UVA CS 4501: Machine Learning

Lecture 17: Support Vector Machine (nonlinear) Kernel Trick and in Practice

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Where are we ? → Five major sections of this course

- Regression (supervised)
- ☐ Classification (supervised)
- Unsupervised models
- Learning theory
- ☐ Graphical models

Today

- Support Vector Machine (SVM)
 - ✓ History of SVM
 - ✓ Large Margin Linear Classifier
 - ✓ Define Margin (M) in terms of model parameter
 - ✓ Optimization to learn model parameters (w, b)
 - ✓ Non linearly separable case
 - ✓ Optimization with dual form
 - ✓ Nonlinear decision boundary
 - ✓ Practical Guide

Dual SVM for linearly separable case - Training / Testing

Our dual target function:
$$\max_{\alpha} \sum_{i} \alpha_{i} - \frac{1}{2} \sum_{i,j} \alpha_{i} \alpha_{j} y_{i} y_{j} \mathbf{x}_{i}^{T} \mathbf{x}_{j}$$

$$\sum_{i} \alpha_{i} y_{i} = 0$$

$$\alpha_i \ge 0$$

 $\forall i$

Dot product for all training samples

Dot product with ("all" ??) training samples

To evaluate a new sample x_{ts} we need to compute:

$$\mathbf{w}^{\mathrm{T}} \mathbf{x}_{ts} + b = \sum_{\mathbf{i}} \alpha_{\mathbf{i}} \mathbf{y}_{\mathbf{i}} \mathbf{x}_{\mathbf{i}}^{\mathrm{T}} \mathbf{x}_{ts} + b$$

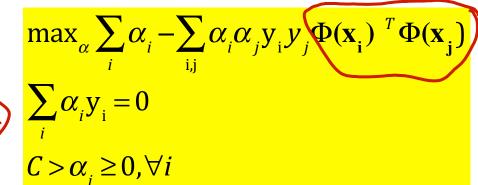


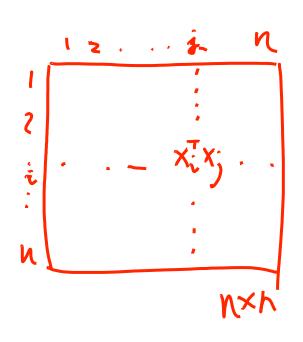
$$\widehat{y}_{ts} = \operatorname{sign}\left(\sum_{i \in SupportVectors} \alpha_i y_i \left(\mathbf{x}_i^T \mathbf{x}_{ts}\right) + b\right)$$

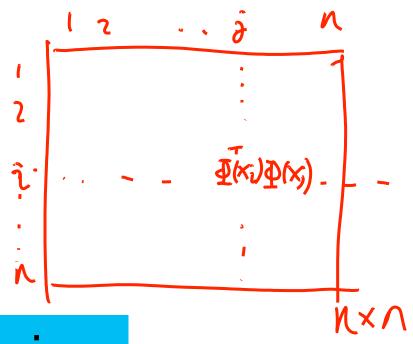
$$\max_{\alpha} \sum_{i} \alpha_{i} - \frac{1}{2} \sum_{i,j} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{i}^{T} x_{j}$$

$$\sum_{i} \alpha_{i} y_{i} = 0$$

$$C > \alpha_i \ge 0, \forall i$$



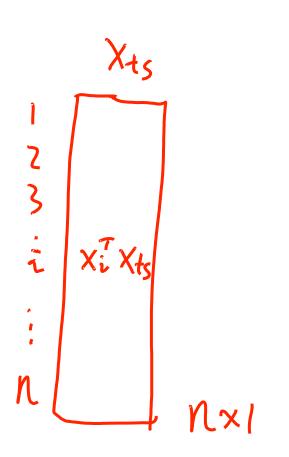




Training

$$\mathbf{w}^{\mathrm{T}} \mathbf{x}_{ts} + b = \sum_{\mathbf{i}} \alpha_{\mathbf{i}} \mathbf{y}_{\mathbf{i}} \mathbf{x}_{\mathbf{i}}^{\mathrm{T}} \mathbf{x}_{ts} + b$$

$$\widehat{y}_{ts} = \operatorname{sign}\left(\sum_{i \in SupportVectors} \alpha_i y_i \left(\mathbf{x}_i^T \mathbf{x}_{ts}\right) + b\right)$$



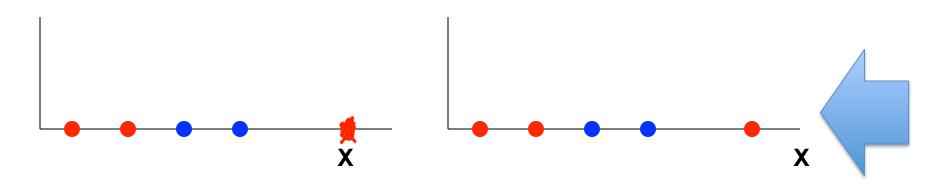


Testing

Classifying in 1-d

Can an SVM correctly classify this data?

