Generative and discriminative classification

Machine Learning and Object Recognition 2017-2018

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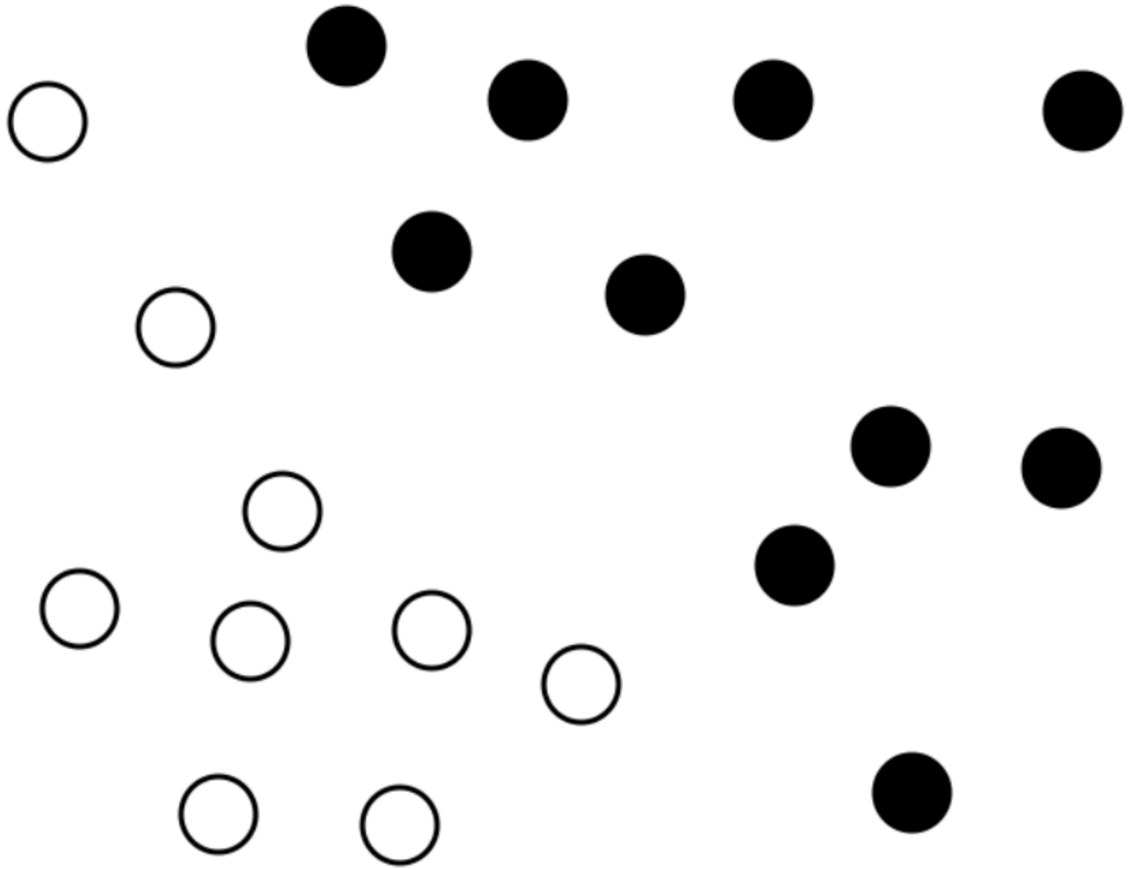
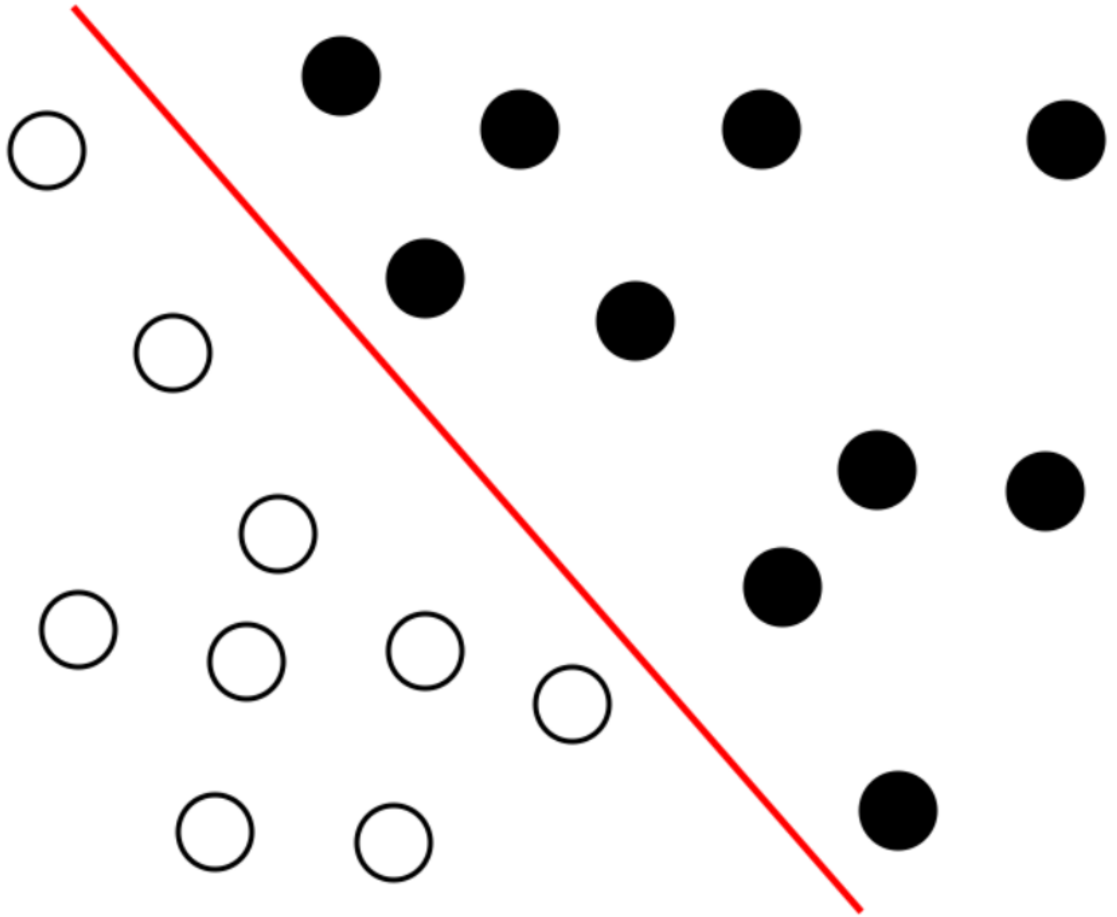
Classification in its simplest form

- Given training data labeled for two or more classes



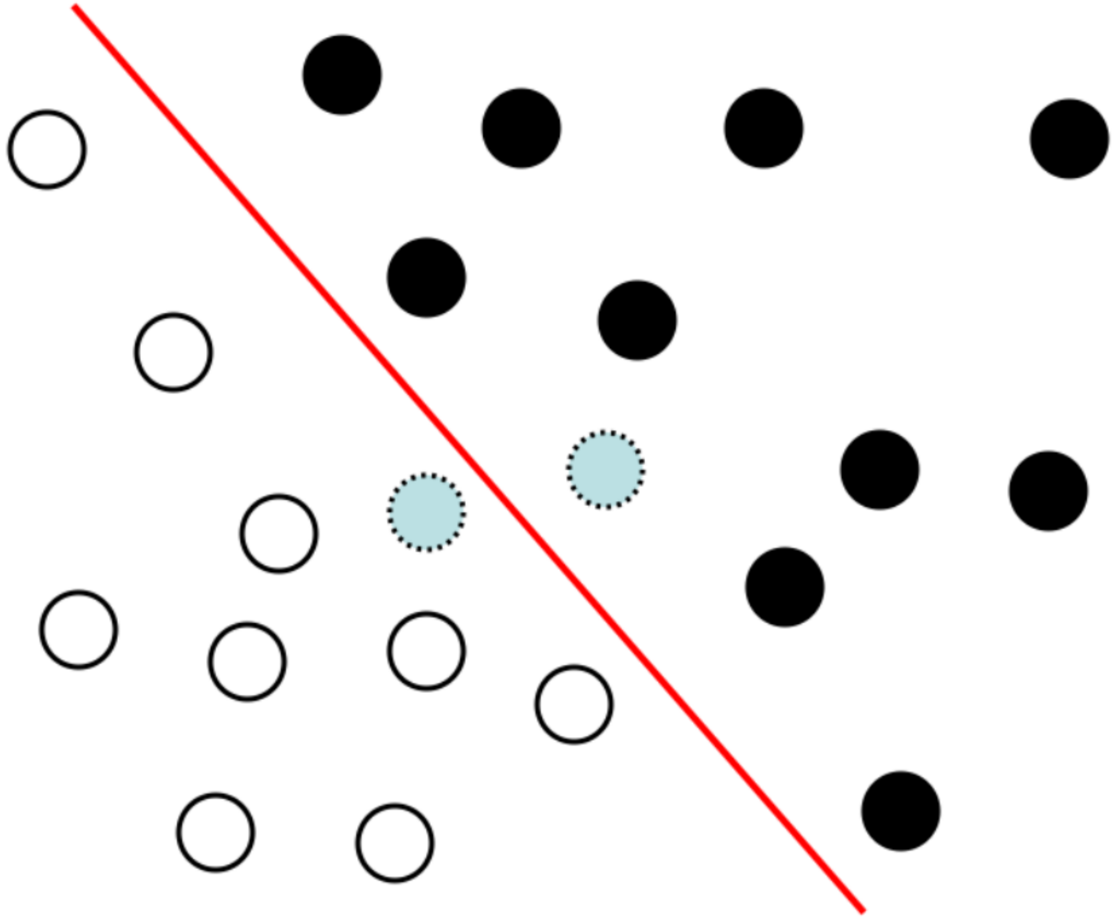
Classification in its simplest form

- Given training data labeled for two or more classes
- Determine a surface that separates those classes



Classification in its simplest form

- 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 examples in category-level recognition

- Image classification: Predict if labels are relevant or not for a given image
- For example: Person = yes, TV = yes, car = no, ...

Classification examples in category-level recognition

- Category localization: predict object bounding boxes
- Classify each possible bounding box as containing the category or not
- Report most confidently classified boxes

Classification examples in category-level recognition

- Semantic segmentation: classify pixels to object categories
- As many classifications as pixels
- Each one based on region around the pixel

Classification

- Goal is to predict for data the corresponding class label

- **Data points x**, e.g. image but could be anything
  - Formatted as vectors, or other
- **Class labels y**, two or more possible discrete values
  - In binary case: “positive” and “negative” class

- **Classifier**: function f(x) that assigns a class to x
  - Possibly gives probabilities over the classes
  - Partitions the input space into regions associated with classes
  - Shape of these regions depends on the family of classifiers used

- **Training data**: pairs (x,y) of inputs x with known class label y

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

Generative classification: principle

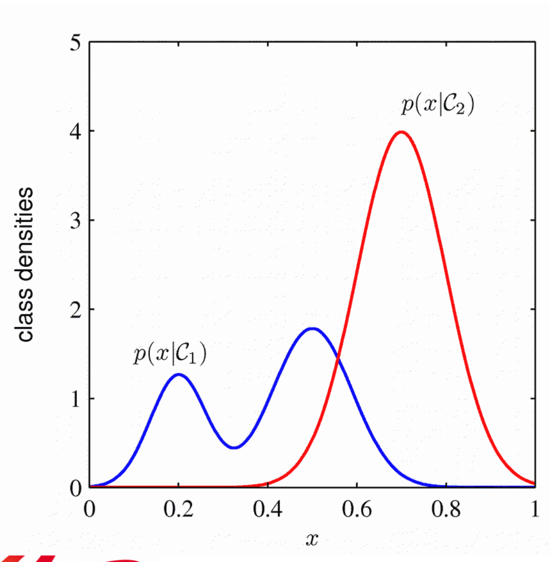
- Model the class conditional distribution over data x for each class y: $p(x|y)$
  - Data of the class can be sampled (generated) from this distribution
- Estimate the a-priori probability that a class will appear $p(y)$

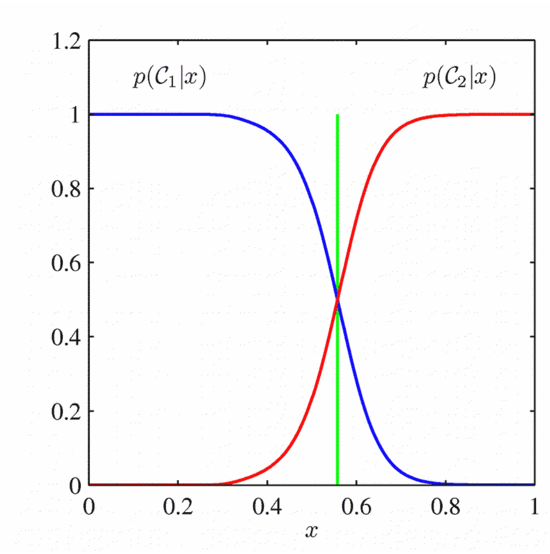
- Infer the probability over classes using Bayes' rule of conditional probability

