Generative and discriminative classification techniques

Machine Learning and Category Representation 2014-2015

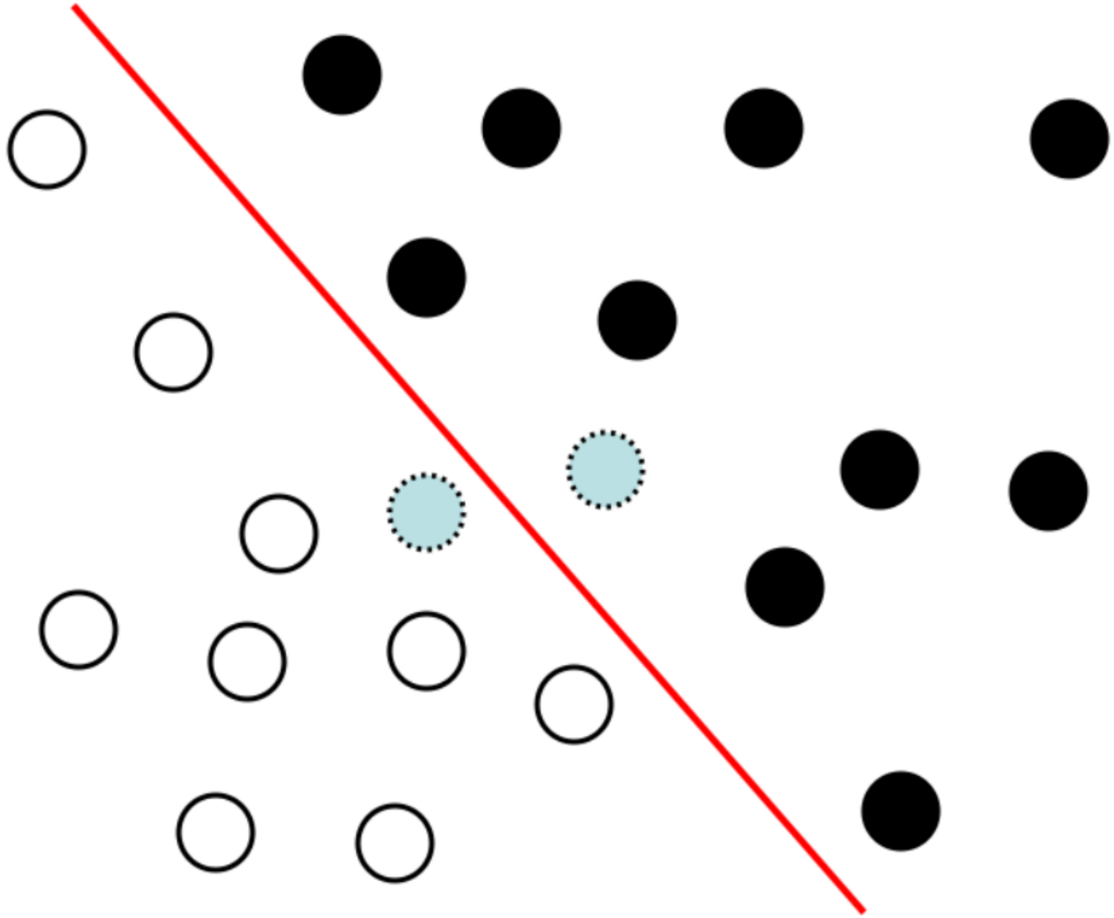
Jakob Verbeek, December 12, 2014

Course website:

http://lear.inrialpes.fr/~verbeek/MLCR.14.15

Classification

- Given training data labeled for two or more classes
- Determine a surface that separates those classes
- Use that surface to predict the class membership of new data



Classification

- Goal is to predict for a test data input the corresponding class label.
  - **Data input x**, eg. image but could be anything, format may be vector or other
  - **Class label y**, can take one out of at least 2 discrete values, can be more

  - In binary classification we often refer to one class as “positive”, and the other as “negative”

- Classifier: function f(x) that assigns a class to x, or probabilities over the classes.

- Training data: pairs (x,y) of inputs x, and corresponding class label y.

- Learning a classifier: determine function f(x) from some family of functions based on the available training data.

- Classifier partitions the input space into regions where data is assigned to a given class
  - Specific form of these boundaries will depend on the family of classifiers used

Generative classification: principle

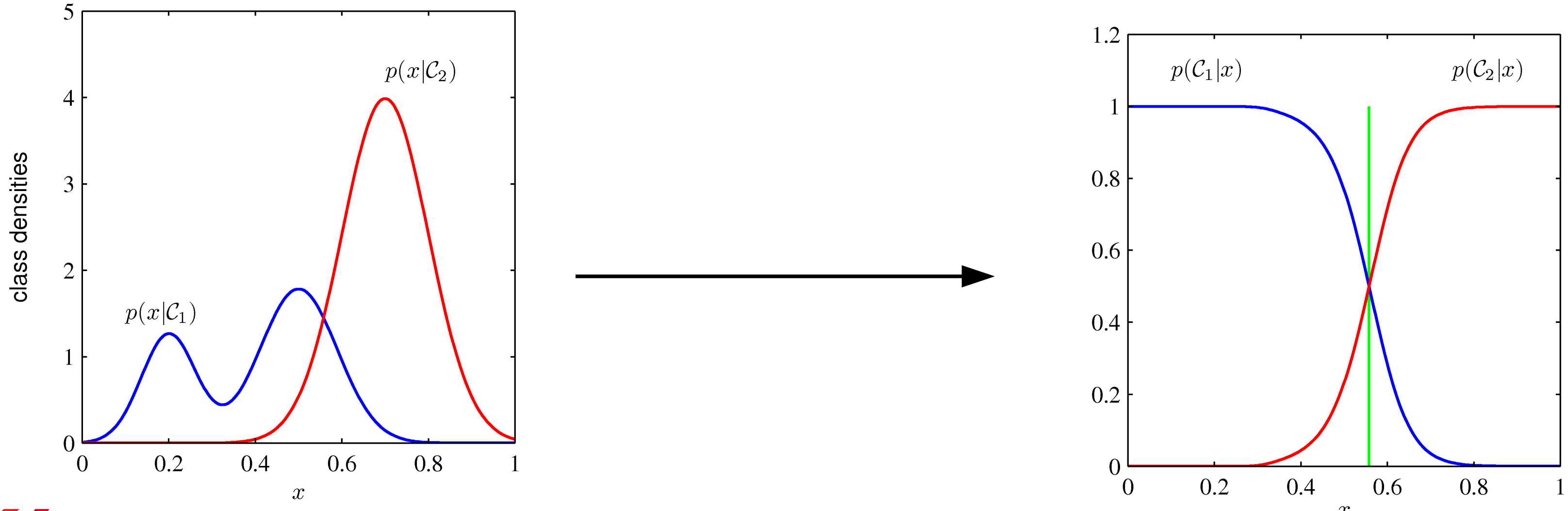
- Model the class conditional distribution over data x for each class y: $p(x|y)$
  - Data of the class can be sampled (generated) from this distribution
- Estimate the a-priori probability that a class will appear $p(y)$

- Infer the probability over classes using Bayes' rule of conditional probability

$$p(y|x) = \frac{p(y)\,p(x|y)}{p(x)}$$

- Unconditional distribution on x is obtained by marginalizing over the class y

$$p(x) = \sum_y p(y)\,p(x|y)$$



Generative classification: practice

- In order to apply Bayes' rule, we need to estimate two distributions.

- A-priori class distribution
  - In some cases the class prior probabilities are known in advance.
  - If the frequencies in the training data set are representative for the true class probabilities, then estimate the prior by these frequencies.
  - More elaborate methods exist, but not discussed here.

- Class conditional data distributions
  - Select a class of density models
    - Parametric model, e.g. Gaussian, Bernoulli, …
    - Semi-parametric models: mixtures of Gaussian, Bernoulli, ...
    - Non-parametric models: histograms, nearest-neighbor method, …
    - Or more structured models taking problem knowledge into account.
  - Estimate the parameters of the model using the data in the training set associated with that class.

Estimation of the class conditional model

- Given a set of n samples from a certain class, and a family of distributions.
  $X=\{x_{1,} \ldots, x_n\}$ $P=\{p_\theta(x); \theta \in \Theta\}$
- Question how do we quantify the fit of a certain model to the data, and how do we find the best model defined in this sense?

- Maximum a-posteriori (MAP) estimation: use Bayes' rule again as follows:
  - Assume a prior distribution over the parameters of the model $p(\theta)$
  - Then the posterior likelihood of the model given the data is
    $$p(\theta|X)=p(x|\theta)\,p(\theta)/p(X)$$
  - Find the most likely model given the observed data
    $$\hat{\theta}=\operatorname{argmax}_\theta p(\theta|X)=\operatorname{argmax}_\theta \{\ln p(\theta)+\ln p(X|\theta)\}$$

- Maximum likelihood parameter estimation: assume prior over parameters is uniform (for bounded parameter spaces), or “near uniform” so that its effect is negligible for the posterior on the parameters.
  - In this case the MAP estimator is given by $\hat{\theta}=\operatorname{argmax}_\theta p(X|\theta)$
  - For i.id. samples:
    $$\hat{\theta}=\operatorname{argmax}_\theta \prod_{i=1}^{n} p(x_i|\theta)=\operatorname{argmax}_\theta \sum_{i=1}^{n} \ln p(x_i|\theta)$$