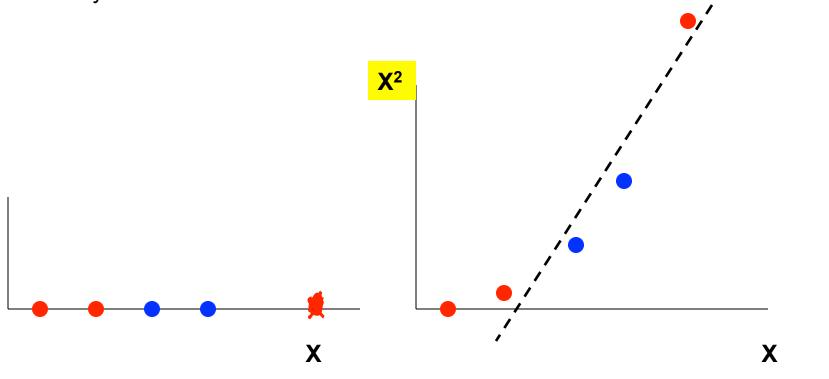
What about this?



Classifying in 1-d Separable In nonlinear

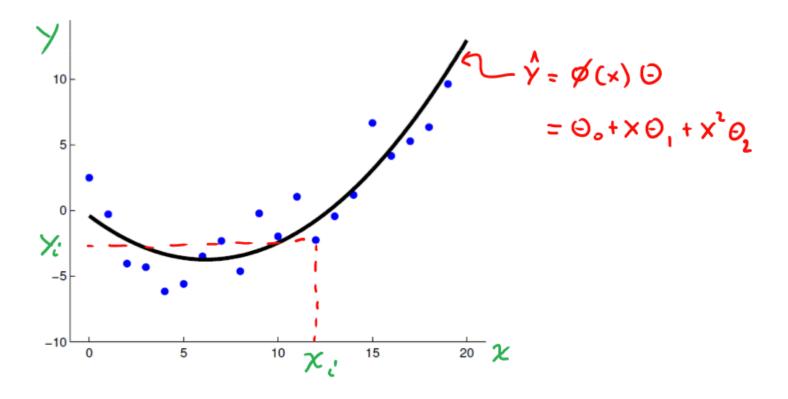
Can an SVM correctly classify this data?

And now? (extend with polynomial basis)



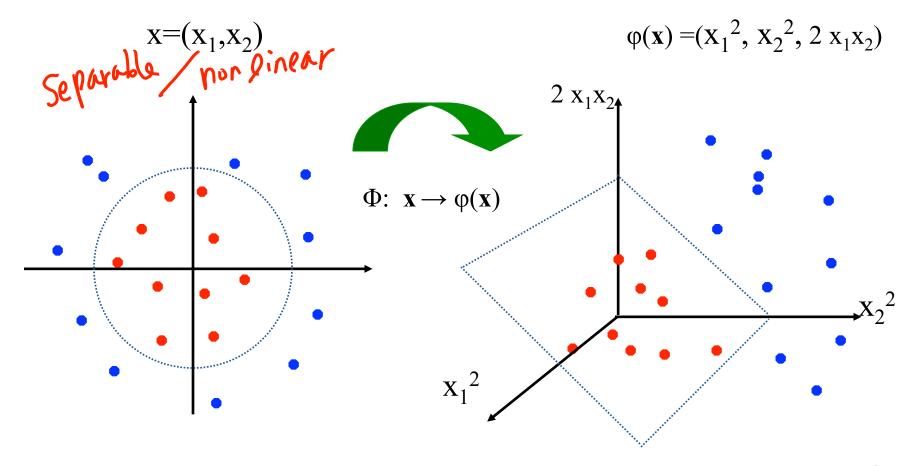
RECAP: Polynomial regression

For example, $\phi(x) = [1, x, x^2]$



Non-linear SVMs: 2D

• The original input space (x) can be mapped to some higher-dimensional feature space ($\phi(\mathbf{x})$) where the training set is separable:



Non-linear SVMs: 2D

• The original input space (x) can be mapped to some higher-dimensional feature space ($\phi(\mathbf{x})$) where the training set is separable:

$$x=(x_1,x_2)$$
 $\phi(x)=(x_1^2,x_2^2,\ 2x_1x_2)$

If data is mapped into sufficiently high dimension, then samples will in general be linearly separable;

N data points are in general separable in a space of N-1 dimensions or more!!!

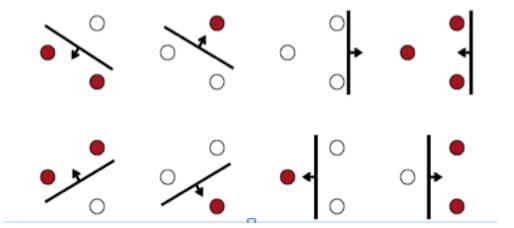
A little bit theory: Vapnik-Chervonenkis (VC) dimension

If data is mapped into sufficiently high dimension, then samples will in general be linearly separable;

N data points are in general separable in a space of N-1 dimensions or more!!!