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

- Distribution on x is obtained by marginalizing the class label y

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



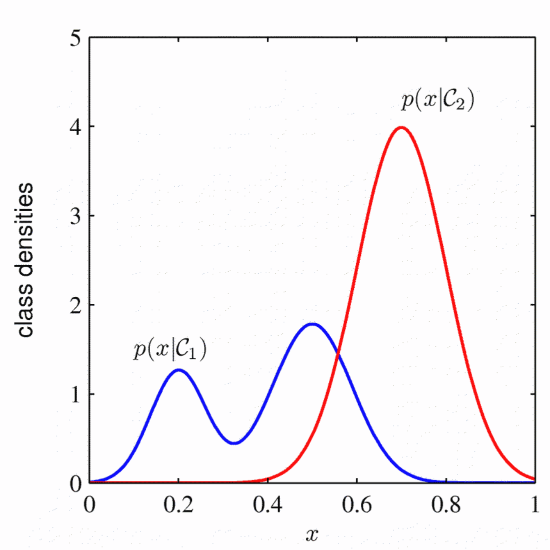


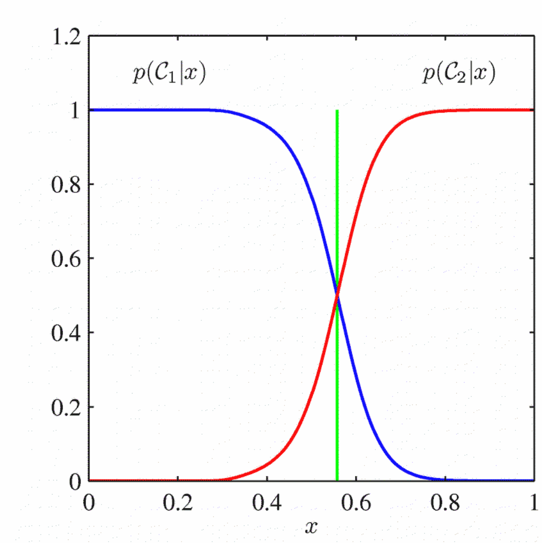
Generative classification methods

- Generative probabilistic methods use Bayes' rule for prediction
  - Problem is reformulated as one of density estimation

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

- Adding new classes to the model is easy:
  - Existing class conditional models stay as they are
  - Estimate p(x|new class) from training examples of new class
  - Re-estimate class prior probabilities





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.

- 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
  $X = \{x_{1,} \ldots, x_n\}$ $\qquad P = \{p_\theta(x); \theta \in \Theta\}$
- 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
    $$\hat{\theta} = \text{argmax}_\theta\, p(\theta|X) = \text{argmax}_\theta \{\ln p(\theta) + \ln p(X|\theta)\}$$

- 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 $\hat{\theta} = \text{argmax}_\theta\, p(X|\theta)$
  - For i.id. samples:
    $$\hat{\theta} = \text{argmax}_\theta \prod_{i=1}^{n} p(x_i|\theta) = \text{argmax}_\theta \sum_{i=1}^{n} \ln p(x_i|\theta)$$

Density estimation for class-conditional models

- Any type of data distribution may be used, preferably one that is modeling the data well, so that we can hope for accurate classification results.

- If we do not have a clear understanding of the data generating process, we can use a generic approach,

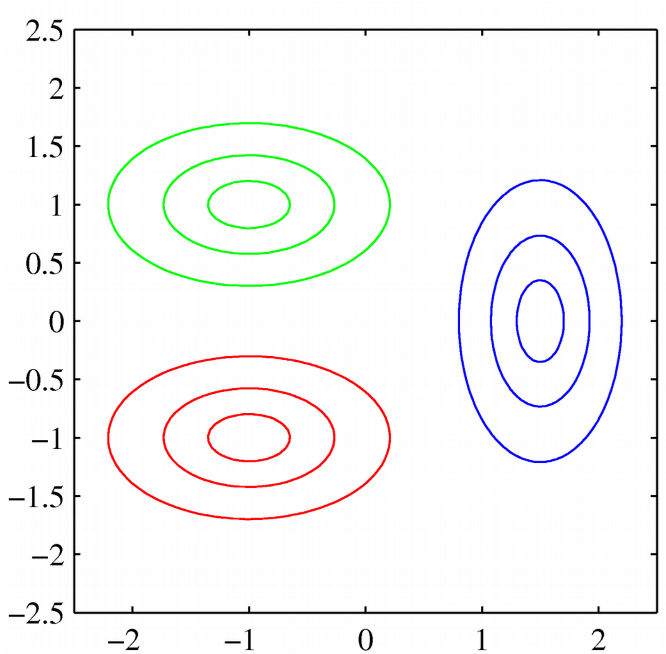
  - Gaussian distribution, or other reasonable parametric model
    - Estimation often in closed form or relatively simple process

  - Mixtures of parametric models
    - Estimation using EM algorithm, not more complicated than single parametric model

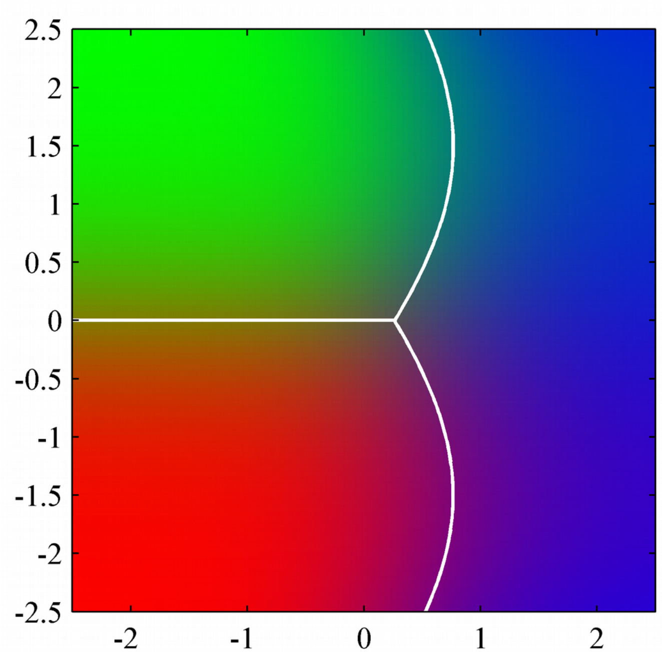
  - Non-parametric models can adapt to any data distribution given enough data for estimation. Examples: (multi-dimensional) histograms, and nearest neighbors.
    - Estimation often trivial, given a single smoothing parameter.

Example of generative classification

- Three-class example in 2D with parametric model
  - Single Gaussian model per class, uniform class prior
  - Exercise 1: how is this model related to the Gaussian mixture model we looked at before for clustering ?
  - Exercise 2: characterize surface of equal class probability when the covariance matrices are the same for all classes



$p(x|y)$



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

Histogram density estimation

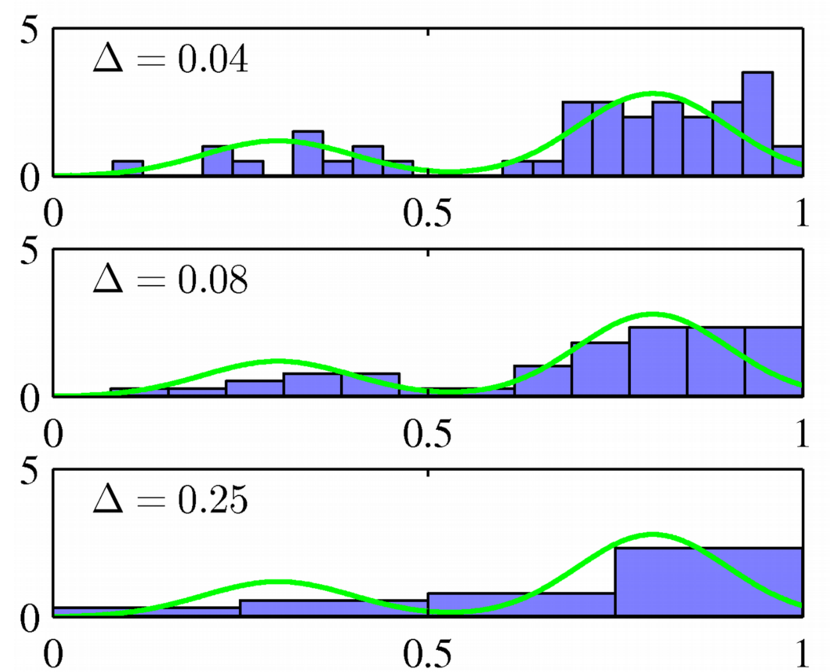
- Suppose we have *N* data points use a histogram with *C* cells
- Consider maximum likelihood estimator

$$\hat{\theta} = \mathrm{argmax}_{\theta} \sum_{i=1}^{n} \ln p_{\theta}(x_i) = \mathrm{argmax}_{\theta} \sum_{c=1}^{C} n_c \ln \theta_c$$

- Take into account constraint that density should integrate to one

$$\sum_{k=1}^{C} v_k \theta_k = 1$$

- Maximum likelihood estimator $\theta_i = \frac{n_i}{v_i N}$



- Some observations:
  - Discontinuous density estimate
  - Cell size determines smoothness
  - Number of cells scales exponentially with the dimension of the data

The Naive Bayes model

- Histogram estimation, and other methods, scale poorly with data dimension
  - Fine division of each dimension: many empty bins
  - Rough division of each dimension: poor density model
  - Even for one cut per dimension: 2^D cells, eg. a million cells in 20 dims.

- The number of parameters can be made linear in the data dimension by assuming independence between the dimensions

$$p(x)=\prod_{d=1}^{D} p(x_d)$$

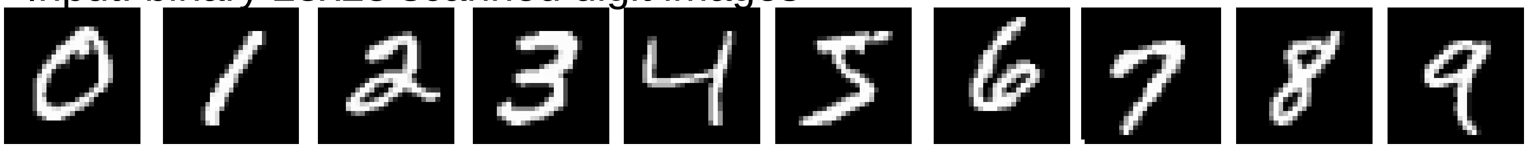
- For example, for histogram model: we estimate a histogram per dimension
  - Only D x C parameters to estimate, instead of C^D: Factorization

- Independence assumption can be unrealistic for high dimensional data
  - Classification performance may still be good using derived p(y|x)
  - Assuming only partial independence relaxes this problem

- Principle can be applied to estimation with any type of density estimate

Example of a naïve Bayes model

- Hand-written digit classification
  - Input: binary 28x28 scanned digit images

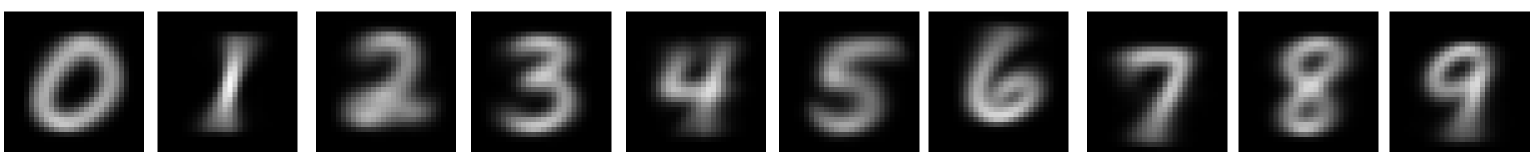


  - Desired output: class label of image

- Generative model over 28 x 28 pixel images: 2^{784} possible images
  - Independent Bernoulli model for each class
  - Probability per pixel per class
  - Maximum likelihood estimator given by average pixel values per class

$$p(x|y=c) = \prod_d p(x^d|y=c)$$

$$p(x^d=1|y=c) = \theta_{cd}$$



- Classify using Bayes' rule, yields linear classifier

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

k-nearest-neighbor density estimation: principle

- **Instead of having fixed cells** as in histogram method
  - **Center cell on the test sample** for which we evaluate the density
  - Fix number of samples in the cell, find the corresponding **cell size**

- Probability to find a point in a sphere ***A*** centered on $\boldsymbol{x_0}$ with volume ***v*** is

$$P(x \in A) = \int_A p(x)\,dx$$

- Assume density is approximately constant in the region

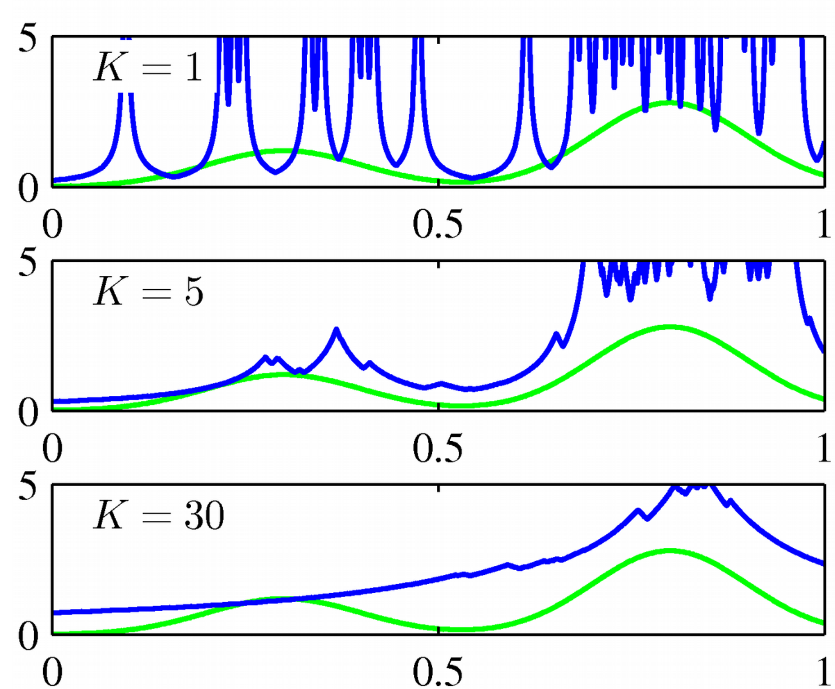
$$P(x \in A) = \int_A p(x)\,dx \approx \int_A p(x_0)\,dx = p(x_0)\,v_A$$

- Alternatively: estimate ***P*** from the fraction of training data in ***A****:* $P(x \in A) \approx \frac{k}{N}$
  - Total N data points, k in the sphere ***A***

- Combine the above to obtain estimate $p(x_0) \approx \frac{k}{N v_A}$
  - Same per-cell density estimate as in histogram estimator
- Note: density estimates not guaranteed to integrate to one!