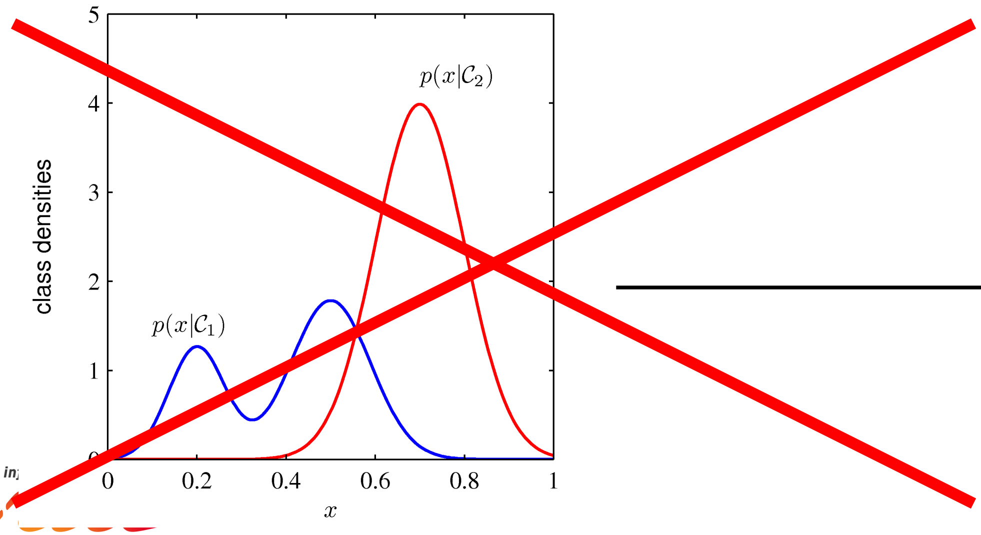
Summary generative classification methods

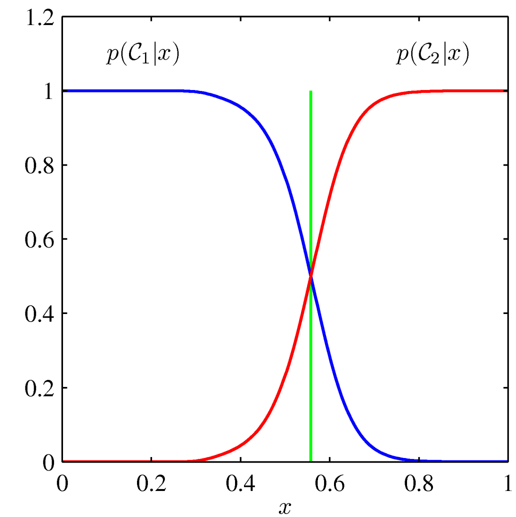
- (Semi-) Parametric models, e.g. p(x|y) is Gaussian, or mixture of …
  - Pros: no need to store training data, just the class conditional models
  - Cons: may fit the data poorly, and might therefore lead to poor classification result

- Non-parametric models:
  - Pros: flexibility, no assumptions distribution shape, “learning” is trivial.
    KNN can be used for anything that comes with a distance.
  - Cons of histograms:
    - Only practical in low dimensional data (<5 or so), application in high dimensional data leads to exponentially many and mostly empty cells
    - Naïve Bayes modeling in higher dimensional cases
  - Cons of k-nearest neighbors
    - Need to store all training data (memory cost)
    - Computing nearest neighbors (computational cost)

Discriminative classification methods

- Generative classification models
  - Model the density of inputs x from each class p(x|y)
  - Estimate class prior probability p(y)
  - Use Bayes' rule to infer distribution over class given input
- In discriminative classification methods we directly estimate class probability given input: p(y|x)
  - Choose class of decision functions in feature space
  - Estimate function that maximizes performance on the training set
  - Classify a new pattern on the basis of this decision rule.

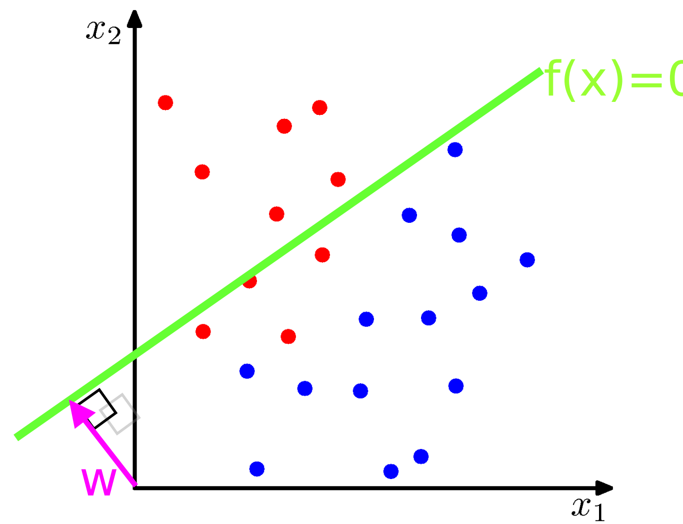




Binary linear classifier

- Decision function is linear in the features:

$$f(x) = w^T x + b = b + \sum_{i=1}^{d} w_i x_i$$



- Classification based on the sign of f(x)
- Orientation is determined by **w**
  - **w** is the surface normal
- Offset from origin is determined by *b*
- Decision surface is (d-1) dimensional hyper-plane orthogonal to **w**, given by

$$f(x) = w^T x + b = 0$$

- Exercise: What happens in 3d with ***w***=(1,0,0) and *b* = - 1?

Binary linear classifier

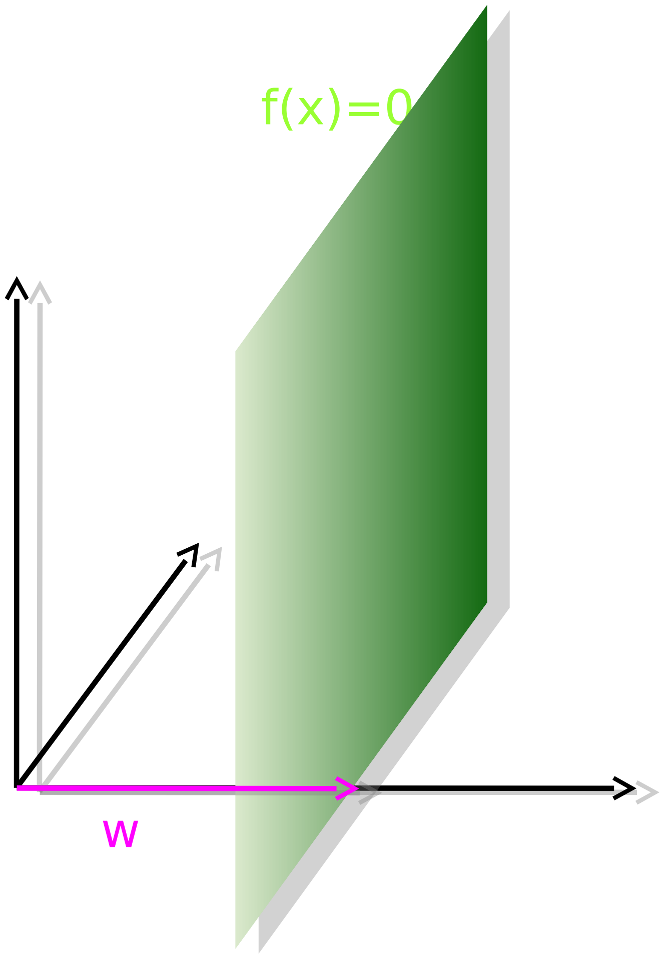
- Decision surface for w=(1,0,0) and b = -1

$$f(x) = w^T x + b = 0$$

$$b + \sum_{i=1}^{d} w_i x_i = 0$$

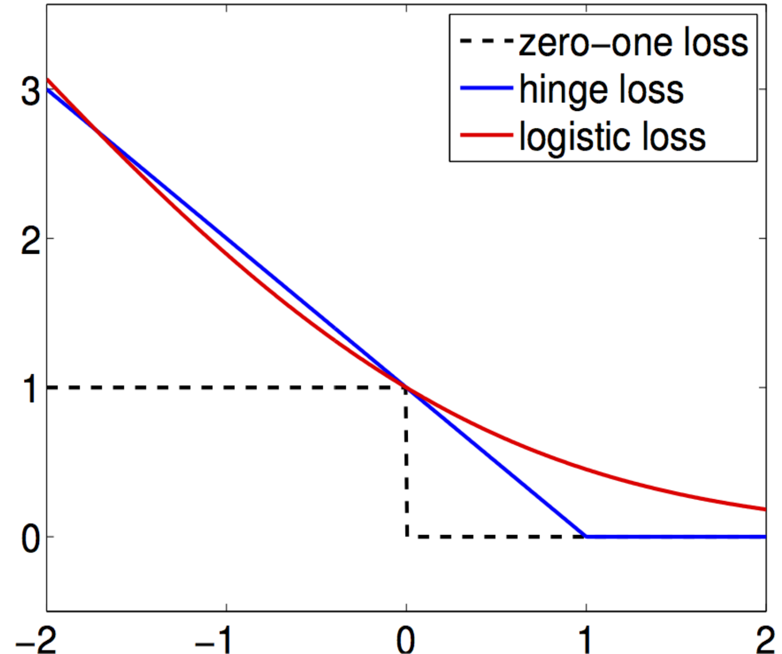
$$x_1 - 1 = 0$$

$$x_1 = 1$$



Common loss functions for classification

- Assign class label using $y = sign(f(x))$
- Measure model quality using loss function
  - Zero-One loss: $L(y_i, f(x_i)) = [y_i f(x_i) \leq 0]$
  - Hinge loss: $L(y_i, f(x_i)) = max(0, 1 - y_i f(x_i))$
  - Logistic loss: $L(y_i, f(x_i)) = \log_2 (1 + e^{-y_i f(x_i)})$