VC dimension of the set of oriented lines in R² is 3

 It can be shown that the VC dimension of the family of oriented separating hyperplanes in R^N is at least N+1

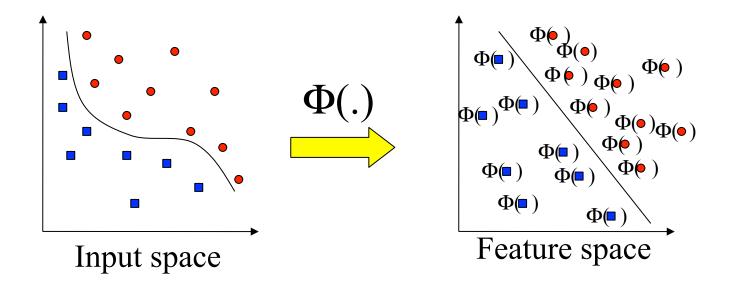


If data is mapped into sufficiently high dimension, then samples will in general be linearly separable;

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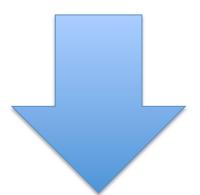
- Possible problems
 - High computation burden due to high-dimensionality
 - Many more parameters to estimate



SVM solves these two issues simultaneously

- "Kernel tricks" for efficient computation
- Dual formulation only assigns parameters to samples, not to features

- SVM solves these two issues simultaneously
 - "Kernel tricks" for efficient computation
 - Dual formulation only assigns parameters to samples, not features



(1). "Kernel tricks" for efficient computation

Never represent features explicitly

☐ Compute dot products in closed form

Very interesting theory – Reproducing Kernel Hilbert Spaces

Not covered in detail here

$$K(\mathbf{x}_i, \mathbf{x}_j) \equiv \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$$
 is called the kernel function.

- Linear kernel (we've seen it)
- $K(\mathbf{x},z) = \mathbf{x}^T z$



Polynomial kernel (we will see an example)

$$K(\mathbf{x},z) = \left(1 + \mathbf{x}^T z\right)^d = \Phi(\mathbf{x}) \Phi(\mathbf{y})$$

where d = 2, 3, ... To get the feature vectors we concatenate all dth order polynomial terms of the components of x (weighted appropriately)

Radial basis kernel

$$K(\mathbf{x},z) = \exp\left(-r\left\|\mathbf{x}-z\right\|^{2}\right) = \Phi(\mathbf{x}) \Phi(\mathbf{z})$$

In this case., r is hyperpara. The feature space of the RBF kernel has an infinite number of dimensions

Never represent features explicitly

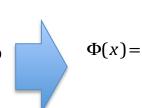
- ☐ Compute dot products with a closed form
- Very interesting theory Reproducing Kernel Hilbert Spaces
 - Not covered in detail here

Example: Quadratic kernels

$$K(\mathbf{x},z) = \left(1 + \mathbf{x}^T z\right)^d \qquad \left(1 + \mathbf{x}^T z\right)^T$$

$$K(\mathbf{x},z) := \Phi(\mathbf{x})^T \Phi(z)$$

 \bullet Consider all quadratic terms for $x_{1},\,x_{2}\,\ldots\,x_{p}$



$$\max_{\alpha} \sum_{i} \alpha_{i} - \sum_{i,j} \alpha_{i} \alpha_{j} y_{i} y_{j} \Phi(\mathbf{x}_{i})^{T} \Phi(\mathbf{x}_{j})$$
$$\sum_{i} \alpha_{i} y_{i} = 0$$
$$\alpha_{i} \ge 0 \qquad \forall i$$

$$\begin{array}{c}
1\\
\sqrt{2}x_1\\
\vdots\\
\sqrt{2}x_p
\end{array}$$

$$\begin{array}{c}
x_1^2\\
\vdots\\
x_p^2\\
\end{array}$$

$$\begin{array}{c}
\sqrt{2}x_1x_2\\
\vdots\\
\sqrt{2}x_{p-1}x_p
\end{array}$$

$$K(\mathbf{x},z) = (1+\mathbf{x}^{T}z)^{2} \quad \left(d=2\right), \quad \left(P=2\right) \quad \left(\chi = (\chi_{1},\chi_{2})\right) \\ k(\chi,\delta) = \left(1+\chi_{1}\delta_{1}+\chi_{2}\delta_{2}\right)^{2} \quad \Rightarrow \left(0(P)\right) \\ \left(P^{2}\right) \quad \left(P$$

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The kernel trick

p^d*n^2 operations if using the basis function representations in building a poly-kernel matrix

