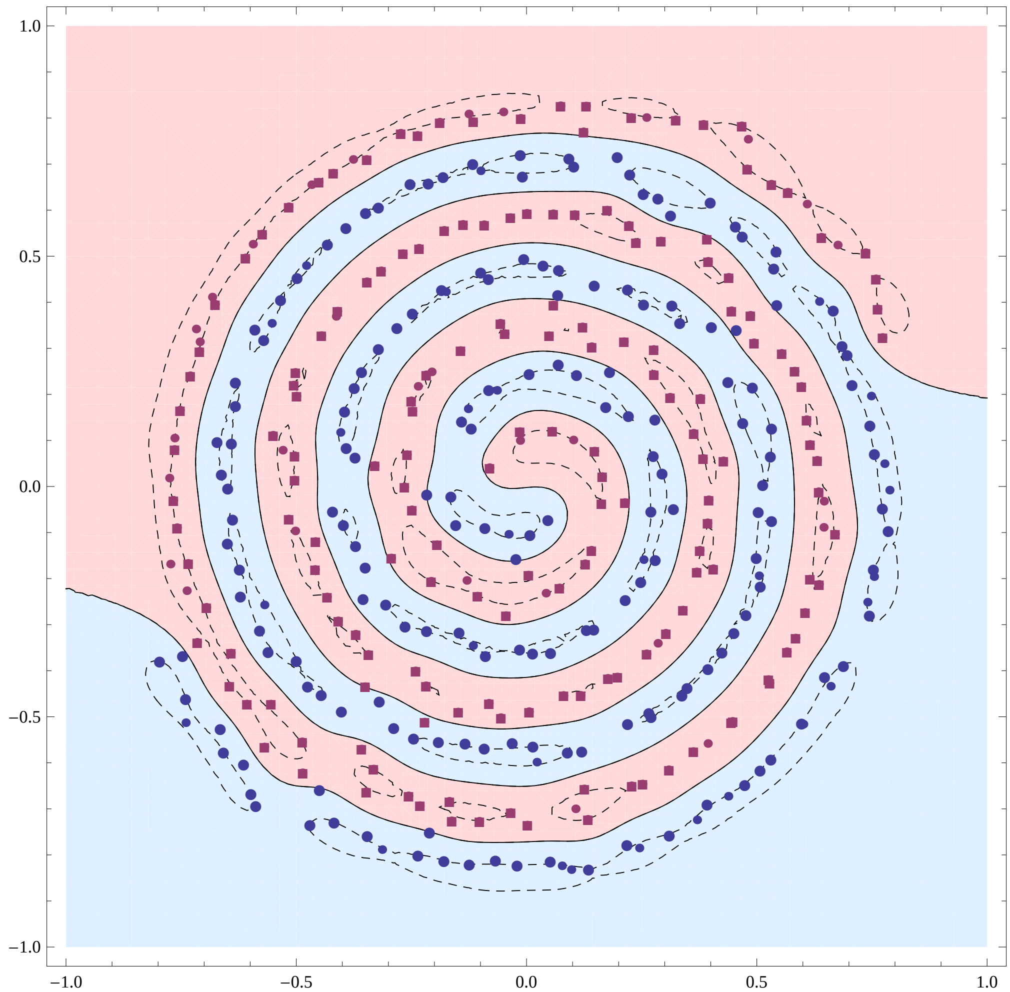

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Show[rbfPlotShading2, rbfPlot2, tPlot]
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