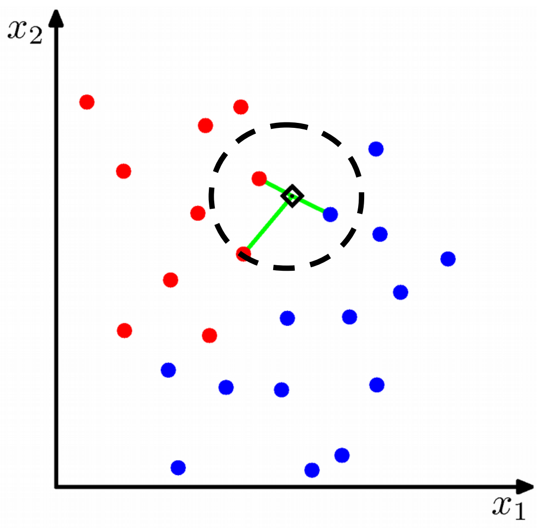
k-nearest-neighbor density estimation: practice

- Procedure in practice:
  - Choose ***k***
  - For given ***x***, find k-th neighbor to compute the volume with k samples
  - Estimate density with $p(x) \approx \frac{k}{Nv}$
- Volume of a sphere with radius ***r*** in ***d*** dimensions is $v(r,d) = \frac{2r^d \pi^{d/2}}{\Gamma(d/2+1)}$
- What effect does ***k*** have?
  - Data sampled from mixture of Gaussians plotted in green
  - Larger ***k***, larger region, smoother estimate
  - Similar effect as cell size for histogram estimation



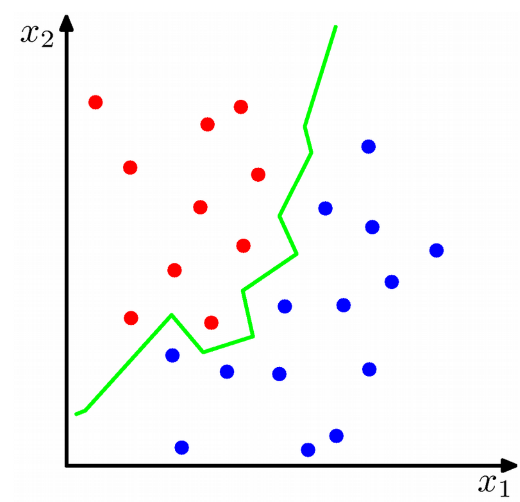
K-nearest-neighbors for classification

- Use Bayes' rule with kNN density estimation for p(x|y)
  - Find sphere volume v to capture ***k*** data points for estimate $p(x)=\frac{k}{Nv}$
  - Use the same sphere for each class for estimates $p(x|y=c)=\frac{k_c}{N_c v}$
  - Estimate class prior probabilities $p(y=c)=\frac{N_c}{N}$
  - Calculate class posterior distribution as fraction of k neighbors in class c



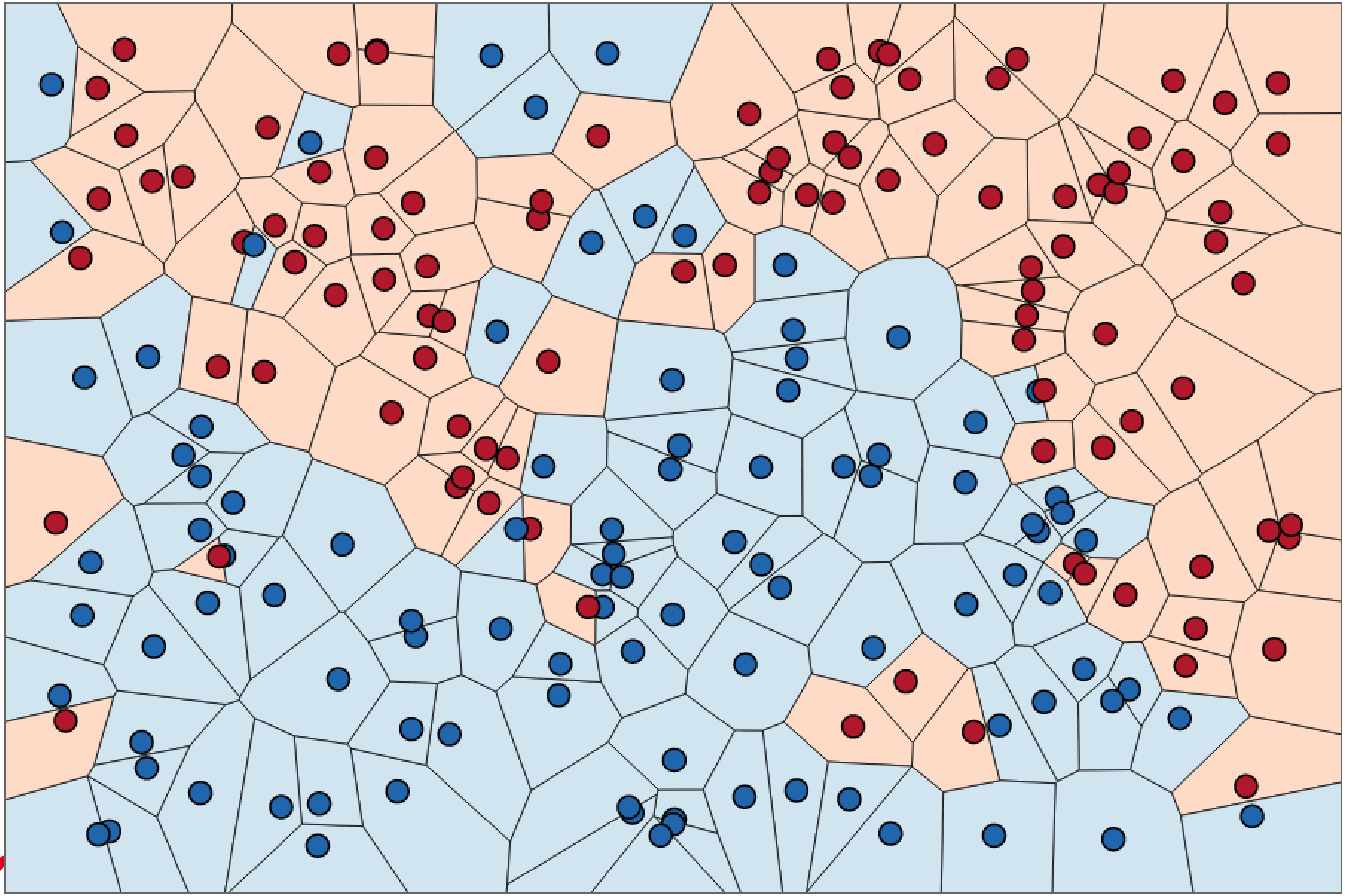
(a)

$$p(y=c|x)=\frac{p(y=c)\,p(x|y=c)}{p(x)}$$
$$=\frac{1}{p(x)}\frac{k_c}{Nv}$$
$$=\frac{k_c}{k}$$

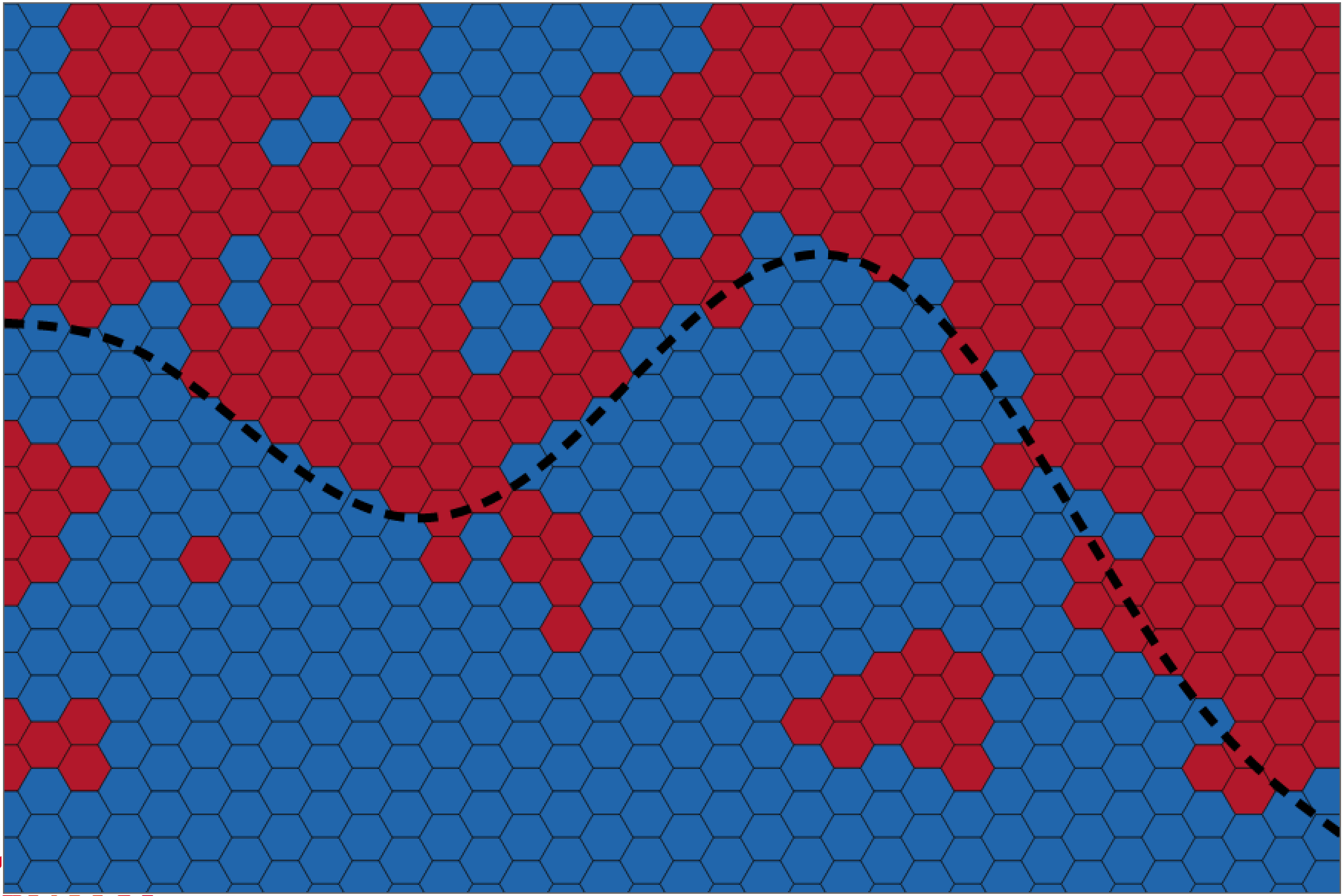


(b)