So, if we define the **kernel function** as follows, there is no need to carry out basis function explicitly

$$K(\mathbf{x},z) = (x^T z + 1)^{d=2}$$



p*n^2 operations in building a
poly-kernel matrix for training

$$\max_{\alpha} \sum_{i} \alpha_{i} - \frac{1}{2} \sum_{i,j} \alpha_{i} \alpha_{j} y_{i} y_{j} K(\mathbf{x}_{i}, \mathbf{x}_{j})$$

$$\sum_{i} \alpha_{i} y_{i} = 0$$

$$C > \alpha_i \ge 0, \forall i \in train$$

Summary: Modification Due to Kernel Trick

- Change all inner products to kernel functions
- For training,

Original Linear

$$\max_{\alpha} \sum_{i} \alpha_{i} - \frac{1}{2} \sum_{i,j} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{i}^{T} x_{j}$$

$$\sum_{i} \alpha_{i} y_{i} = 0$$

$$C > \alpha_{i} \ge 0, \forall i \in train$$

With kernel function - nonlinear

$$\max_{\alpha} \sum_{i} \alpha_{i} - \frac{1}{2} \sum_{i,j} \alpha_{i} \alpha_{j} y_{i} y_{j} K(\mathbf{x}_{i}, \mathbf{x}_{j})$$

$$\sum_{i} \alpha_{i} y_{i} = 0$$

$$C > \alpha_{i} \ge 0, \forall i \in train$$

Summary: Modification Due to Kernel Function

For testing, the new data x_ts

$$\widehat{y_{ts}} = \operatorname{sign}\left(\sum_{i \in \operatorname{train}} \alpha_i y_i x_i^T x_{ts} + b\right)$$

With kernel function - nonlinear

$$\widehat{y_{ts}} = \operatorname{sign}\left(\sum_{i \in \text{supportVectors}} \alpha_i y_i K(\mathbf{x_i}, \mathbf{x_{ts}}) + b\right)$$

An example: Support vector machines with polynomial kernel

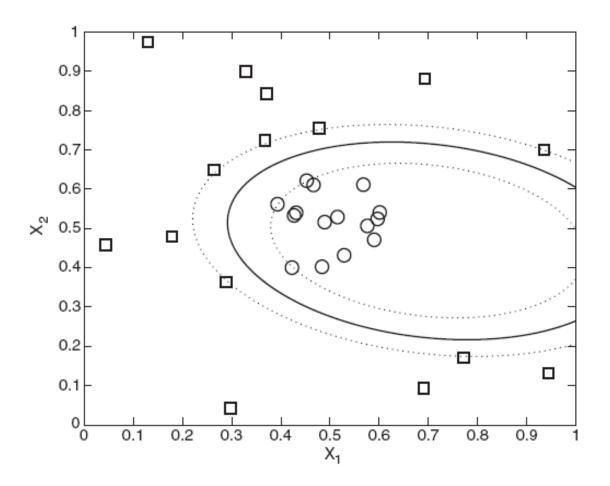


Figure 5.29. Decision boundary produced by a nonlinear SVM with polynomial kernel.

Kernel Trick: Implicit Basis Representation

- For some kernels (e.g. RBF) the implicit transform basis form \phi(x) is infinitedimensional!
 - But calculations with kernel are done in original space, so computational burden and curse of dimensionality aren't a problem.

$$K(\mathbf{x},z) = \exp\left(-r||\mathbf{x}-z||^2\right)$$

p*n^2 operations in building a RBF-kernel matrix for training → Gaussian RBF Kernel corresponds to an infinite-dimensional vector space.

YouTube video of Caltech: Abu-Mostafa explaining this in more detail https://www.youtube.com/watch? v=XUj5JbQihlU&t=25m53s

Kernel Functions (Extra)

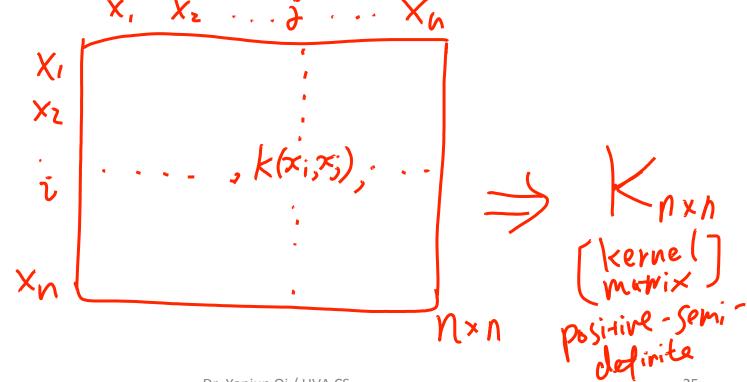
- In practical use of SVM, only the kernel function (and not basis function) is specified
- Kernel function can be thought of as a similarity measure between the input objects
- Not all similarity measure can be used as kernel function, however Mercer's condition states that any positive semi-definite kernel K(x, y), i.e. $\sum_{i \in K} K(x_i, x_j) c_i c_j \ge 0$

*33

can be expressed as a dot product in a high dimensional space.