Common loss functions for classification

- Assign class label using $y = sign(f(x))$
  - Zero-One loss: $L(y_i, f(x_i)) = [y_i f(x_i) \geq 0]$
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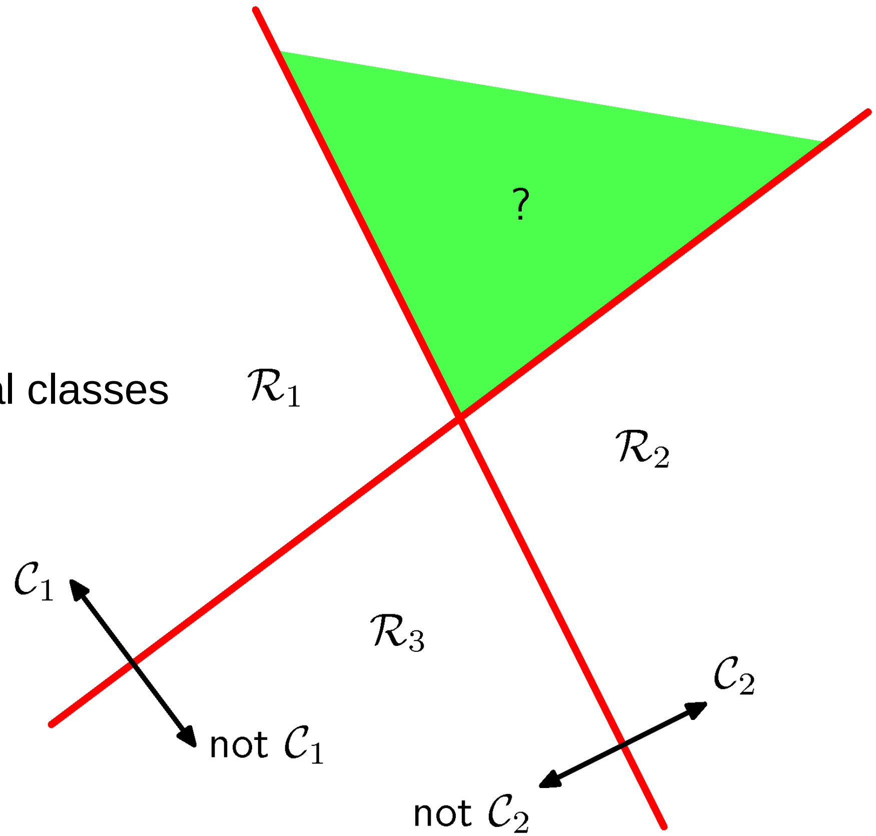
  - Logistic loss: $L(y_i, f(x_i)) = \log_2(1 + e^{-y_i f(x_i)})$
- The zero-one loss counts the number of misclassifications, which is the "ideal" empirical loss.
  - Discontinuity at zero makes optimization intractable.
- Hinge and logistic loss provide continuous and convex upperbounds, which can be optimized in tractable manner.
- Convexity does, however, not guarantee better performance than non-convex counterparts in practice!

Dealing with more than two classes

- First idea: construction from multiple binary classifiers
  - Learn binary “base” classifiers independently

- One vs rest approach:
  - 1 vs (2 & 3)
  - 2 vs (1 & 3)
  - 3 vs (1 & 2)

- Problem: Region claimed by several classes

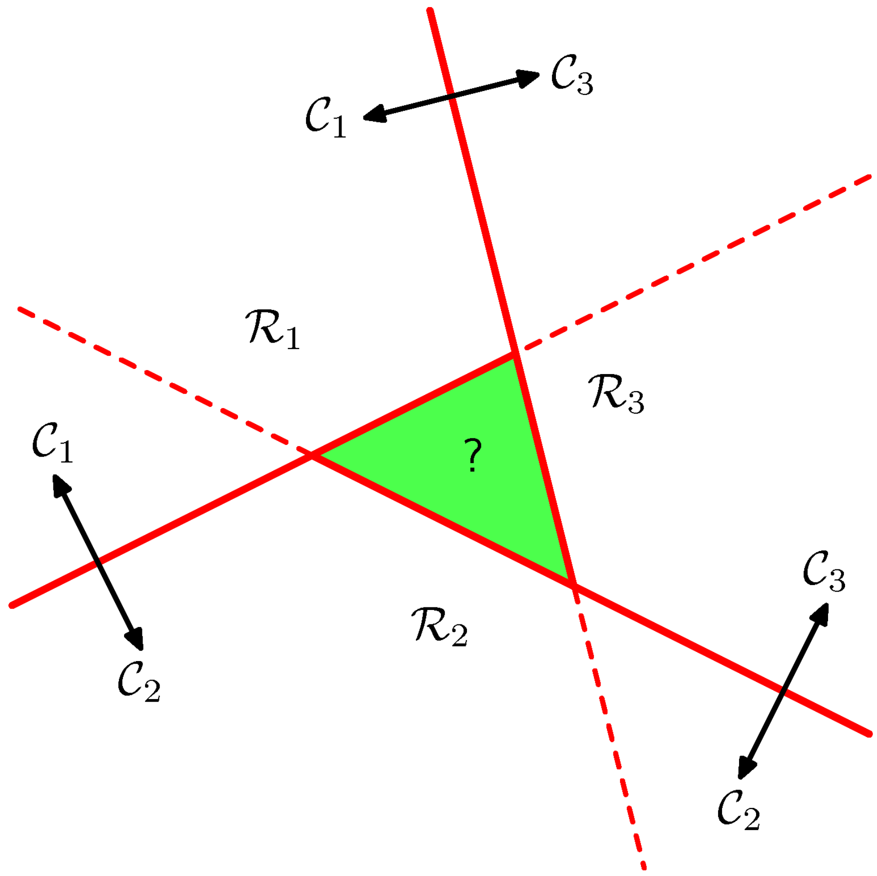


Dealing with more than two classes

- First idea: construction from multiple binary classifiers
  - Learn binary “base” classifiers independently

- One vs one approach:
  - 1 vs 2
  - 1 vs 3
  - 2 vs 3

- Problem: conflicts in some regions



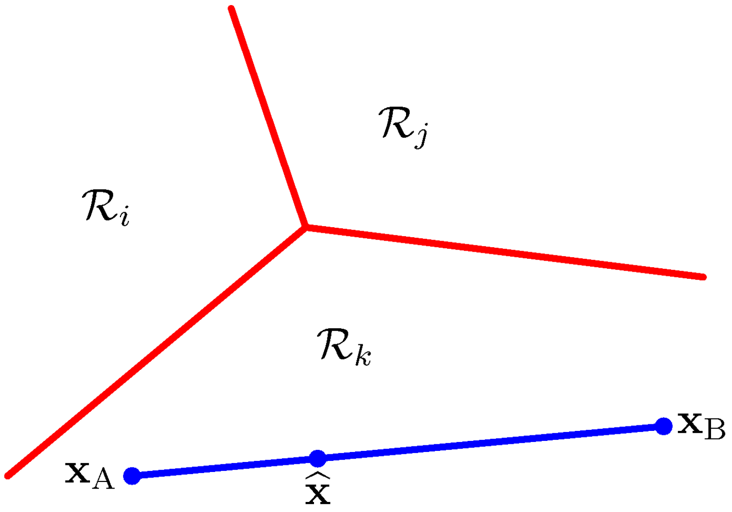
Dealing with more than two classes

- Instead: define a separate linear score function for each class

$$f_k(x) = w_k^T x + b_k$$

- Assign sample to the class of the function with maximum value

$$y = \arg\max_k f_k(x)$$



- Exercise 1: give the expression for points where two classes have equal score

- Exercise 2: show that the set of points assigned to a class is convex
  - If two points fall in the region, then also all points on connecting line

Logistic discriminant for two classes

- Map linear score function to class probabilities with sigmoid function

$$p(y=+1|x)=\sigma(w^T x+b)$$

  - For binary classification problem, we have by definition

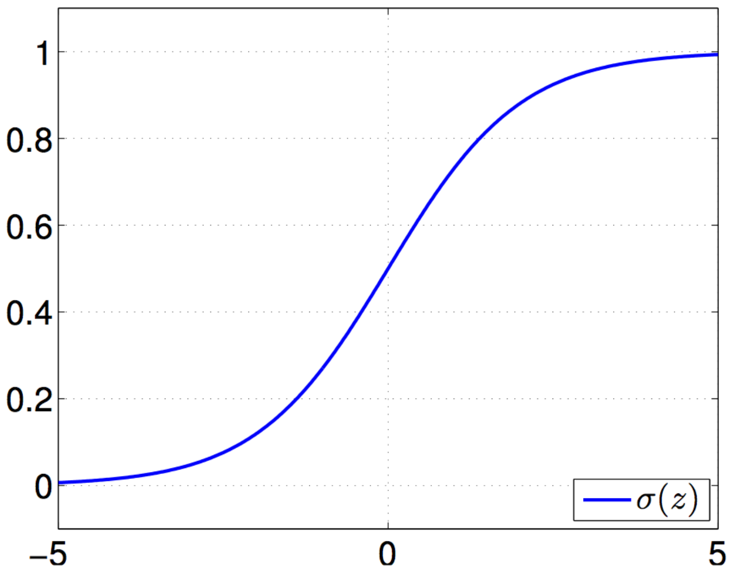
$$p(y=-1|x)=1-p(y=+1|x)$$

  - Exercise: show that

$$p(y=-1|x)=\sigma(-(w^T x+b))$$

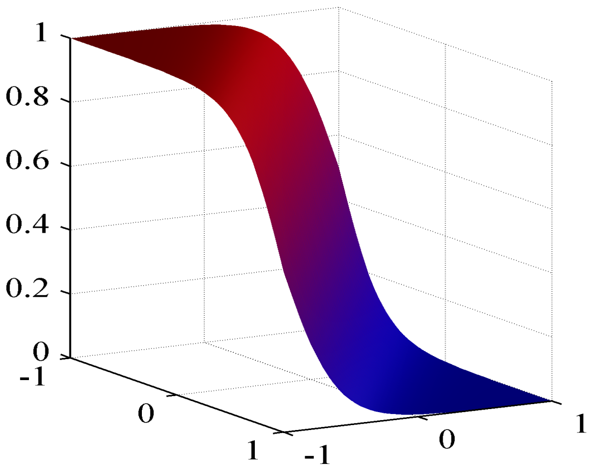
  - Therefore:

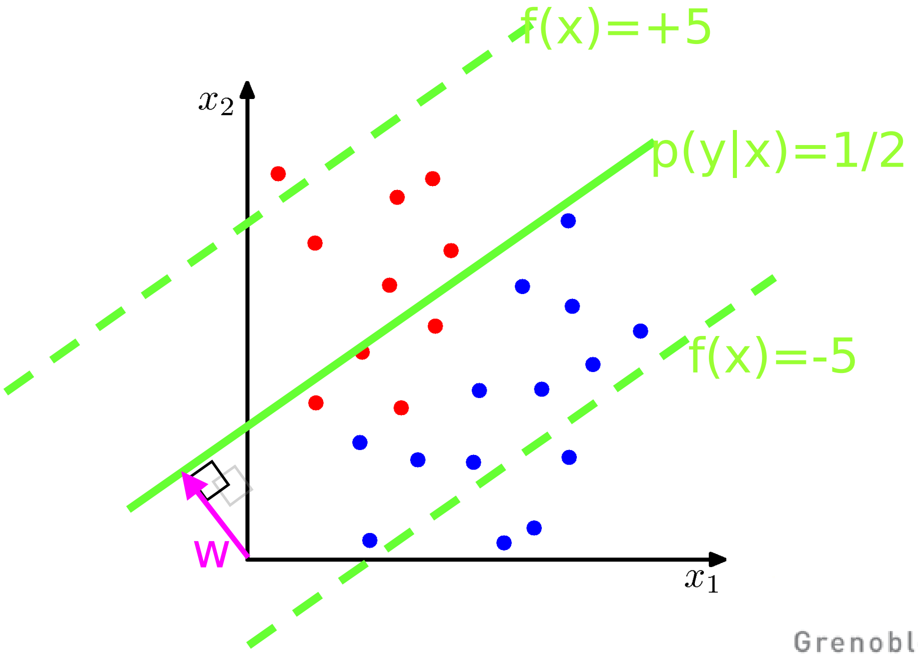
$$p(y|x)=\sigma(y(w^T x+b))$$



Logistic discriminant for two classes

- Map linear score function to class probabilities with sigmoid function
- The class boundary is obtained for p(y|x)=1/2, thus by setting linear function in exponent to zero





Multi-class logistic discriminant

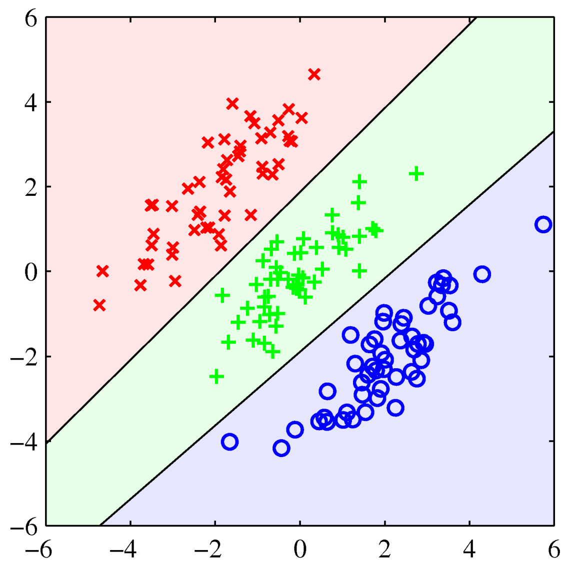
- Map score function of each class to class probabilities with "soft-max" function
  - Absorb bias into w and x

$$f_k(x) = w_k^T x \qquad\qquad p(y=c|x) = \frac{\exp(f_c(x))}{\sum_{k=1}^{K} \exp(f_k(x))}$$

  - The class probability estimates are non-negative, and sum to one.
  - Relative probability of most likely class increases exponentially with the difference in the linear score functions

$$\frac{p(y=c|x)}{p(y=k|x)} = \frac{\exp(f_c(x))}{\exp(f_k(x))} = \exp(f_c(x) - f_k(x))$$

  - For any given pair of classes we find that they are equally likely on a hyperplane in the feature space



Maximum likelihood parameter estimation

- Maximize the log-likelihood of predicting the correct class label for training data
  - Predictions are made independently, so sum log-likelihood of all training data

$$L=\sum_{n=1}^{N} \log p\left(y_n|x_n\right)$$

- Derivative of log-likelihood as intuitive interpretation

Indicator function
1 if y_n=k, else 0

$$\frac{\partial L}{\partial \boldsymbol{w}_k}=\sum_{n=1}^{N}\left(\left[y_n=k\right]-p\left(y=k|\boldsymbol{x}_n\right)\right)\boldsymbol{x}_n$$

Expected value of each feature, weighting points by p(y|x), should equal empirical expectation.

- No closed-form solution, but log-likelihood is concave in parameters
  - no local optima, use general purpose convex optimization methods
  - For example: gradient-based method started from w=0
    - ***w*** is linear combination of data points

Maximum a-posteriori (MAP) parameter estimation

- Let us assume a zero-mean Gaussian prior distribution on w
  - We expect "small" weight vectors
- Find w that maximizes posterior likelihood

$$\hat{w} = \mathrm{argmax}_w \sum_{n=1}^{N} \ln p(y_n | x_n, w) + \sum_k \ln p(w_k)$$

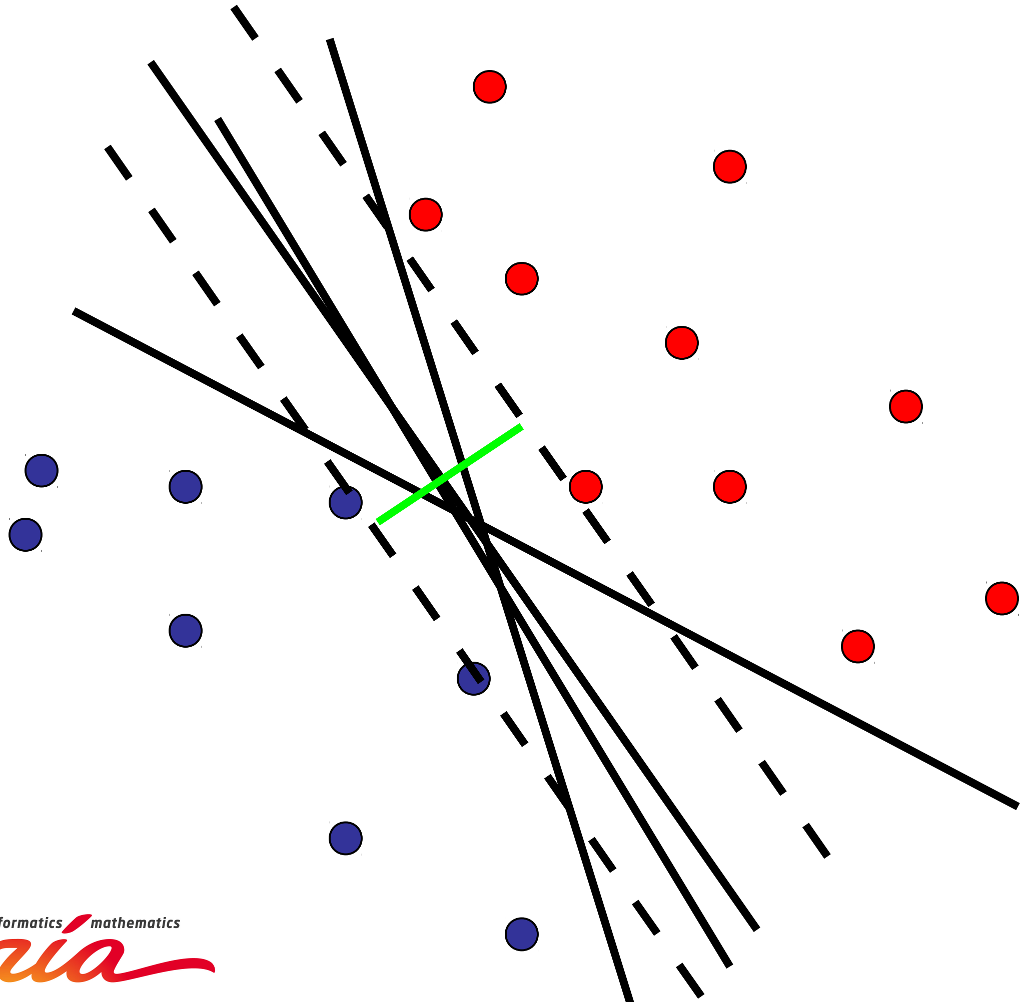
- Can be rewritten as following "penalized" maximum likelihood estimator:

$$\hat{w} = \mathrm{argmax}_w \sum_{n=1}^{N} \ln p(y_n | x_n, w) - \lambda \frac{1}{2} \sum_k \|w_k\|_2^2$$

  - where non-negative lambda is the inverse variance of the Gaussian prior
- Penalty for "large" w, bounds the scale of w in case of separable data
- Exercise: show that for separable data the norm of the optimal w's would be infinite without using the penalty term.

Support Vector Machines

- Find linear function to separate positive and negative examples
- Which function best separates the samples ?
  - Function inducing the largest margin



$$y_i = +1 \quad : \quad w^T x_i + b > 0$$
$$y_i = -1 \quad : \quad w^T x_i + b < 0$$

Support vector machines

- Witout loss of generality, define function value at the margin as +/- 1
- Now constrain w to that all points fall on correct side of the margin:

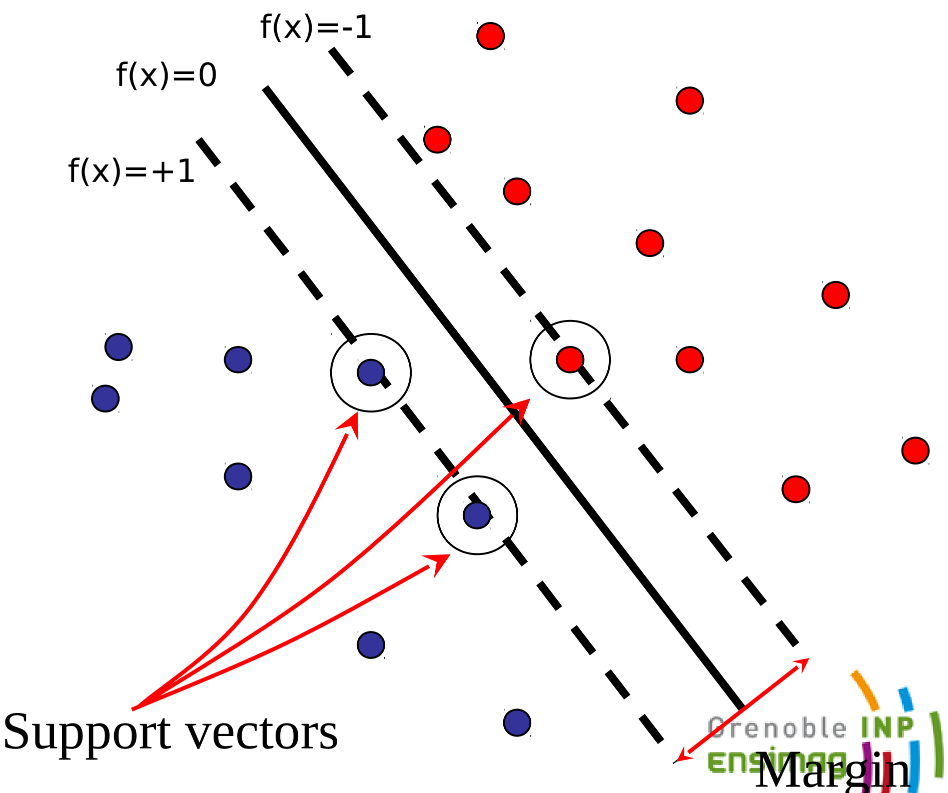
$$y_i\left(w^T x_i + b\right) \geq 1$$

- By construction we have that the “support vectors”, the ones that define the margin, have function values

$$w^T x_i + b = y_i$$

- Express the size of the margin

  in terms of w.