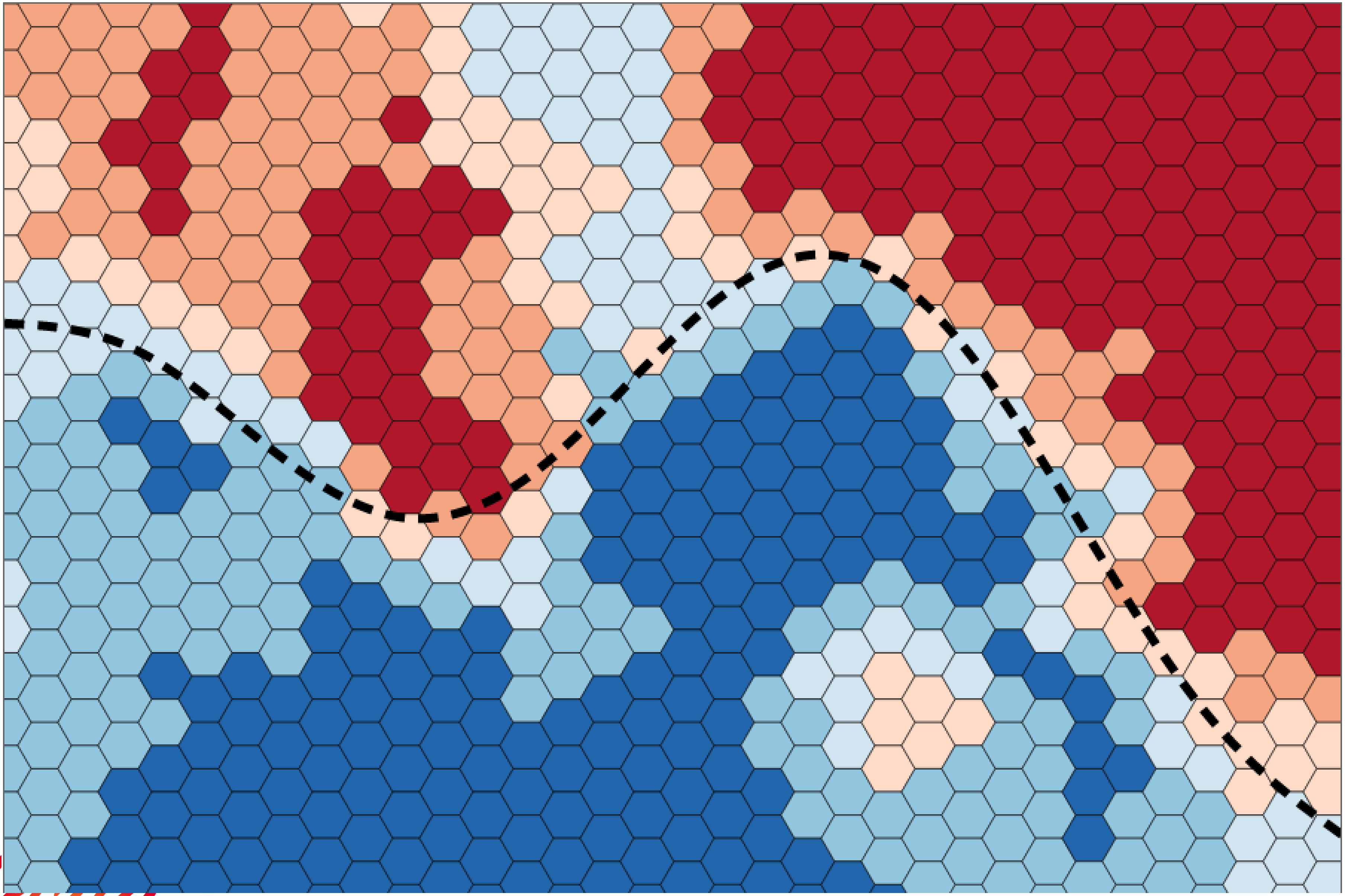
Smoothing effects for large values of k: data set



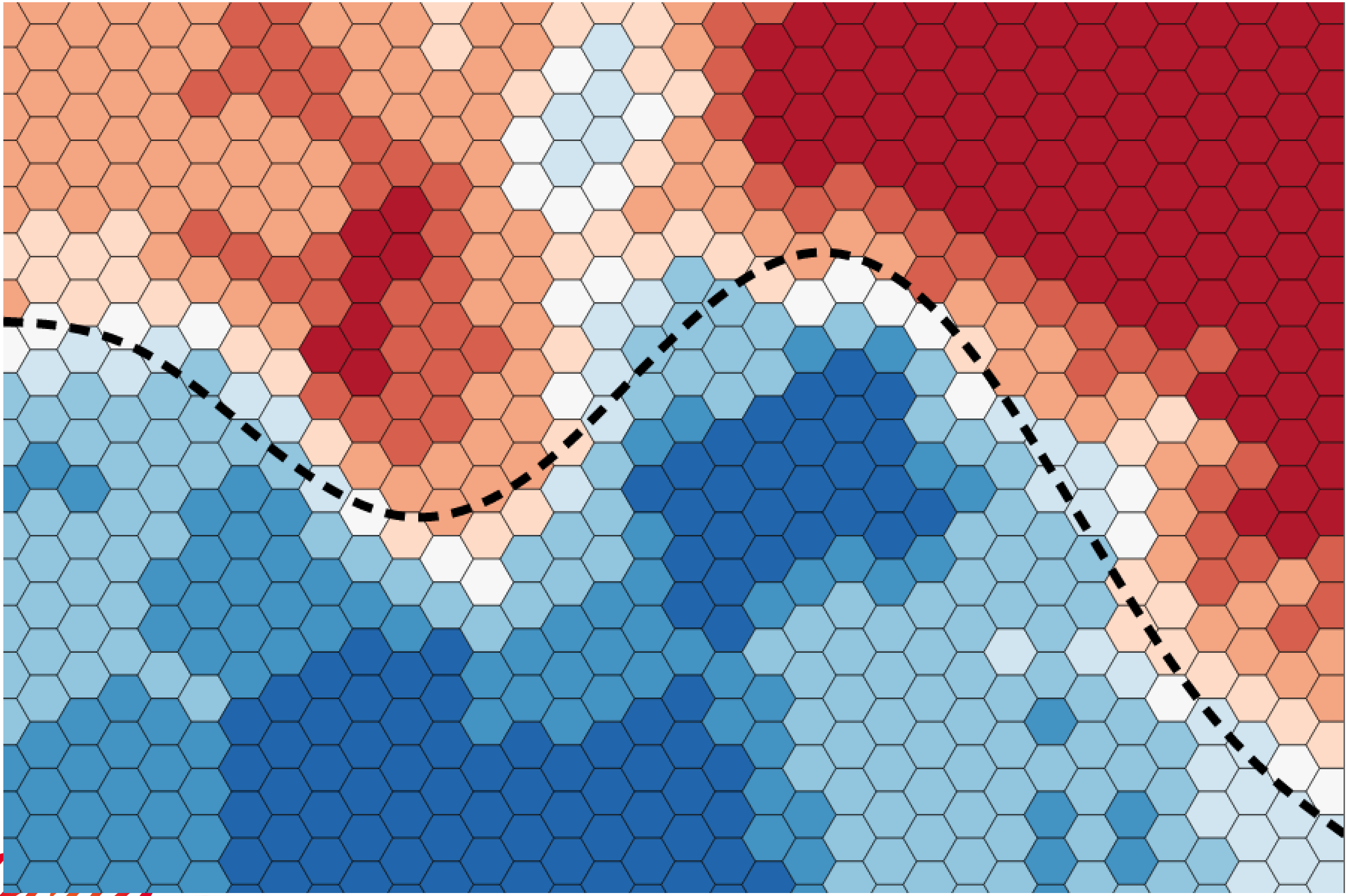
Smoothing effects for large values of k, k=1



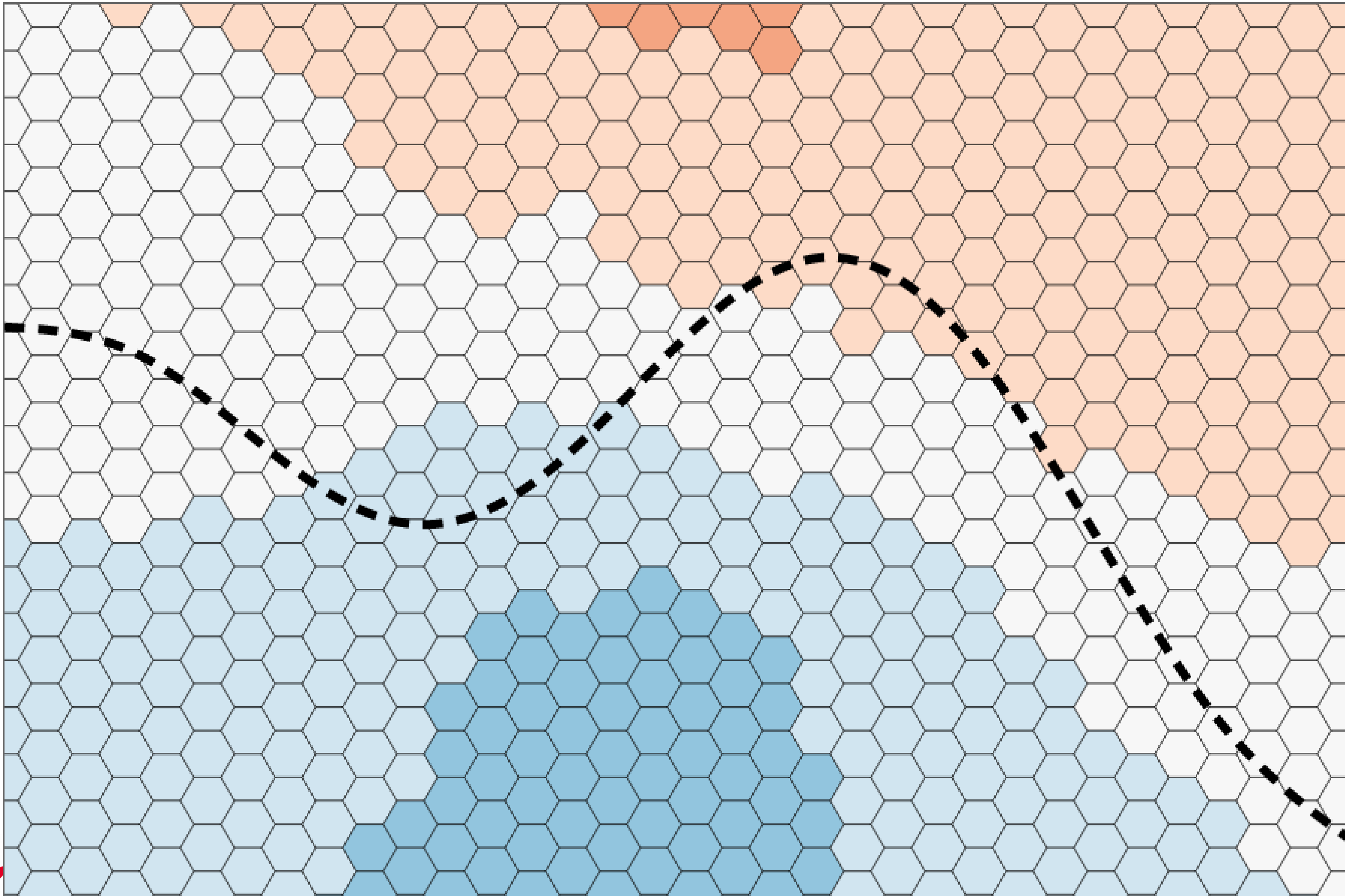
Smoothing effects for large values of k, k=5



Smoothing effects for large values of k, k=10



Smoothing effects for large values of k, k=100



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)

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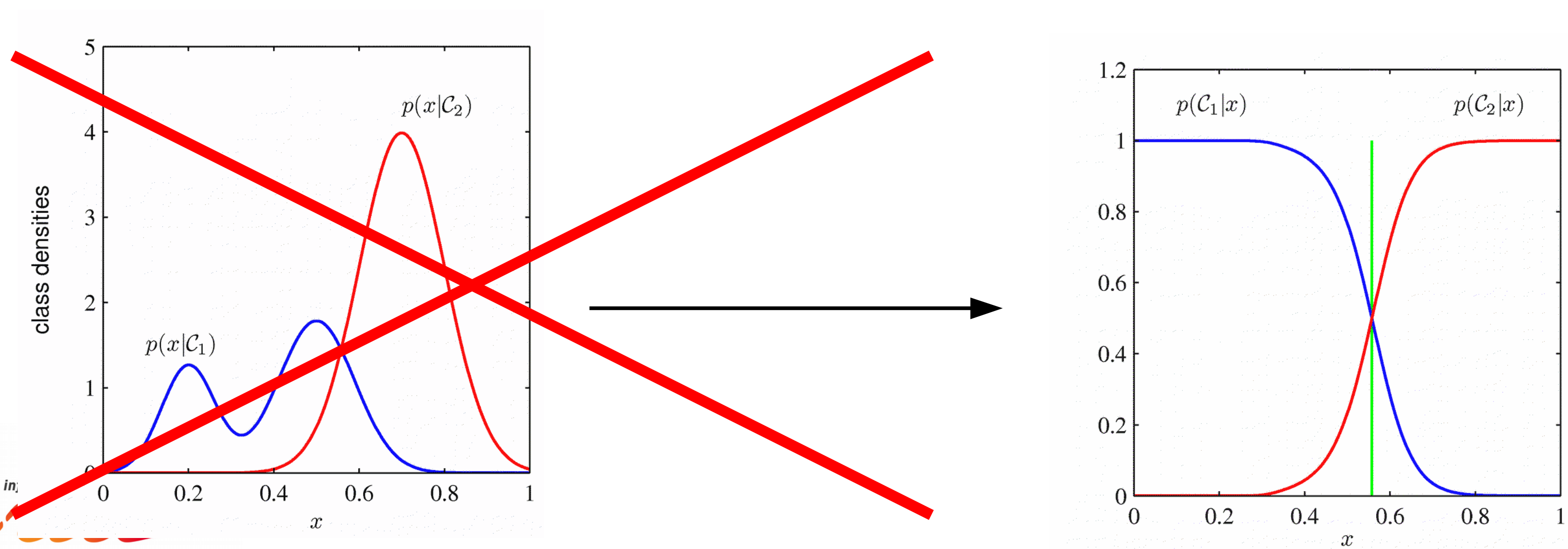
Discriminative classification methods