Kernel Matrix

 Kernel function creates the kernel matrix, which summarize all the data



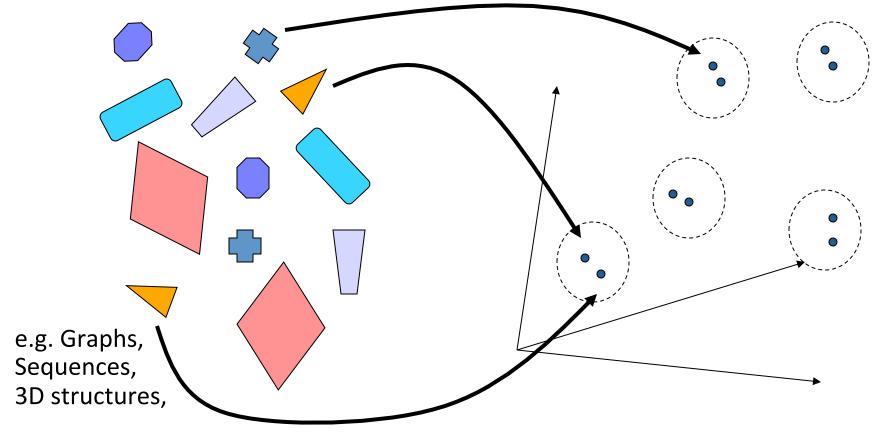
Choosing the Kernel Function

- Probably the most tricky part of using SVM.
- The kernel function is important because it creates the kernel matrix, which summarize all the data
- Many principles have been proposed (diffusion kernel, Fisher kernel, string kernel, tree kernel, graph kernel, ...)
 - Kernel trick has helped Non-traditional data like strings and trees able to be used as input to SVM, instead of feature vectors
- In practice, a low degree polynomial kernel or RBF kernel with a reasonable width is a good initial try for most applications.

Kernel trick has helped Nontraditional data like strings and trees able to be used as input to SVM, instead of feature vectors

k(x,z)

Vector vs. Relational data



Original Space

Feature Space

Mercer Kernel vs. Smoothing Kernel

 The Kernels used in Support Vector Machines are different from the Kernels used in LocalWeighted / Kernel Regression.

- We can think
 - Support Vector Machines' kernels as Mercer
 Kernels
 - Local Weighted / Kernel Regression's kernels as
 Smoothing Kernels

Why do SVMs work?

- ☐ If we are using huge features spaces (e.g., with kernels), how come we are not overfitting the data?
 - ✓ Number of parameters remains the same (and most are set to 0)
 - ✓ While we have a lot of input values, at the end we only care about the support vectors and these are usually a small group of samples
 - ✓ The minimization (or the maximizing of the margin) function acts as a sort of regularization term leading to reduced overfitting

Why SVM Works? (Extra)

- Vapnik argues that the fundamental problem is not the number of parameters to be estimated. Rather, the problem is about the flexibility of a classifier
- Vapnik argues that the flexibility of a classifier should not be characterized by the number of parameters, but by the capacity of a classifier
 - This is formalized by the <u>"VC-dimension"</u> of a classifier
- The SVM objective can also be justified by structural risk minimization: the empirical risk (training error), plus a term related to the generalization ability of the classifier, is minimized
- Another view: the SVM loss function is analogous to ridge regression. The term $\frac{1}{2} |w|^2$ "shrinks" the parameters towards zero to avoid overfitting

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Software

- A list of SVM implementation can be found at
 - http://www.kernel-machines.org/software.html
- Some implementation (such as LIBSVM) can handle multi-class classification
- SVMLight is among one of the earliest implementation of SVM
- Several Matlab toolboxes for SVM are also available

Summary: Steps for Using SVM in HW

- Prepare the feature-data matrix
- Select the kernel function to use
- Select the parameter of the kernel function and the value of C
 - You can use the values suggested by the SVM software, or you can set apart a validation set to determine the values of the parameter
- Execute the training algorithm and obtain the α_i
- Unseen data can be classified using the α_i and the support vectors

Practical Guide to SVM

- From authors of as LIBSVM:
 - A Practical Guide to Support Vector Classification Chih-Wei Hsu, Chih-Chung Chang, and Chih-Jen Lin, 2003-2010
 - http://www.csie.ntu.edu.tw/~cjlin/papers/guide/guide.pdf

LIBSVM

- http://www.csie.ntu.edu.tw/~cjlin/libsvm/
 - ✓ Developed by Chih-Jen Lin etc.
 - √ Tools for Support Vector classification
 - ✓ Also support multi-class classification
 - √ C++/Java/Python/Matlab/Perl wrappers
 - ✓ Linux/UNIX/Windows
 - ✓ SMO implementation, fast!!!