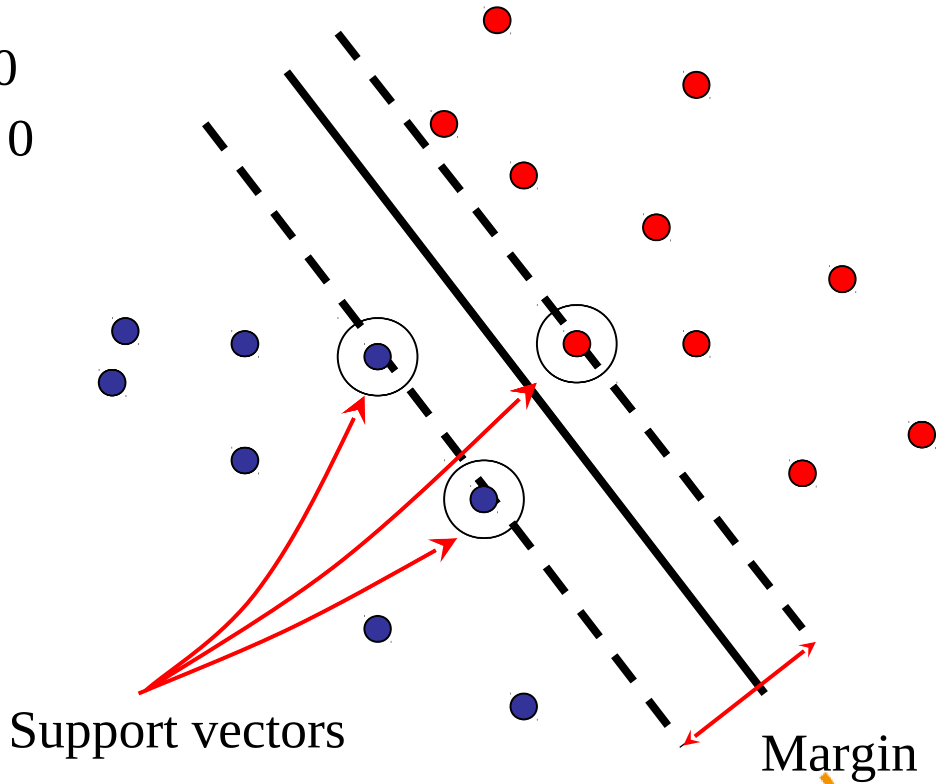
Support vector machines

- Let's consider a support vector x from the positive class $f(x)=w^T x+b=1$
- Let z be its projection on the decision plane
  - Since w is normal vector to the decision plane, we have $z=x-\alpha w$
  - and since z is on the decision plane $f(z)=w^T(x-\alpha w)+b=0$
- Solve for alpha

$$w^T(x-\alpha w)+b=0$$
$$w^T x+b-\alpha w^T w=0$$
$$\alpha w^T w=1$$
$$\alpha=\frac{1}{\|w\|_2^2}$$

- Margin is twice distance from x to z

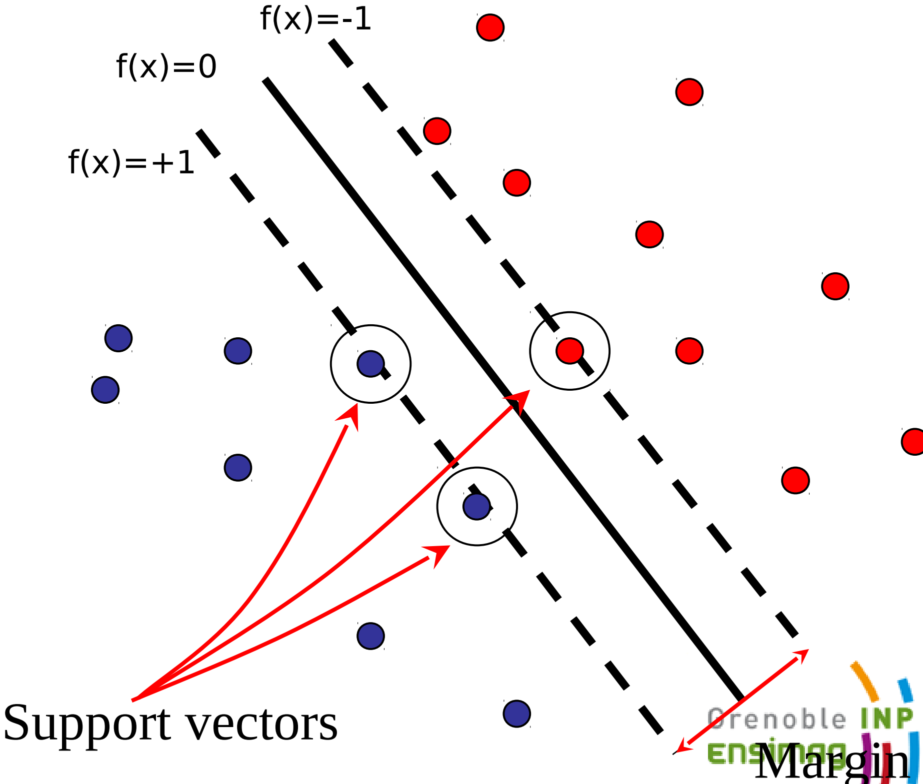
$$\|x-z\|_2=\|x-(x-\alpha w)\|_2$$
$$\|\alpha w\|_2=\alpha\|w\|_2$$
$$\frac{\|w\|_2}{\|w\|_2^2}=\frac{1}{\|w\|_2}$$



Support vector machines

- To find the maximum-margin separating hyperplane, we
  - Maximize the margin, while ensuring correct classification
  - Minimize the norm of w, s.t. $\forall_i:\ y_i(w^T x_i + b) \geq 1$
- Solve using quadratic program with linear inequality constraints over p+1 variables

$$argmin_{w,b} \frac{1}{2} w^T w$$
$$\text{subject to } y_i(w^T x_i + b) \geq 1$$

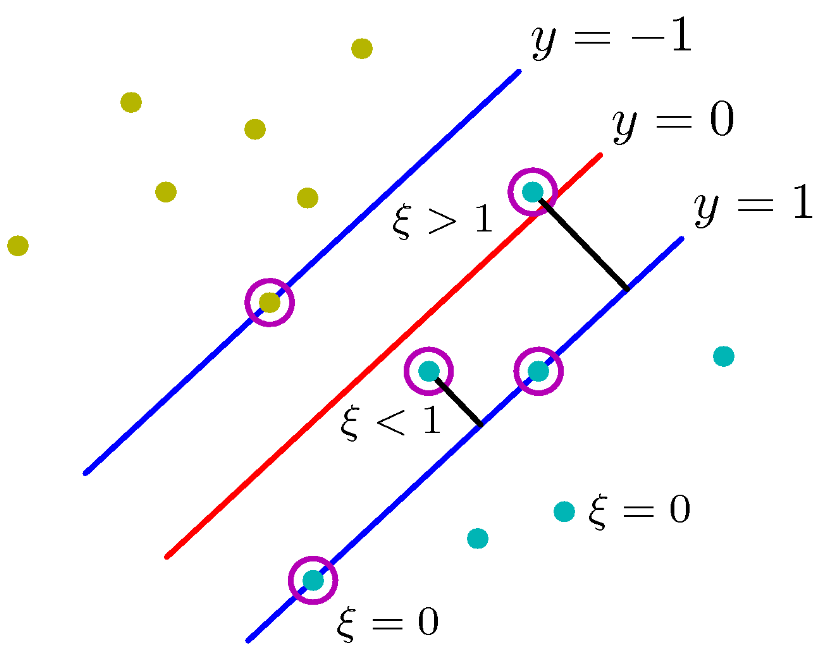


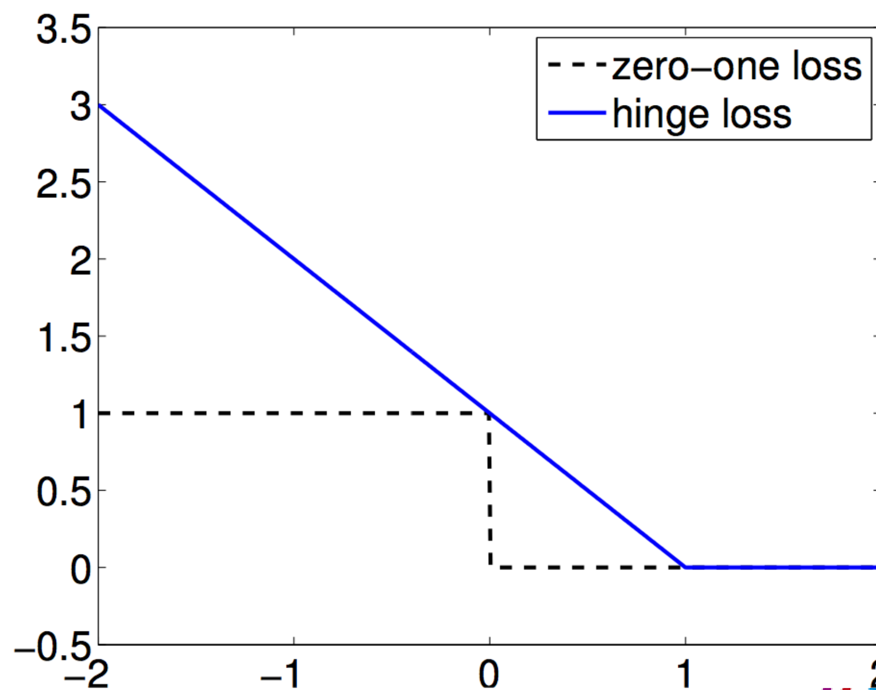
Support vector machines: inseperable classes