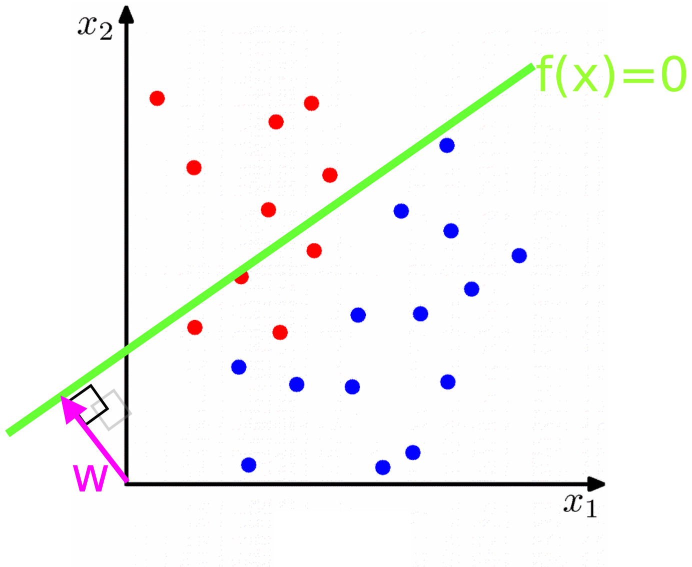
- Generative classification models
  - Model the density of inputs x from each class p(x|y)
  - Estimate class prior probability p(y)
  - Use Bayes' rule to infer distribution over class given input
- In discriminative classification methods we directly estimate class probability given input: p(y|x)
  - 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**
- Offset from origin is determined by *b*

- Decision surface is (d-1) dimensional hyper-plane orthogonal to **w**, given by

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

Common loss functions for classification

- Assign class label using $y = sign(f(x))$
- Quantify model accuracy using “loss function”

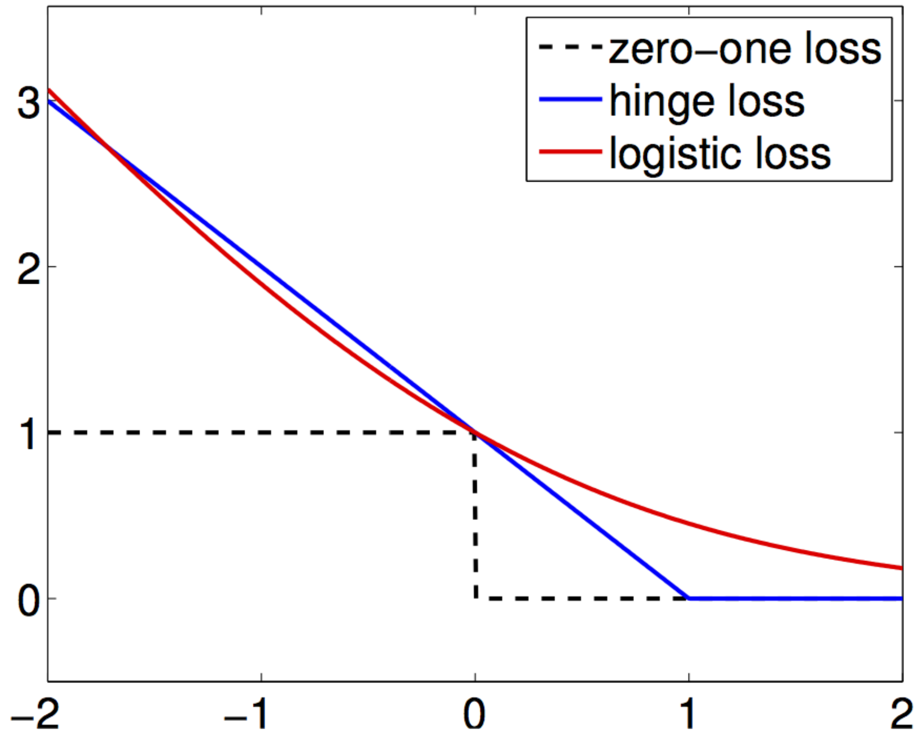
- The zero-one loss counts the number of misclassifications

$$L(y_i, f(x_i)) = [y_i f(x_i) < 0]$$

  - Corresponds directly to number of errors
  - Discontinuity at zero, constant elsewhere w.r.t. f
  - Not useful to derive gradient signal to improve model f

Common loss functions for classification

- Hinge and logistic loss provide continuous and convex upper bounds on zero-one loss, which allow for continuous optimization
  - Hinge loss: $L(y_i, f(x_i)) = max(0, 1 - y_i f(x_i))$
  - Logistic loss: $L(y_i, f(x_i)) = \log_2(1 + e^{-y_i f(x_i)})$
- Both penalize f if it gives the wrong sign with large magnitude

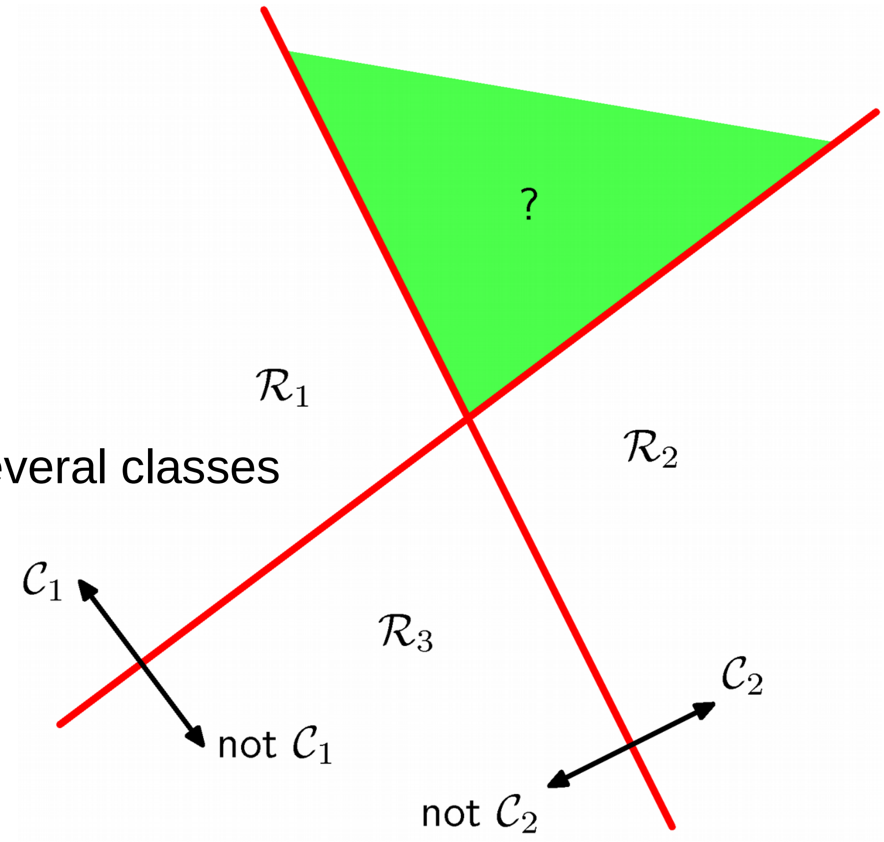


Dealing with more than two classes

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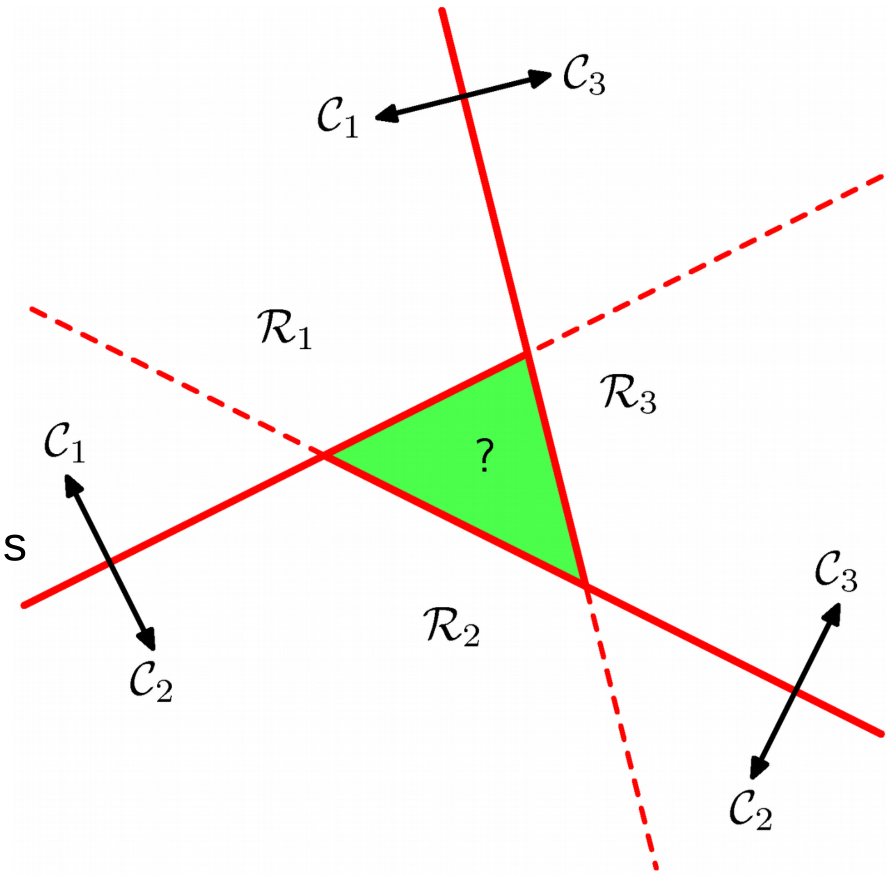
- One vs one approach:
  - 1 vs 2
  - 1 vs 3
  - 2 vs 3



- Problem: conflicts in some regions

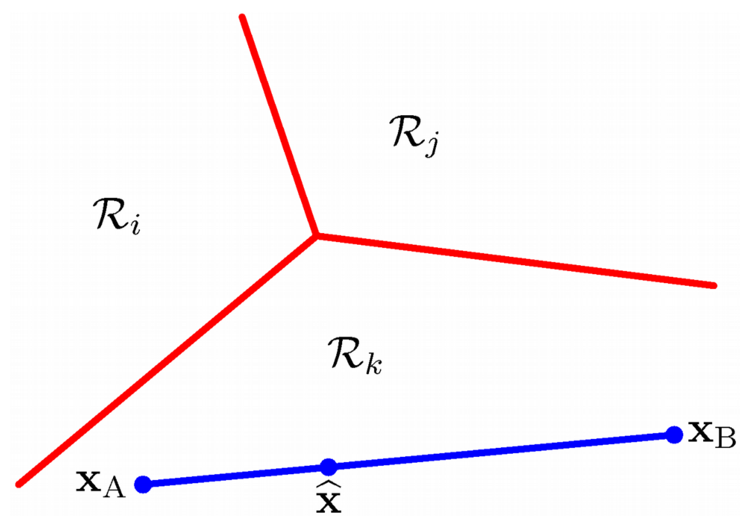
Dealing with more than two classes

- 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
  - For any two points in the set, the points on connecting line are too

Logistic discriminant for two classes

- Map linear score function to class probabilities with sigmoid function

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

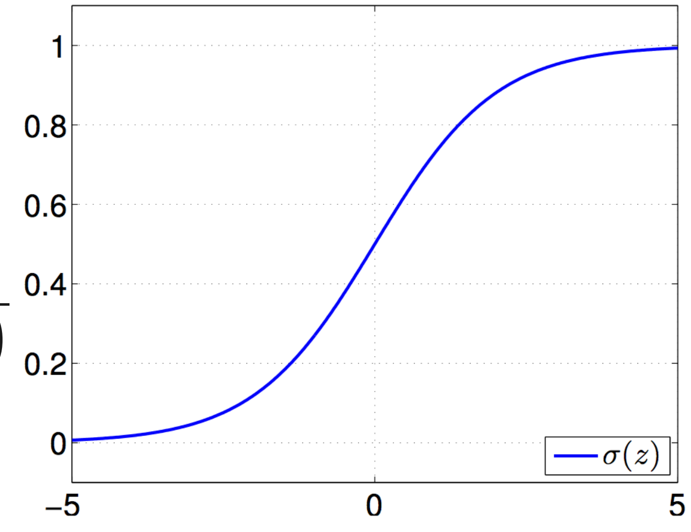
  - For binary classification problem, we have by definition