(a) Data file formats for LIBSVM

Training.dat

```
+1 1:0.708333 2:1 3:1 4:-0.320755
```

-1 1:0.583333 2:-1 4:-0.603774 5:1

+1 1:0.166667 2:1 3:-0.333333 4:-0.433962

-1 1:0.458333 2:1 3:1 4:-0.358491 5:0.374429

• • •

Testing.dat

(b) Feature Preprocessing

- (1) Categorical Feature
 - Recommend using m numbers to represent an mcategory attribute.
 - Only one of the m numbers is one, and others are zero.

For example, a three-category attribute such as {red, green, blue} can be represented as (0,0,1), (0,1,0), and (1,0,0)

Feature Preprocessing

- (2) Scaling before applying SVM is very important
 - to avoid attributes in greater numeric ranges dominating those in smaller numeric ranges.
 - to avoid numerical difficulties during the calculation
 - Recommend linearly scaling each attribute to the range [1, +1] or [0, 1].

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For i-th feature (olumn sparaton) on $X_{n \times p}$)

(centering: $X_i - X_i \Rightarrow E(X_i) = 0$ Scaling: $a \times i + b \Rightarrow e_i \cdot X_i - \min(X_i)$ Normalization: $\Rightarrow \begin{cases} E(X_i) = 0 \\ Var(X_i) = 1 \end{cases}$

Of course we have to use the same method to scale both training and testing data. For example, suppose that we scaled the first attribute of training data from [-10, +10] to [-1, +1]. If the first attribute of testing data lies in the range [-11, +8], we must scale the testing data to [-1.1, +0.8]. See Appendix B for some real examples.

If training and testing sets are separately scaled to [0, 1], the resulting accuracy is lower than 70%.

- \$ python easy.py svmguide4.scale svmguide4.t.scale
 Accuracy = 69.2308% (216/312) (classification)
 Using the same scaling factors for training and testing sets, we obtain much better
- accuracy.
- \$../svm-scale -1 0 -s range4 svmguide4 > svmguide4.scale
 \$../svm-scale -r range4 svmguide4.t > svmguide4.t.scale
- \$ python easy.py svmguide4.scale svmguide4.t.scale
 Accuracy = 89.4231% (279/312) (classification)

\$../svm-scale -1 0 svmguide4 > svmguide4.scale

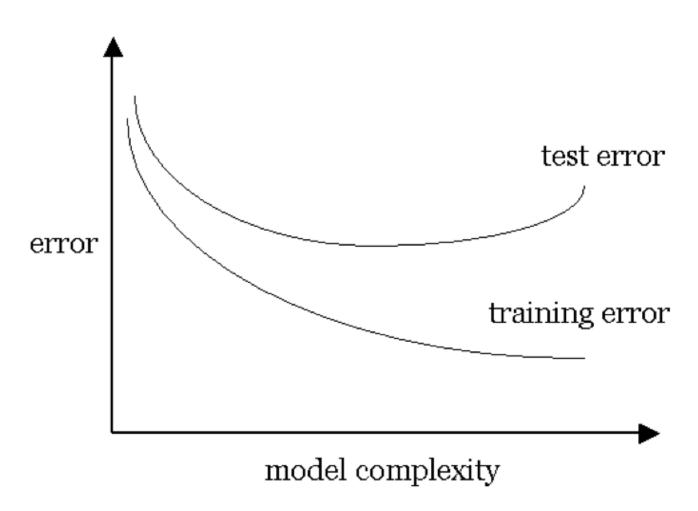
\$../svm-scale -1 0 svmguide4.t > svmguide4.t.scale

Feature Preprocessing

- (3) missing value
 - Very very tricky !
 - Easy way: to substitute the missing values by the mean value of the variable
 - A little bit harder way: imputation using nearest neighbors
 - Even more complex: e.g. EM based (beyond the scope)

(c) Model Selection

Our goal: find the model M which minimizes the test error:

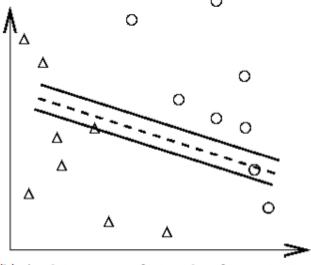


(c) Model Selection (e.g. for linear kernel)

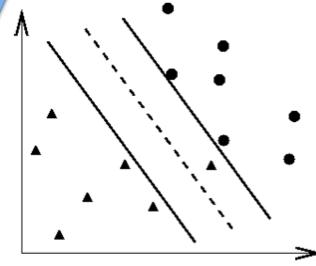
• linear: $K(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^T \mathbf{x}_j$.