- For non-separable classes we incorporate hinge-loss

$$L(y_i, f(x_i)) = max(0, 1 - y_i f(x_i))$$

- Recall: convex and piecewise linear upper bound on zero/one loss.
  - Zero if point on the correct side of the margin
  - Otherwise given by absolute difference from score at margin





Support vector machines: inseperable classes

- Minimize penalized loss function

$$min_{w,b} \quad \lambda \frac{1}{2} w^T w \; + \; \sum_i max\left(0, 1 - y_i\left(w^T x_i + b\right)\right)$$

  - Quadratic function, plus **piecewise linear functions**.

- Transformation into a quadratic program
  - Define "slack variables" that measure the loss for each data point
  - Should be non-negative, and at least as large as the loss

$$min_{w,b,\{\xi_i\}} \quad \lambda \frac{1}{2} w^T w \; + \; \sum_i \xi_i$$

$$\text{subject to } \forall_i : \; \xi_i \geq 0 \text{ and } \xi_i \geq 1 - y_i\left(w^T x_i + b\right)$$

- Solution of the quadratic program has the property that w is a linear combination of the data points.

SVM solution properties

- Optimal w is a linear combination of data points $w = \sum_{n=1}^{N} \alpha_n y_n x_n$

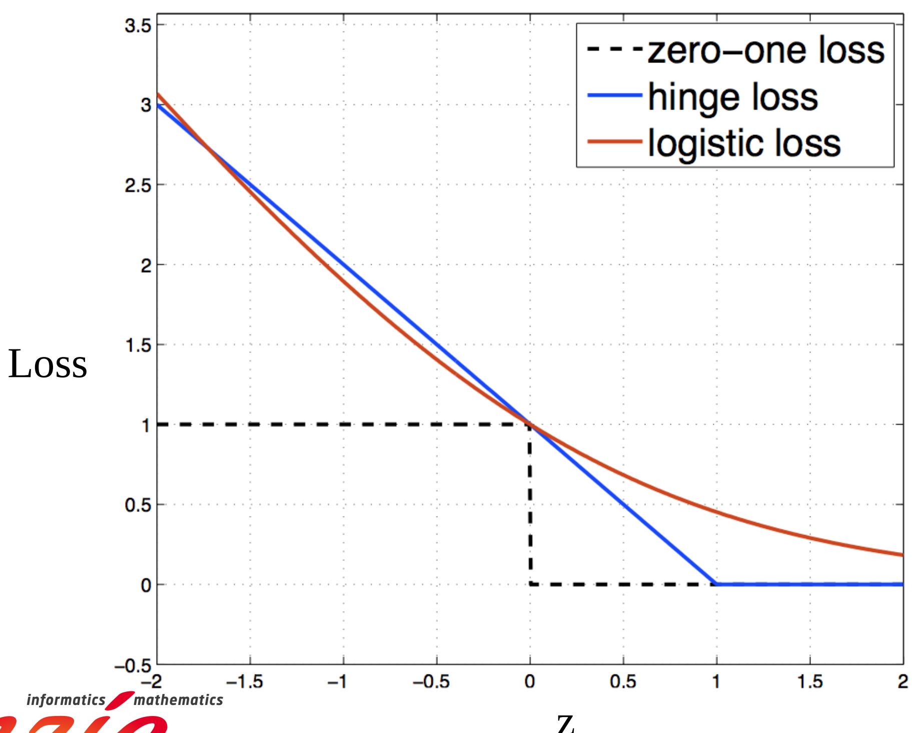
- Weights (alpha) are zero for all points on the correct side of the margin
  - Points on the margin also have non-zero weight

- Classification function thus has form $f(x) = w^T x + b = \sum_{n=1}^{N} \alpha_n y_n \boxed{x_n^T x} + b$
  - relies only on inner products between the test point $\boldsymbol{x}$ and data points with non-zero alpha's

- Solving the optimization problem also requires access to the data only in terms of inner products $\boldsymbol{x}_i \cdot \boldsymbol{x}_j$ between pairs of training points

Relation SVM and logistic regression

- A classification error occurs when sign of the function does not match the sign of the class label: the zero-one loss $z = y_i f(x_i) \leq 0$
- Consider error minimized when training classifier:
  - Non-separable SVM, hinge loss: $\xi_i = max(0, 1 - y_i f(x_i)) = max(0, 1 - z)$
  - Logistic loss: $-\log p(y_i | x_i) = -\log \sigma(y_i f(x_i)) = \log(1 + \exp(-z))$



- L2 penalty for SVM motivated by margin between the classes
- For Logistic discriminant we find it via MAP estimation with a Gaussian prior
- Both lead to efficient optimization
  - Hinge-loss is piece-wise linear: quadratic programming
  - Logistic loss is smooth : smooth convex optimization methods

Summary of discriminative linear classification

- Two most widely used linear classifiers in practice:
  - Logistic discriminant (supports more than 2 classes directly)
  - Support vector machines (multi-class extensions possible)

- For both, in the case of binary classification
  - Criterion that is minimized is a convex bound on zero-one loss
  - weight vector **w** is a linear combination of the data points $w = \sum_{n=1}^{N} \alpha_n x_n$

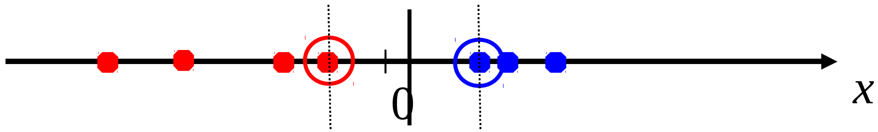
- This means that we only need the inner-products between data points to calculate the linear functions

$$
\begin{aligned}
f(x) &= w^T x + b \\
&= \sum_{n=1}^{N} \alpha_n x_n^T x + b \\
&= \sum_{n=1}^{N} \alpha_n k(x_n, x) + b
\end{aligned}
$$

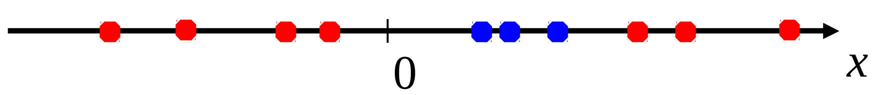
  - The “kernel” function k(,) computes the inner products

Nonlinear Classification

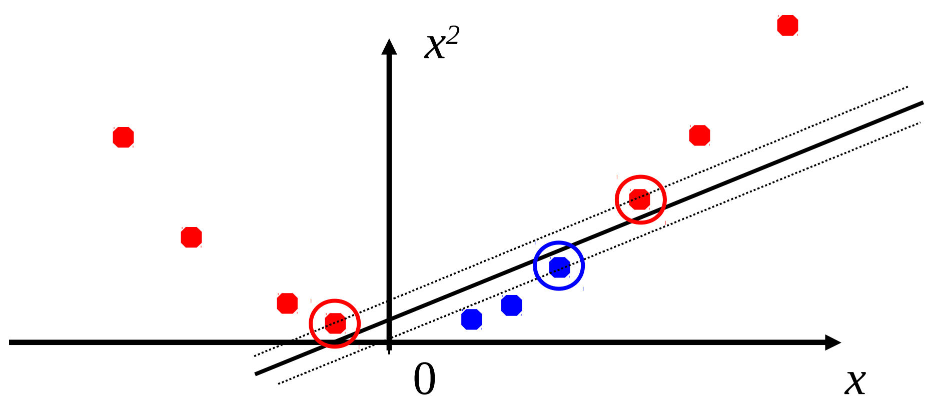
- 1 dimensional data that is linearly separable



- But what if the data is not linearly seperable?



