Advanced Learning Models

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http://lear.inrialpes.fr/people/mairal/teaching/2015-2016/MSIAM/

informatics mathematics

Practical Organization

- 6 lectures of 3h each, 8h15 – 11h15, Room H204
- Homework
  - Theoretical exercises covering material from lectures 1 to 4
  - To be handed in on January 21, 2016 (lecture 5)
  - Electronic format or printed
- Practical project
  - Solve a classification/prediction task with method of choice
  - 2 page report, code, and results
  - To be handed-in after exam period, exact date to be decided
- Students receiving 3 credits for the course choose to do either only homework, or only practical project

Course content

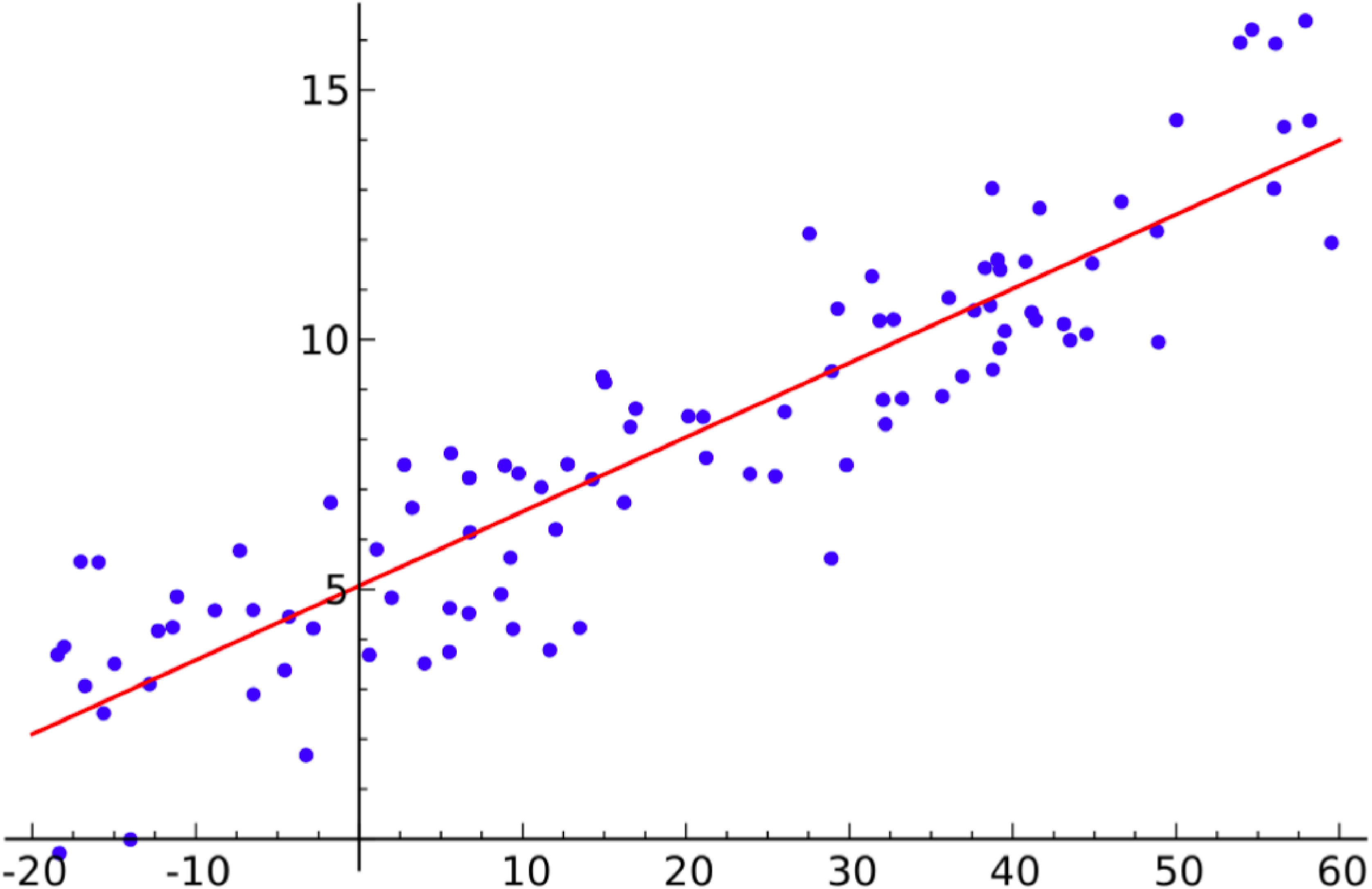
- Lecture 1
  - Introduction
  - Linear classification
  - Non-linear classification with kernels
  - Kernel-trick more generally
  - Bias-variance decomposition

- Lectures 2,3,4 (Julien Mairal)
  - Theory on kernels

- Lectures 5,6 (Jakob Verbeek)
  - Fisher kernel
  - Convolutional and recurrent neural networks