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

  - Exercise: show that

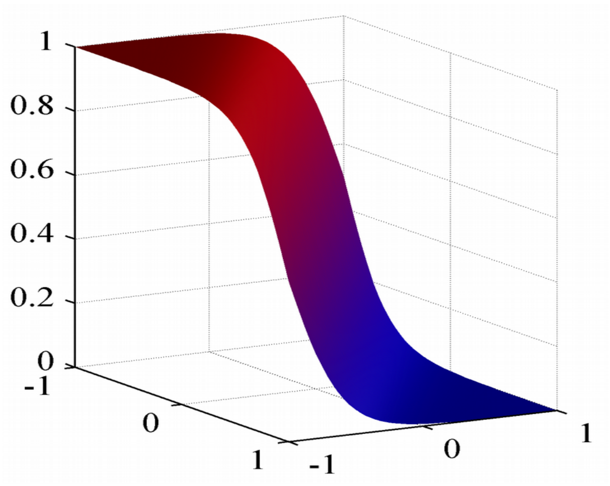
$$p(y|x)=\sigma(y(w^T x+b))$$

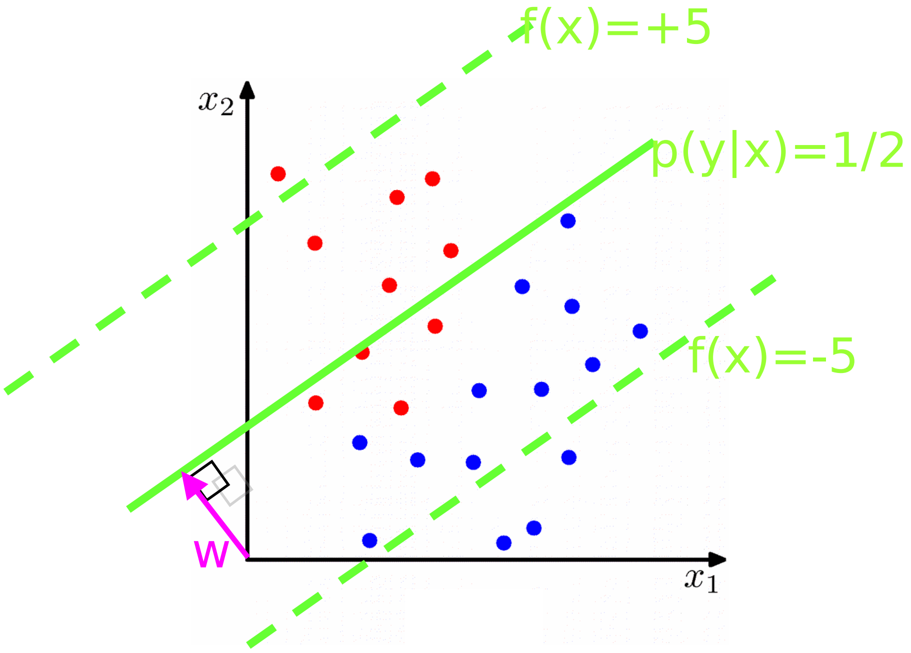
$$\sigma(z)=\frac{1}{1+\exp(-z)}$$



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

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

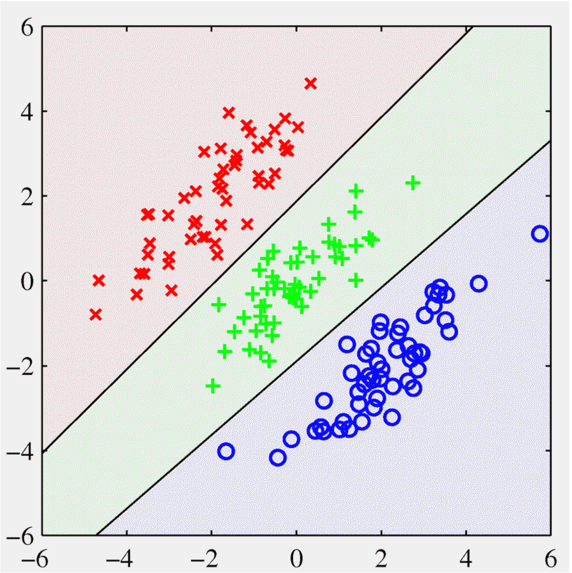
  - The class probability estimates are non-negative, and sum to one.

- Probabilities invariant for additive constants, only score differences matter
  - Relative probability exponential function of difference in score functions

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

- Any given pair of classes are equally likely

  on a hyperplane in the feature space



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Maximum likelihood parameter estimation

- Maximize the log-likelihood of predicting the correct class label for training data
  - Assume independent predictions, so sum log-likelihood of all training data

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

- Derivative of log-likelihood has intuitive interpretation

Indicator function
1 if y_n=k, else 0

$$\frac{\partial L}{\partial w_k} = \sum_{n=1}^{N} \left([y_n = k] - p(y = k | x_n) \right) x_n = \sum_{n=1}^{N} \alpha_n x_n$$

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 method
  - For example: gradient descent, started from w=0
    - *w* is linear combination of data points
    - Sign of coefficients depends on class labels

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Maximum a-posteriori (MAP) parameter estimation

- Exercise: show that for separable data the w's found by maximum likelihood estimation have infinite norm

- Let us assume a zero-mean Gaussian prior distribution on w
  - We expect weight vectors with a small norm

- Find w that maximizes posterior likelihood

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

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

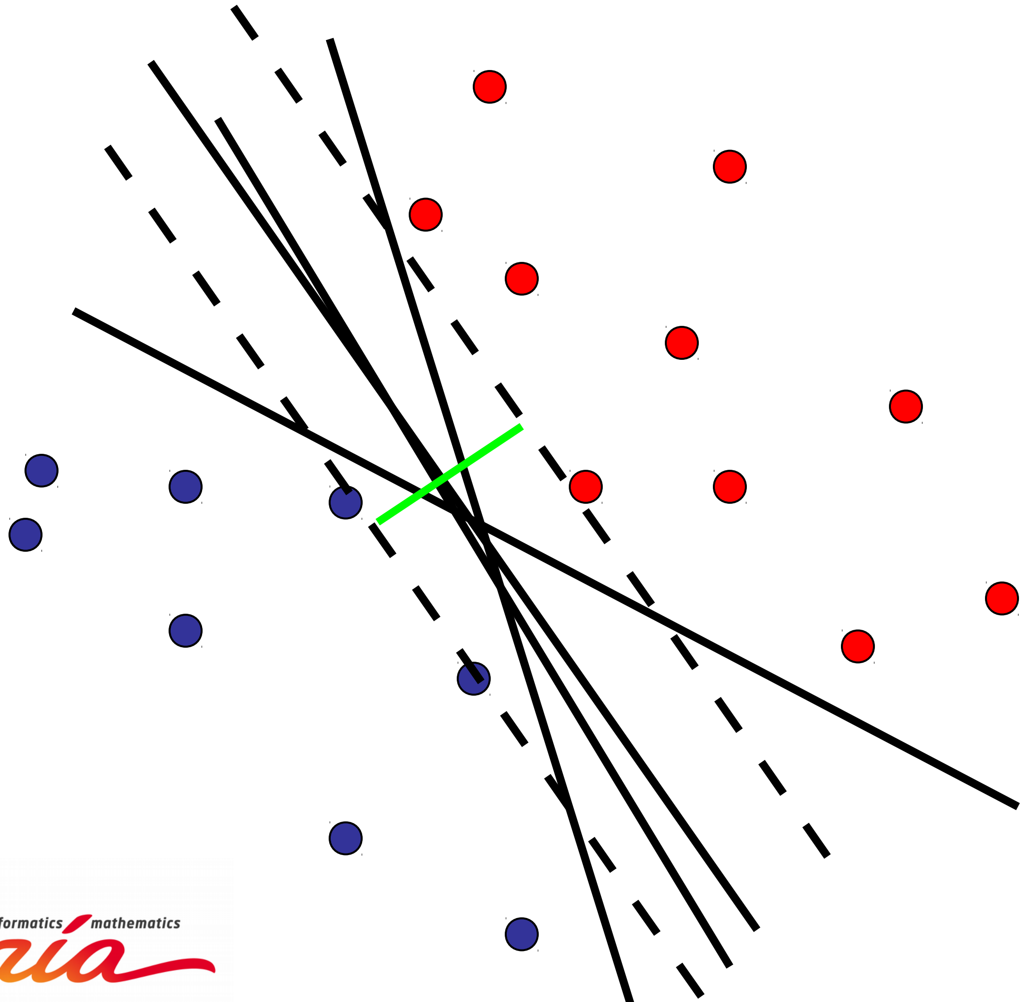
$$\hat{w} = \text{argmax}_w \sum_{n=1}^{N} \ln p(y_n | x_n, w) - \lambda \|w\|_2^2$$

  - With lambda non-negative

- Penalty for "large" w, limits the norm of w in case of separable data

Support Vector Machines

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



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

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Support vector machines

- Without loss of generality, let function value at the margin be +/- 1
  - Can change bias to obtain same absolute function value on each side
  - Can scale w to get +1 and -1 on each side, without changing decisions

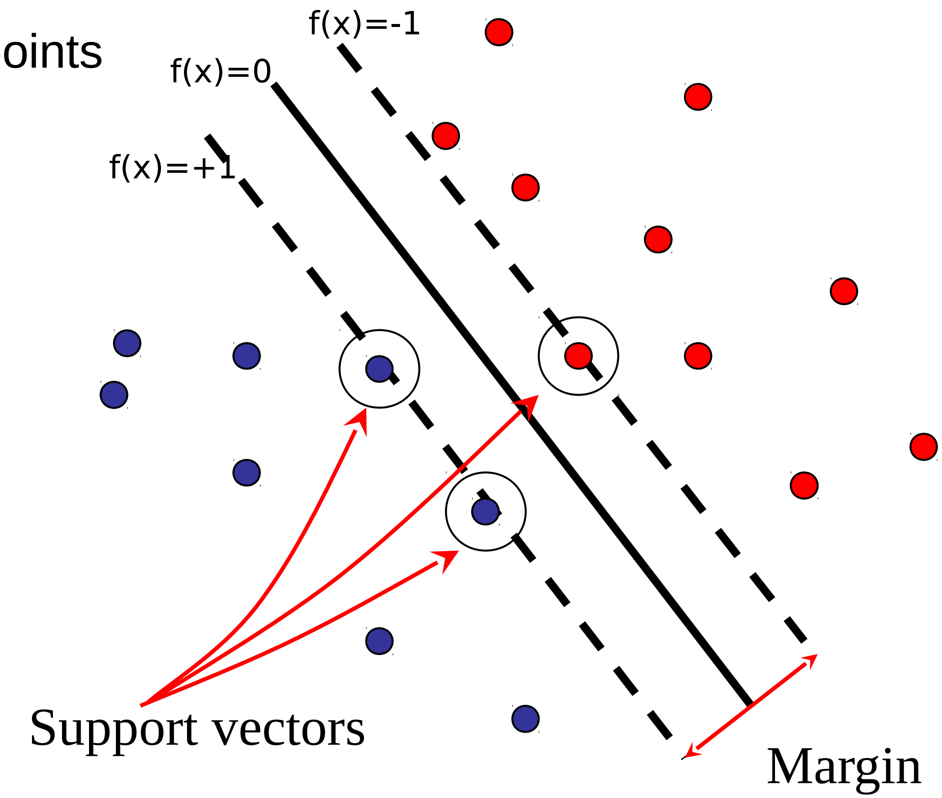
- Now constrain w so that all points fall on correct side of the margin:

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

- The "support vectors" are the data points that define the margin, i.e. having

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

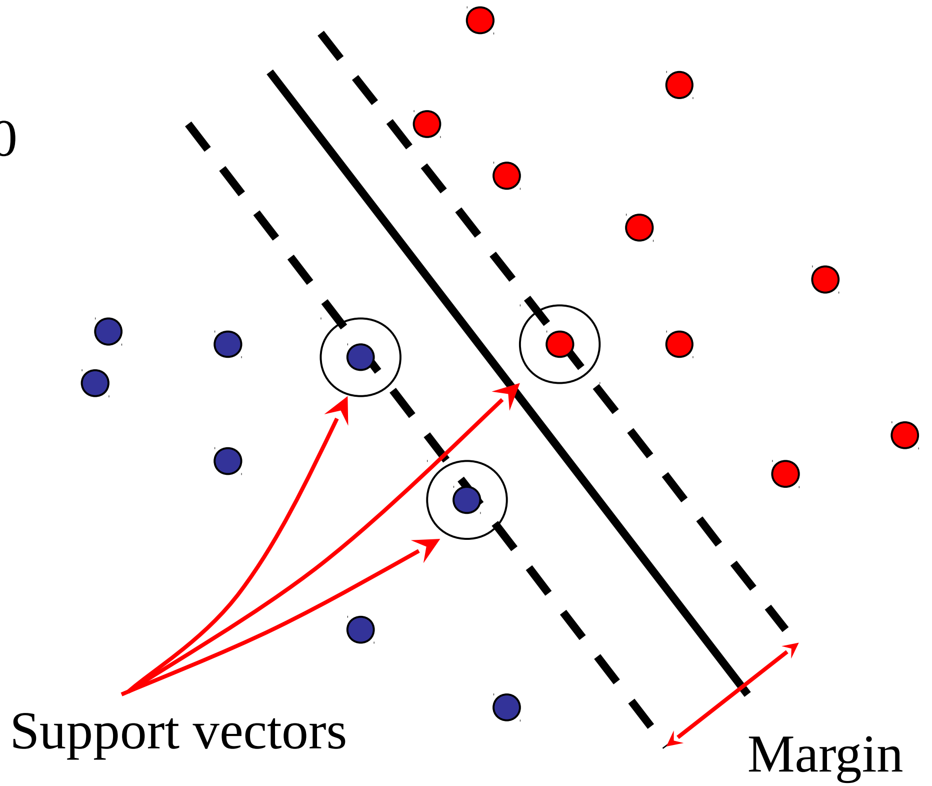
- Quantify the size of the margin in terms of w