- We can map it to a higher-dimensional space:

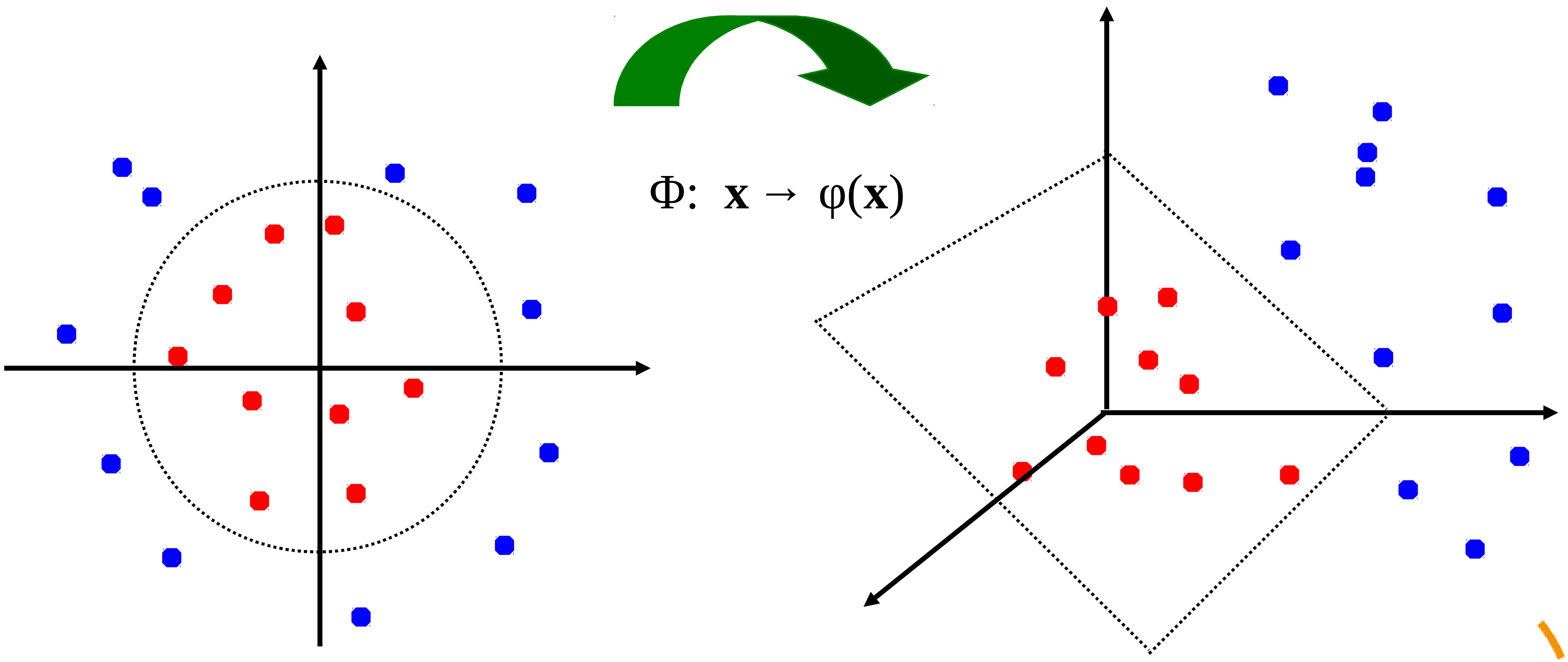


Slide credit: Andrew Moore

Kernels for non-linear classification

- General idea: map the original input space to some higher-dimensional feature space where the training set is separable

- Exercise: find features that could separate the 2d data linearly



Slide credit: Andrew Moore

Nonlinear classification with kernels

- *The kernel trick*: instead of explicitly computing the feature transformation $\boldsymbol{\varphi}(\mathbf{x})$, define a kernel function K such that

$$k(x_i, x_j) = \langle \varphi(x_i), \varphi(x_j) \rangle$$

- Conversely, if a kernel satisfies Mercer's condition then it computes an inner product in some feature space, possibly with large or infinite number of dimensions

  - *Mercer's Condition: The square N x N matrix K with kernel evaluations for any arbitrary N data points should always be a positive definite.*

$$a^T K a = \sum_{i=1}^{N} \sum_{j=1}^{N} a_i a_j [K]_{ij} \geq 0$$

- This gives a **nonlinear decision boundary** in the original space:

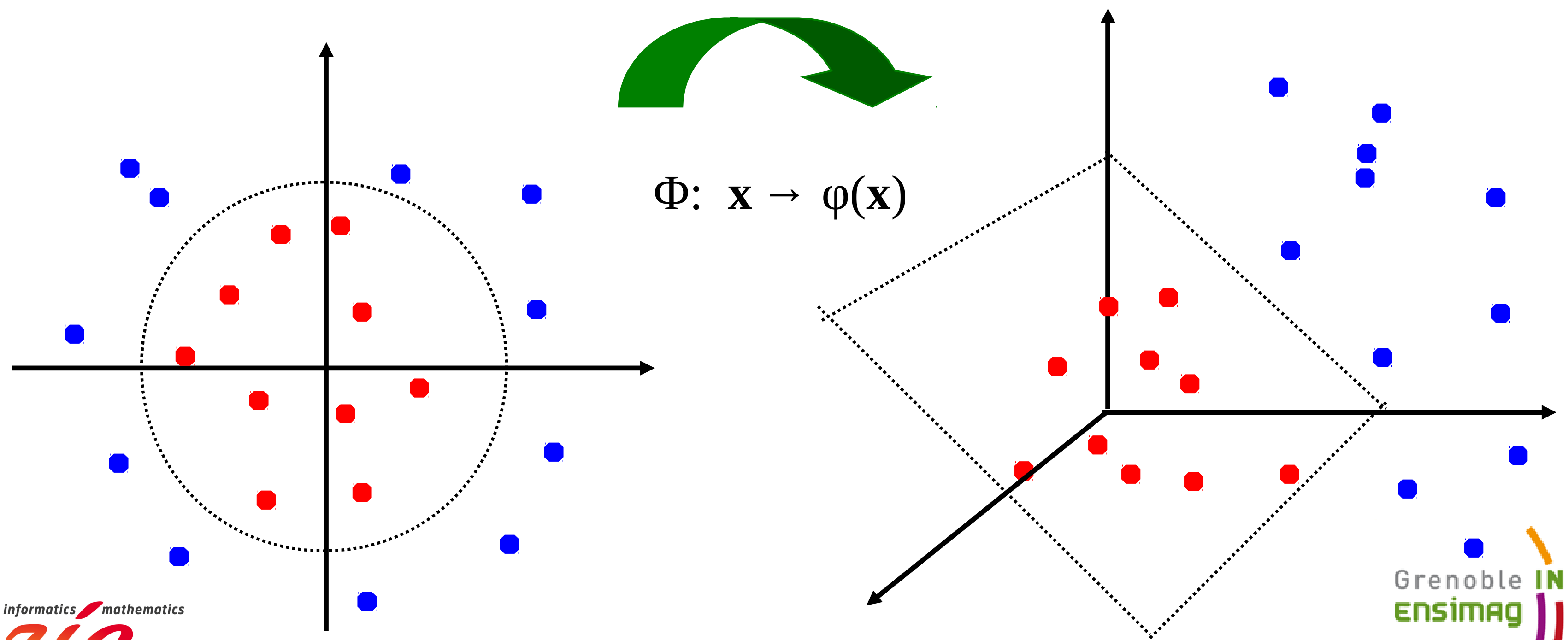
$$\begin{aligned} f(x) &= b + w^T \varphi(x) = b + \sum_i \alpha_i \varphi(x_i)^T \varphi(x) \\ &= b + \sum_i \alpha_i k(x_i, x) \end{aligned}$$

Kernels for non-linear classification

- What is the kernel function that corresponds to this feature mapping ?

$$\varphi(x) = \begin{pmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}\, x_1 x_2 \end{pmatrix}$$

$$\begin{aligned} k(x,y) &= \langle \varphi(x), \varphi(y) \rangle = ? \\ &= x_1^2 y_1^2 + x_2^2 y_2^2 + 2 x_1 x_2 y_1 y_2 \\ &= (x_1 y_1 + x_2 y_2)^2 \\ &= (x^T y)^2 \end{aligned}$$



Kernels for non-linear classification

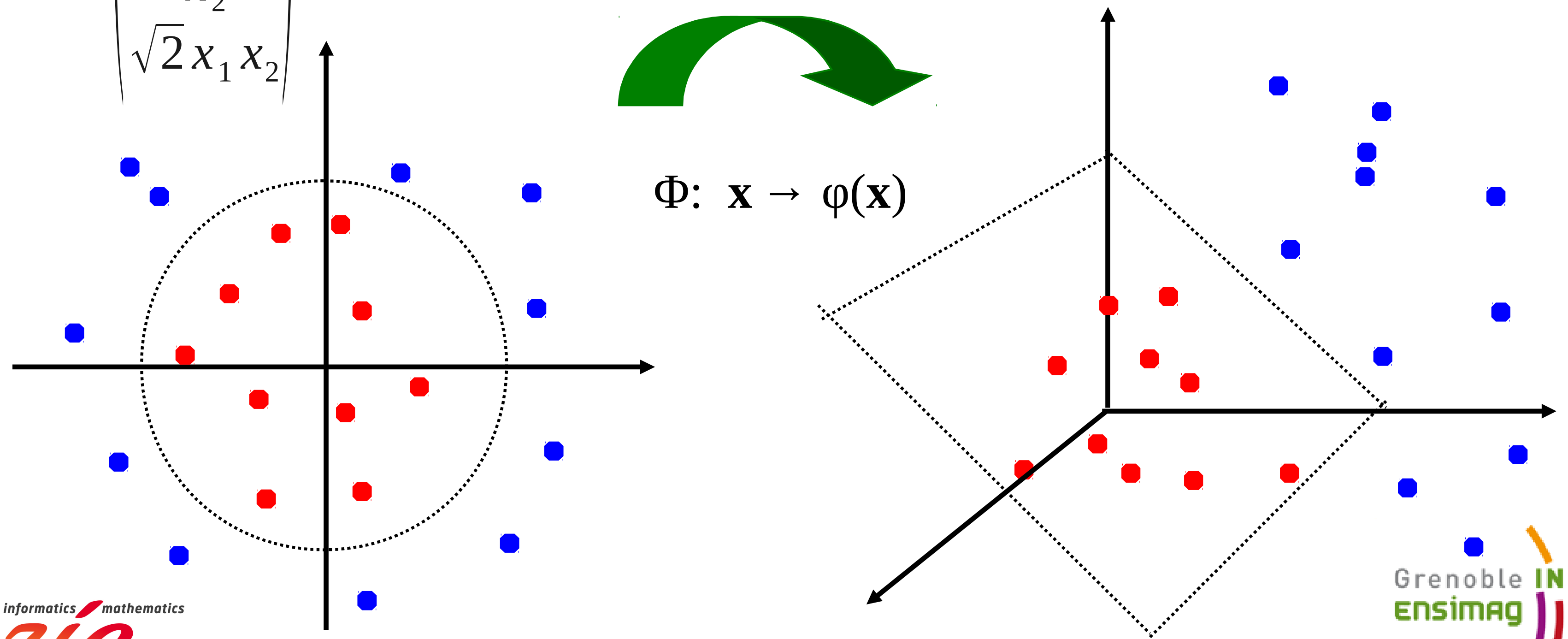
- Suppose we also want to keep the original features to be able to still implement linear functions

$$k(x,y)=\langle\varphi(x),\varphi(y)\rangle=?$$

$$=1+2x^T y+\left(x^T y\right)^2$$

$$=\left(x^T y+1\right)^2$$

$$\varphi(x)=\begin{pmatrix}1\\ \sqrt{2}\,x_1\\ \sqrt{2}\,x_2\\ x_1^2\\ x_2^2\\ \sqrt{2}\,x_1x_2\end{pmatrix}$$