Select the right penalty

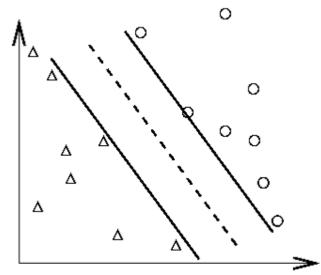
(a) Training data and an overfitting classifier



(b) Applying an overfitting classifier on testing data



(c) Training data and a better classifier



(d) Applying a better classifier on testing data

parameter

(c) Model Selection

• radial basis function (RBF): $K(\mathbf{x}_i, \mathbf{x}_j) = \exp(-\gamma ||\mathbf{x}_i - \mathbf{x}_j||^2), \ \gamma > 0.$ two parameters for an RBF kernel: C and γ

• polynomial: $K(\mathbf{x}_i, \mathbf{x}_j) = (\gamma \mathbf{x}_i^T \mathbf{x}_j + r)^d, \ \gamma > 0.$

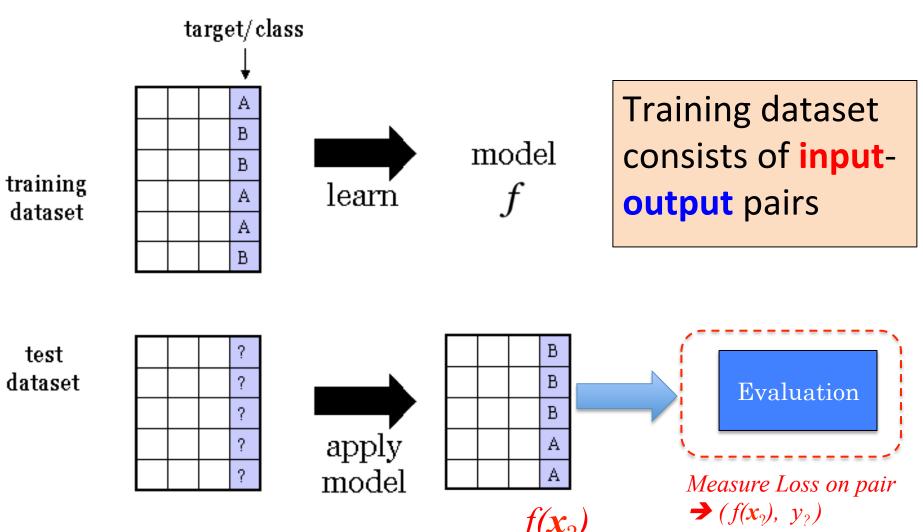
Three parameters for a polynomial kernel

(d) Pipeline Procedures

- (1) train / test
- (2) k-folds cross validation
- (3) k-CV on train to choose hyperparameter / then test

Evaluation Choice-I:

Train and Test



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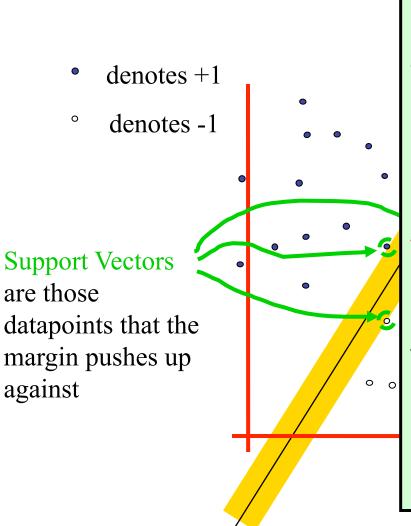
Evaluation Choice-II:

Cross Validation

- Problem: don't have enough data to set aside a test set
- Solution: Each data point is used both as train and test
- Common types:
 - -K-fold cross-validation (e.g. K=5, K=10)
 - -2-fold cross-validation
 - -Leave-one-out cross-validation (LOOCV)

A good practice is: to random shuffle all training sample before splitting

Why Maximum Margin for SVM?



- 1. Intuitively this feels safest.
- 2. If we've made a small error in the location of the boundary (it's been jolted in its perpendicular direction) this gives us least chance of causing a misclassification.
- 3. LOOCV is easy since the model is immune to removal of any non-support-vector datapoints.
- 4. There's some theory (using VC dimension) that is related to (but not the same as) the proposition that this is a good thing.
- 5. Empirically it works very very well.

Evaluation Choice-III:

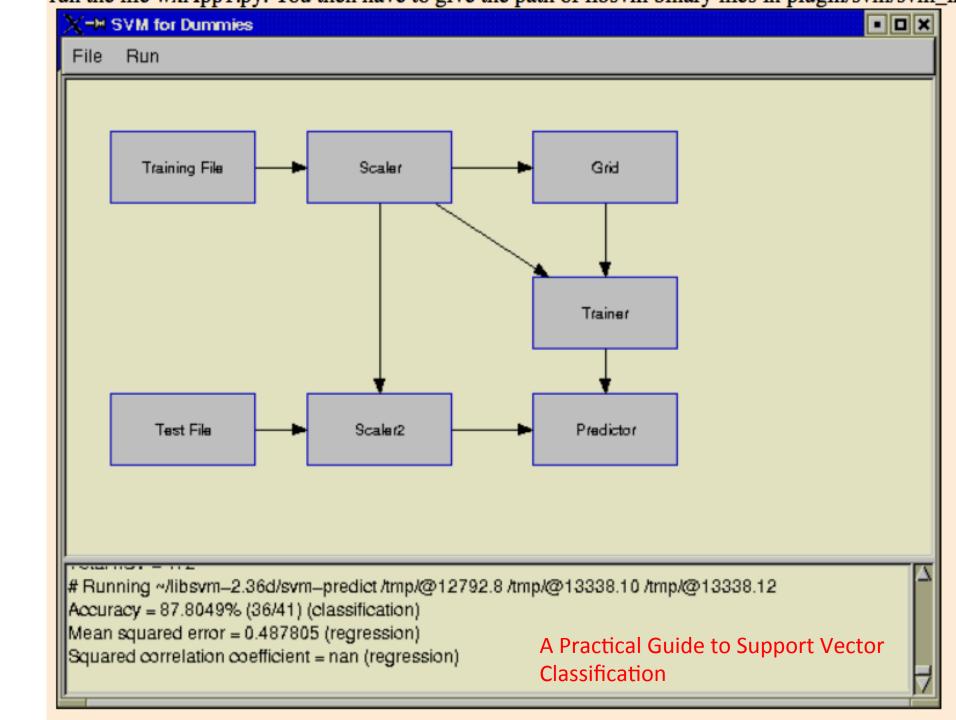
Many beginners use the following procedure now:

- Transform data to the format of an SVM package
- Randomly try a few kernels and parameters
- Test

We propose that beginners try the following procedure first:

- Transform data to the format of an SVM package
- Conduct simple scaling on the data
- Consider the RBF kernel $K(\mathbf{x}, \mathbf{y}) = e^{-\gamma ||\mathbf{x} \mathbf{y}||^2}$
- ullet Use cross-validation to find the best parameter C and γ
- Use the best parameter C and γ to train the whole training set⁵

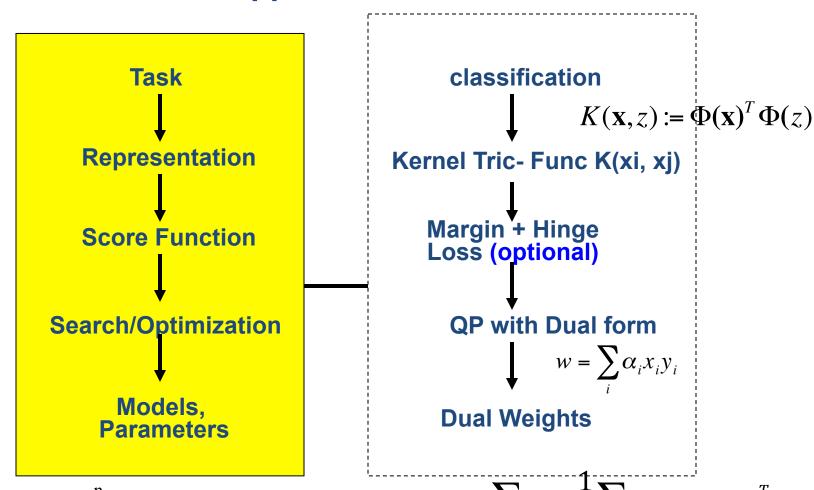




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 - √ File format / LIBSVM
 - √ Feature preprocsssing
 - ✓ Model selection
 - ✓ Pipeline procedure

Support Vector Machine



$$\underset{\mathbf{w},b}{\operatorname{argmin}} \sum_{i=1}^{p} w_i^2 + C \sum_{i=1}^{n} \varepsilon_i$$

subject to $\forall \mathbf{x}_i \in Dtrain : y_i (\mathbf{x}_i \cdot \mathbf{w} + b) \ge 1_{\text{total}} \varepsilon_i / VA \sum_i \alpha_i y_i = 0$,

$$\max_{\alpha} \sum_{i} \alpha_{i} - \frac{1}{2} \sum_{i,j} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{i}^{T} x_{j}$$

$$\alpha_i y_i = 0, \qquad \alpha_i \ge 0$$

 $_{2}$ $\forall i$

References

- Big thanks to Prof. Ziv Bar-Joseph and Prof. Eric Xing
 @ CMU for allowing me to reuse some of his slides
- Elements of Statistical Learning, by Hastie, <u>Tibshirani and Friedman</u>
- Prof. Andrew Moore @ CMU's slides
- Tutorial slides from Dr. Tie-Yan Liu, MSR Asia
- A Practical Guide to Support Vector Classification Chih-Wei Hsu, Chih-Chung Chang, and Chih-Jen Lin, 2003-2010
- Tutorial slides from Stanford "Convex Optimization I Boyd & Vandenberghe