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

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

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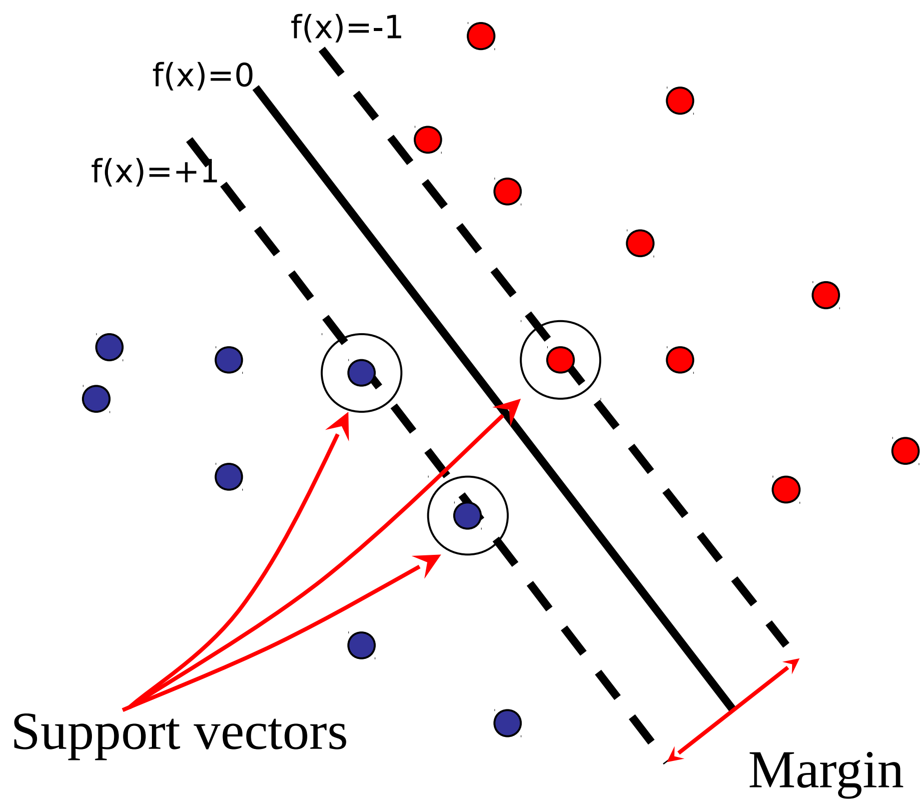
Support vector machines

- 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
  - Linear inequality constraints over w and b

$$argmin_{w,b} \frac{1}{2} w^T w$$

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

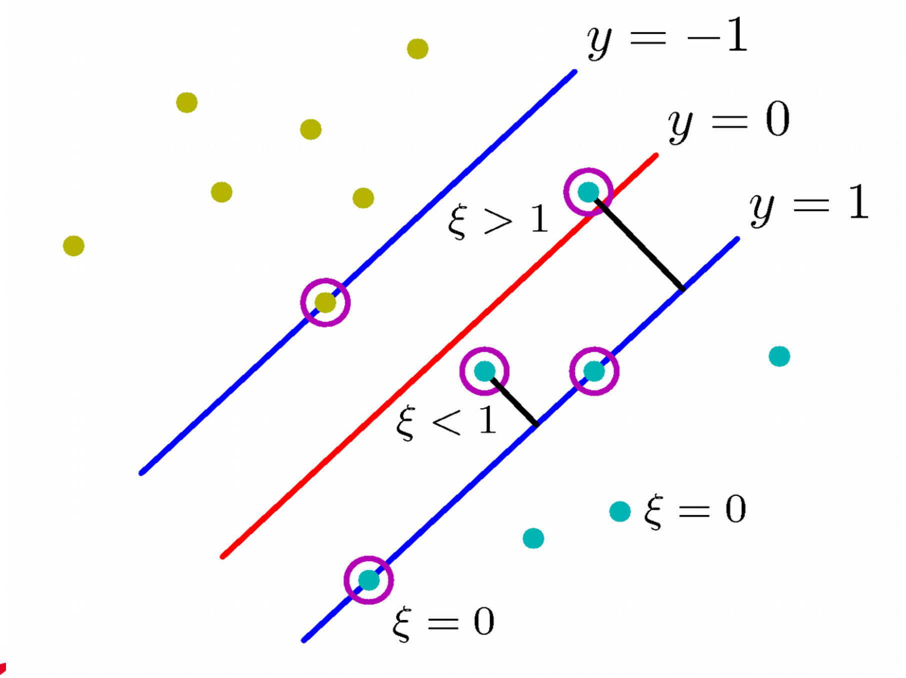


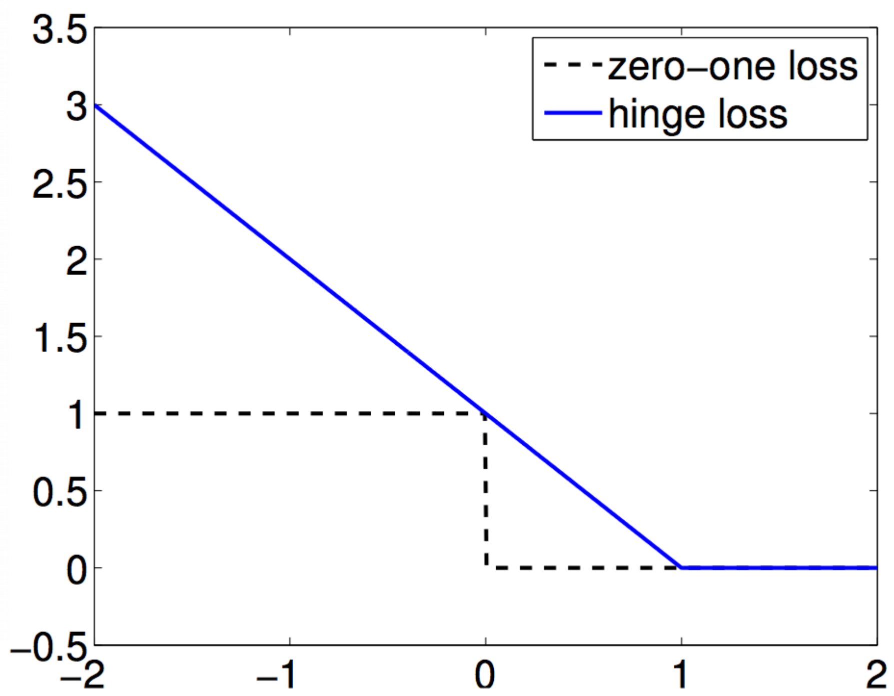
Support vector machines: inseperable classes

- 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 piece-wise 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 **piece-wise 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

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

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

SVM solution properties

- Optimal w is a linear combination of data points $w = \sum_{n=1}^{N} \alpha_n y_n x_n$
- Alpha weights are zero for all points on the correct side of the margin
- Points on the margin, or on the wrong side, have non-zero weight
  - Called support vectors
- 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 ***x*** and training data with non-zero associated alpha's
- Solving the optimization problem alsoonly requires to access the data in terms of inner products between pairs of training points

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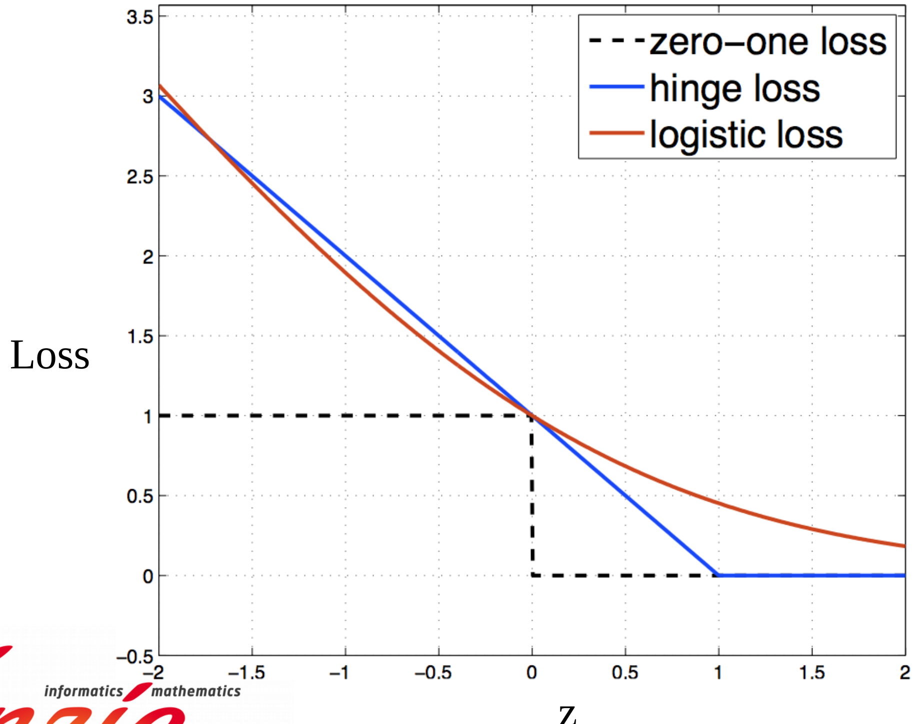
Relation SVM and logistic regression

- 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:
  - Hinge loss: $\xi_i = max(0, 1 - y_i f(x_i)) = max(0, 1 - z)$
  - Logistic loss: $-\log p(y_i | x_i) = -\log \sigma(y_i f(x_i)) = \log(1 + \exp(-z))$



- Both lead to efficient optimization
  - Hinge-loss is piece-wise linear: quadratic programming
  - Logistic loss is smooth : smooth convex optimization methods

- L2 penalty for SVM motivated by margin between the classes
- Found in MAP estimation with Gaussian prior for logistic discriminant

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
  - Optimal weight vector **w** is a linear combination of the data $w = \sum_{n=1}^{N} \alpha_n x_n$

- We only need the inner-products between data points to calculate the train and use linear classifiers

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

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

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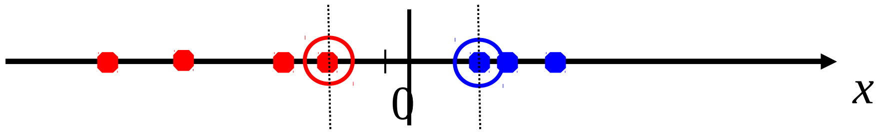
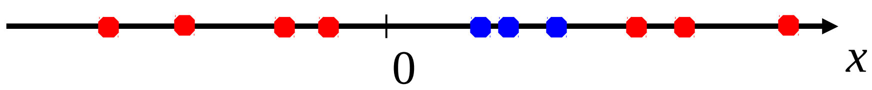
Nonlinear Classification

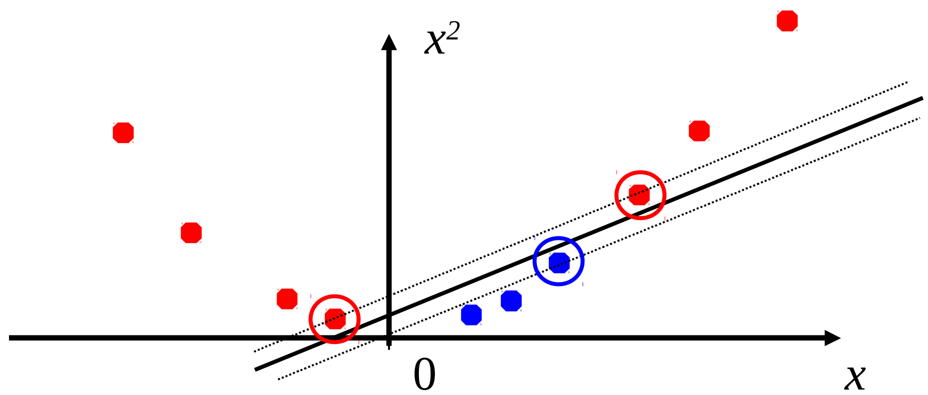
- 1 dimensional data that is linearly separable



- But what if the data is not linearly seperable?