Kernels for non-linear classification

- What happens if we use the same kernel for higher dimensional data
  - Which feature vector $\varphi(x)$ corresponds to it ?

$$k(x,y)=\left(x^T y+1\right)^2=1+2x^T y+\left(x^T y\right)^2$$

  - First term, encodes an additional 1 in each feature vector
  - Second term, encodes scaling of the original features by sqrt(2)
  - Let's consider the third term $\left(x^T y\right)^2=\left(x_1 y_1+\ldots+x_D y_D\right)^2$

$$=\sum_{d=1}^{D}\left(x_d y_d\right)^2+2\sum_{d=1}^{D}\sum_{i=d+1}^{D}\left(x_d y_d\right)\left(x_i y_i\right)$$

$$=\sum_{d=1}^{D}x_d^2 y_d^2+2\sum_{d=1}^{D}\sum_{i=d+1}^{D}\left(x_d x_i\right)\left(y_d y_i\right)$$

  - In total we have 1 + 2D + D(D-1)/2 features !
  - But the kernel is computed as efficiently as dot-product in original space

$$\varphi(x)=\Big(1,\underbrace{\sqrt{2}x_1,\sqrt{2}x_2,\ldots,\sqrt{2}x_D}_{\text{Original features}},\underbrace{x_1^2,x_2^2,\ldots,x_D^2}_{\text{Squares}},\underbrace{\sqrt{2}x_1x_2,\ldots,\sqrt{2}x_1x_D,\ldots,\sqrt{2}x_{D-1}x_D}_{\text{Products of two distinct elements}}\Big)^T$$

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Common kernels for bag-of-word histograms

- Hellinger kernel:

$$k(h_1, h_2) = \sum_d \sqrt{h_1(i)} \times \sqrt{h_2(i)}$$

- Histogram intersection kernel:

$$k(h_1, h_2) = \sum_d min(h_1(d), h_2(d))$$

  - Exercise: find the feature transformation ?

- Generalized Gaussian kernel:

$$k(h_1, h_2) = \exp\left(-\frac{1}{A} d(h_1, h_2)\right)$$

  - *d* can be Euclidean distance, χ^2 distance, Earth Mover's Distance, etc.

See also:
J. Zhang, M. Marszalek, S. Lazebnik, and C. Schmid,
Local features and kernels for classification of texture and object categories: a comprehensive study. Int. Journal of Computer Vision, 2007

Logistic discriminant with kernels

- Let us assume a given kernel, and let us express the classifier functions for each class c as

$$f_c(\boldsymbol{x}_j)=b_c+\sum_{i=1}^{n}\alpha_{ic}\langle\varphi(\boldsymbol{x}_i),\varphi(\boldsymbol{x}_j)\rangle=b_c+\sum_{i=1}^{n}\alpha_{ic}k(\boldsymbol{x}_i,\boldsymbol{x}_j)=b_c+\boldsymbol{\alpha}_c^T\boldsymbol{k}_j$$

  - Where $\boldsymbol{k}_j=\left(k(\boldsymbol{x}_j,\boldsymbol{x}_1),\ldots,k(\boldsymbol{x}_j,\boldsymbol{x}_n)\right)^T$

- Consider the L2 penalty on the weight vector for $\boldsymbol{w}_c=\sum_{i=1}^{n}\alpha_{ic}\varphi(\boldsymbol{x}_i)$

$$\langle\boldsymbol{w}_c,\boldsymbol{w}_c\rangle=\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_{ic}\alpha_{jc}k(\boldsymbol{x}_i,\boldsymbol{x}_j)=\boldsymbol{\alpha}_c^T\boldsymbol{K}\boldsymbol{\alpha}_c$$

  - Where $\boldsymbol{\alpha}_c=\left(\alpha_{1c},\ldots,\alpha_{nc}\right)^T$ and $[\boldsymbol{K}]_{ij}=k(\boldsymbol{x}_i,\boldsymbol{x}_j)$

- MAP estimation of the alpha's and b's amounts to maximize

$$\sum_{i=1}^{n}\ln p(y_i|\boldsymbol{x}_i)-\lambda\frac{1}{2}\sum_{c=1}^{C}\boldsymbol{\alpha}_c^T\boldsymbol{K}\boldsymbol{\alpha}_c$$

Logistic discriminant with kernels

- Recall that $p(y_i|\boldsymbol{x}_i)=\frac{\exp(f_{y_i}(\boldsymbol{x}_i))}{\sum_c \exp f_c(\boldsymbol{x}_i)}$ and $f_c(\boldsymbol{x}_i)=b_c+\boldsymbol{\alpha}_c^T \boldsymbol{k}_i$

- Therefore we want to maximize

$$E(\{\alpha_c\},\{b_c\})=\sum_{i=1}^{n}\left(f_{y_i}(\boldsymbol{x}_i)-\ln\sum_c \exp f_{y_i}(\boldsymbol{x}_i)\right)-\lambda\frac{1}{2}\sum_c \boldsymbol{\alpha}_c^T \boldsymbol{K}\boldsymbol{\alpha}_c$$

- Consider the partial derivative of this function with respect to the b's, and the gradient with respect to the alpha vectors

$$\frac{\partial E}{\partial b_c}=\sum_{i=1}^{n}\left([y_i=c]-p(c|\boldsymbol{x}_i)\right)$$

$$\nabla_{\boldsymbol{\alpha}_c} E=\sum_{i=1}^{n}\left([y_i=c]-p(c|\boldsymbol{x}_i)\right)\boldsymbol{k}_i-\boldsymbol{K}\boldsymbol{\alpha}_c$$

  - Essentially the same gradients as in the linear case, feature vector is replace with a column of the kernel matrix

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Support vector machines with kernels

- Minimize quadratic program

$$min_{\boldsymbol{w},b,\{\xi_i\}} \quad \lambda \frac{1}{2} \boldsymbol{w}^T \boldsymbol{w} \;+\; \sum_i \xi_i$$

$$\text{subject to } \forall_i: \;\; \xi_i \geq 0 \;\text{ and }\; \xi_i \geq 1 - y_i f(\boldsymbol{x}_i)$$

- Let us again define the classification function in terms of kernel evaluations

$$f(\boldsymbol{x}_i) = b + \boldsymbol{\alpha}^T \boldsymbol{k}_i$$

- Then we obtain a quadratic program in b, alpha, and the slack variables xi

$$min_{\boldsymbol{w},b,\{\xi_i\}} \quad \lambda \frac{1}{2} \boldsymbol{\alpha}^T \boldsymbol{K} \boldsymbol{\alpha} \;+\; \sum_i \xi_i$$

$$\text{subject to } \forall_i: \;\; \xi_i \geq 0 \;\text{ and }\; \xi_i \geq 1 - y_i \left(b + \boldsymbol{\alpha}^T \boldsymbol{k}_i \right)$$

SVM with kernels

- Recall that $p(y_i|\boldsymbol{x}_i)=\frac{\exp\left(f_{y_i}(\boldsymbol{x}_i)\right)}{\sum_c \exp f_c(\boldsymbol{x}_i)}$ and $f_c(\boldsymbol{x}_i)=b_c+\boldsymbol{\alpha}_c^T\boldsymbol{k}_i$

- Therefore we want to maximize

$$E(\{\alpha_c\},\{b_c\})=\sum_{i=1}^n\left(f_{y_i}(\boldsymbol{x}_i)-\ln\sum_c \exp f_{y_i}(\boldsymbol{x}_i)\right)-\lambda\frac{1}{2}\sum_c \boldsymbol{\alpha}_c^T\boldsymbol{K}\boldsymbol{\alpha}_c$$

- Consider the partial derivative of this function with respect to the b's, and the gradient with respect to the alpha vectors

$$\frac{\partial E}{\partial b_c}=\sum_{i=1}^n\left([y_i=c]-p(c|\boldsymbol{x}_i)\right)$$

$$\nabla_{\boldsymbol{\alpha}_c}E=\sum_{i=1}^n\left([y_i=c]-p(c|\boldsymbol{x}_i)\right)\boldsymbol{k}_i-\boldsymbol{K}\boldsymbol{\alpha}_c$$

  - Essentially the same gradients as in the linear case, feature vector is replace with a column of the kernel matrix

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Summary linear classification & kernels

- Linear classifiers learned by minimizing convex cost functions
  - Logistic discriminant: smooth objective, minimized using gradient descend
  - Support vector machines: piecewise linear objective, quadratic programming
  - Both require only computing inner product between data points

- Non-linear classification can be done with linear classifiers over new features that are non-linear functions of the original features
  - Kernel functions efficiently compute inner products in (very) high-dimensional spaces, can even be infinite dimensional in some cases.

- Using kernel functions non-linear classification has drawbacks
  - Requires storing the support vectors, may cost lots of memory in practice
  - Computing kernel between new data point and support vectors may be computationally expensive (at least more expensive than linear classifier)

- The "kernel trick" also applies for other linear data analysis techniques
  - Principle component analysis, k-means clustering, …

Reading material

- A good book that covers all machine learning aspects of the course is
  - Pattern recognition & machine learning
    Chris Bishop, Springer, 2006

- For clustering with k-means & mixture of Gaussians read
  - Section 2.3.9
  - Chapter 9, except 9.3.4
  - Optionally, Section 1.6 on information theory

- For classification read
  - Section 2.5, except 2.5.1
  - Section 4.1.1 & 4.1.2
  - Section 4.2.1 & 4.2.2
  - Section 4.3.2 & 4.3.4
  - Section 6.2
  - Section 7.1 start + 7.1.1 & 7.1.2