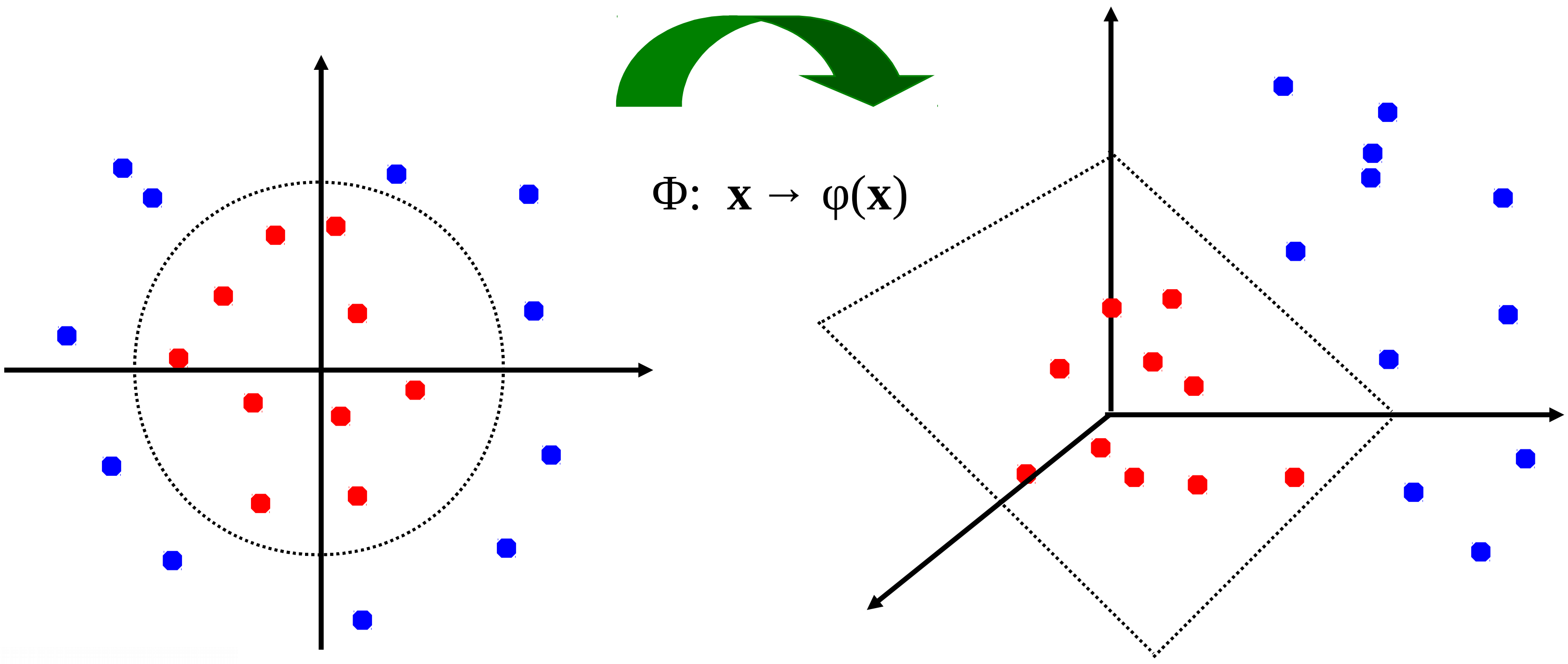
- We can map it to a higher-dimensional space:



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 can linearly separate data in/out a ball in n-dimensional Euclidean space, centered at arbitrary point



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

$$k(\mathbf{x}_i, \mathbf{x}_j) = \boldsymbol{\varphi}(\mathbf{x}_i) \cdot \boldsymbol{\varphi}(\mathbf{x}_j)$$

- Conversely, any positive definite kernel 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 with kernel evaluations for any arbitrary N data points should always be a positive definite matrix*

$$K = [k_{ij}]_{i,j=1}^{N}$$
$$k_{ij} = \phi(x_i)^T \phi(x_j)$$

$$\alpha \neq 0$$
$$\alpha^T K \alpha > 0$$

Nonlinear classification with kernels

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

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

- Generalized linear function
  - Non-linear in original space, linear in new features

$$\phi(x) = \begin{pmatrix} \phi_1(x) \\ \phi_2(x) \\ \vdots \end{pmatrix}$$

- Optimal w is linear combination of training data
  - Linear in space of kernel evaluations
  - Data represented as finite dimensional vector of kernel evaluations with all training data

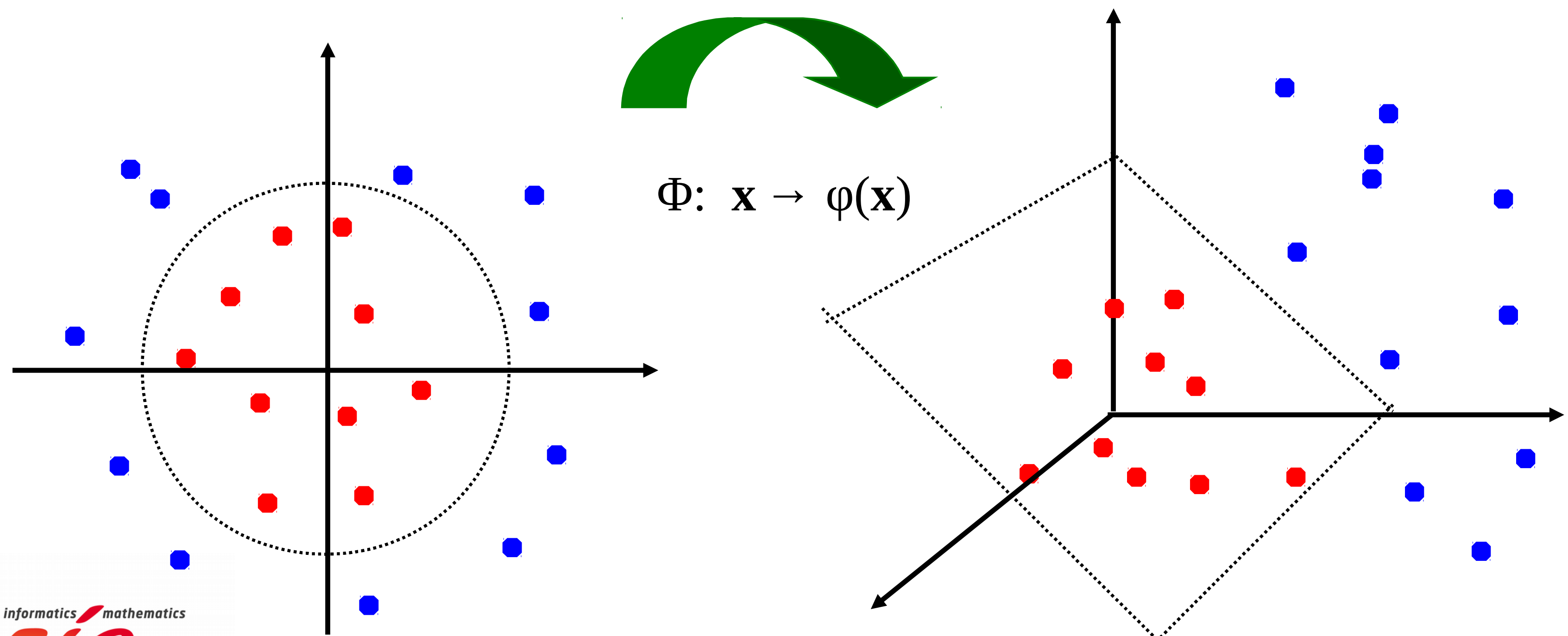
$$\psi(x) = \begin{pmatrix} \phi(x)^T \phi(x_1) \\ \phi(x)^T \phi(x_2) \\ \dots \\ \phi(x)^T \phi(x_N) \end{pmatrix} = \begin{pmatrix} k(x, x_1) \\ k(x, x_2) \\ \dots \\ k(x, x_N) \end{pmatrix}$$

Kernels for non-linear classification

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

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

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



Kernels for non-linear classification

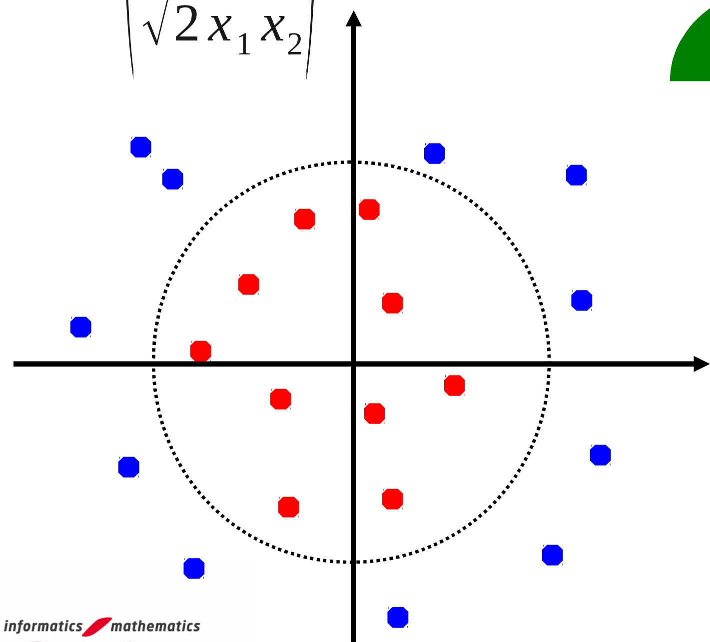
- Suppose we also want to keep the original features to be able to still implement linear functions

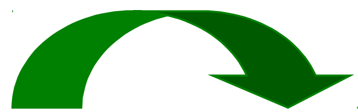
$$k(x,y)=\phi(x)^T\phi(y)=?$$

$$=1+2x^Ty+(x^Ty)^2$$

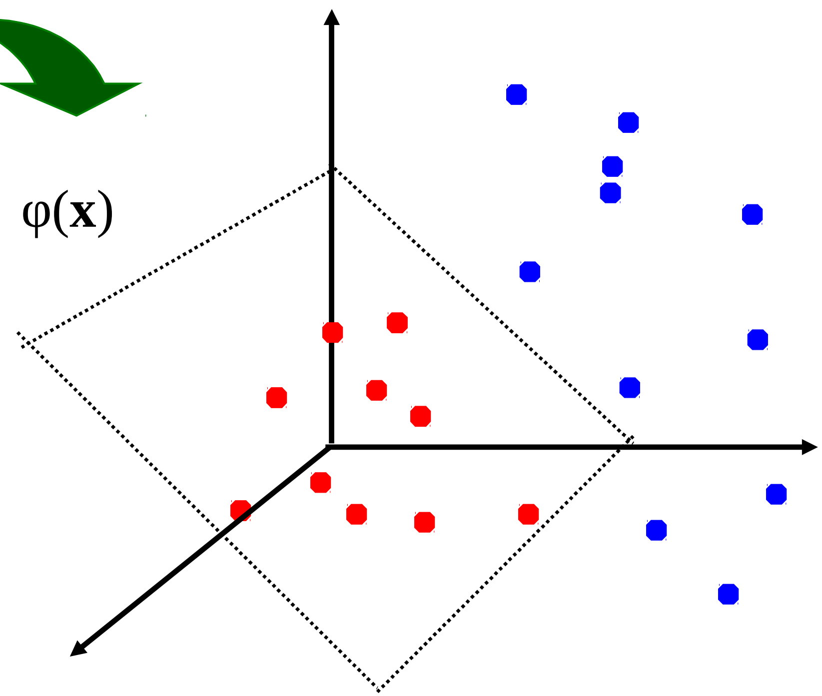
$$=(x^Ty+1)^2$$

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





Φ: $\mathbf{x} \rightarrow \varphi(\mathbf{x})$



Kernels for non-linear classification

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

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

  - 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 $(x^T y)^2=(x_1 y_1+\ldots+x_D y_D)^2$

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

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

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

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

Original features Squares Products of two distinct elements

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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, when h(d) is a bounded integer

- 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 weight vectors $\boldsymbol{w}_c = \sum_{i=1}^{n} \alpha_{ic} \phi(\boldsymbol{x}_i)$
  - Express the score functions using the kernel

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

    - Where $\boldsymbol{k}_j = \left(k(\boldsymbol{x}_j, \boldsymbol{x}_1), \ldots, k(\boldsymbol{x}_j, \boldsymbol{x}_n)\right)^T$
      $\boldsymbol{\alpha}_c = \left(\alpha_{1c}, \ldots, \alpha_{nc}\right)^T$

  - Express the L2 penalty on the weight vectors using the kernel

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

  - Where $[\boldsymbol{K}]_{ij} = k(\boldsymbol{x}_i, \boldsymbol{x}_j)$

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

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

Logistic discriminant with kernels

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

- Plug this into the objective function

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

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

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

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

- The same as the linear case, except that in the gradient the feature vector x is replaced with a column of the kernel matrix

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

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

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

Summary linear classification & kernels

- Linear classifiers learned by minimizing convex cost functions
  - Logistic discriminant: smooth, gradient-based optimization methods
  - Support vector machines: piecewise linear, 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 support vectors, may cost lots of memory in practice
  - Computing kernel between data points may be computationally expensive (at least more expensive than linear classifier)

- The "kernel trick" applies to other linear data analysis techniques
  - Principle component analysis, k-means clustering, regression, ...

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
- Much more on kernels in “Advanced Learning Models” course in MSIAM