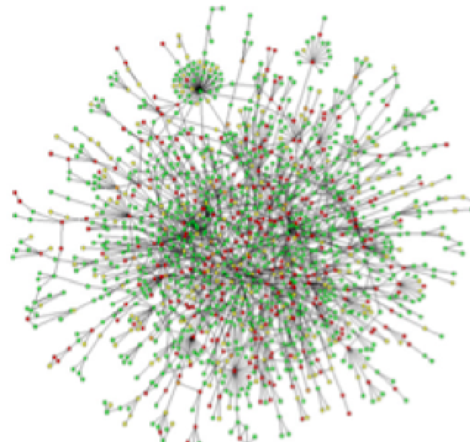
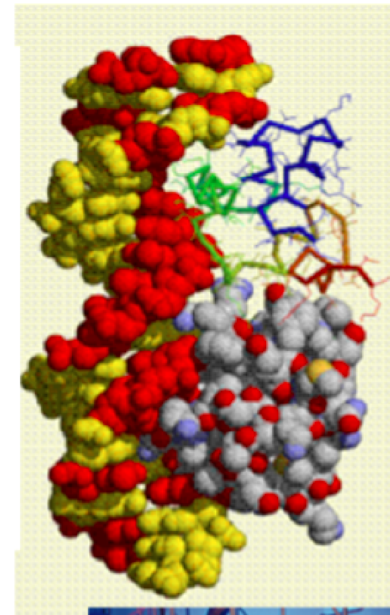
Course content

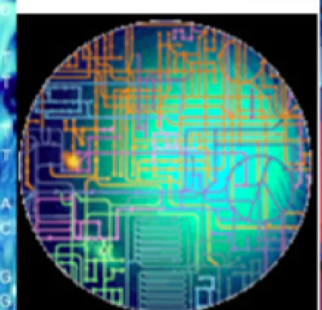
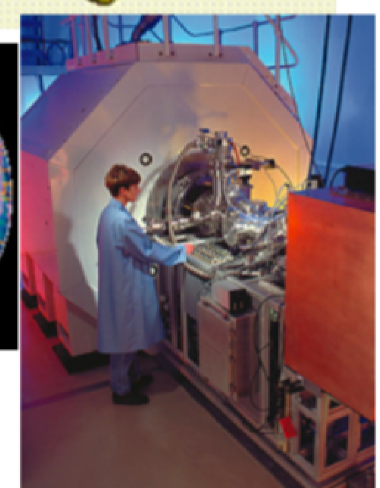
- From classic linear learning problems



Course content

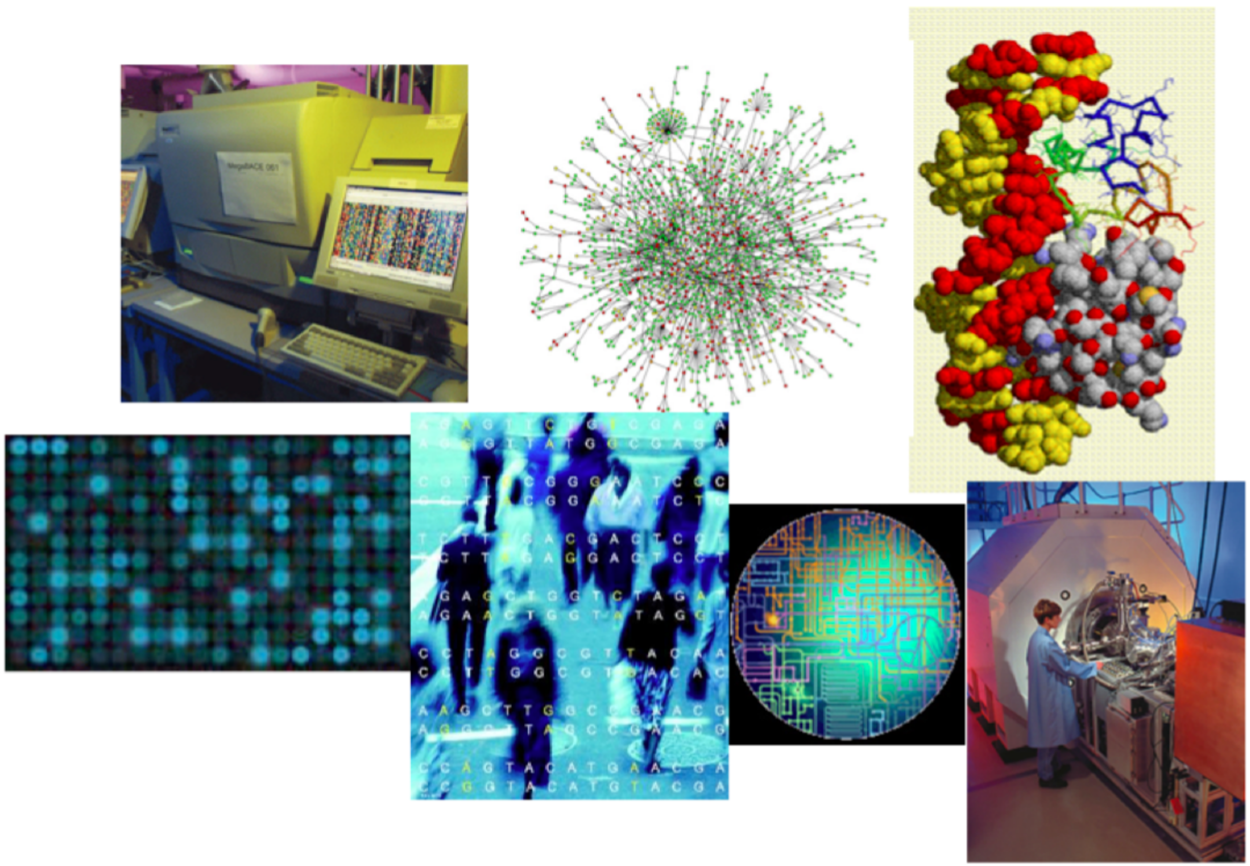
- To current practical learning problems

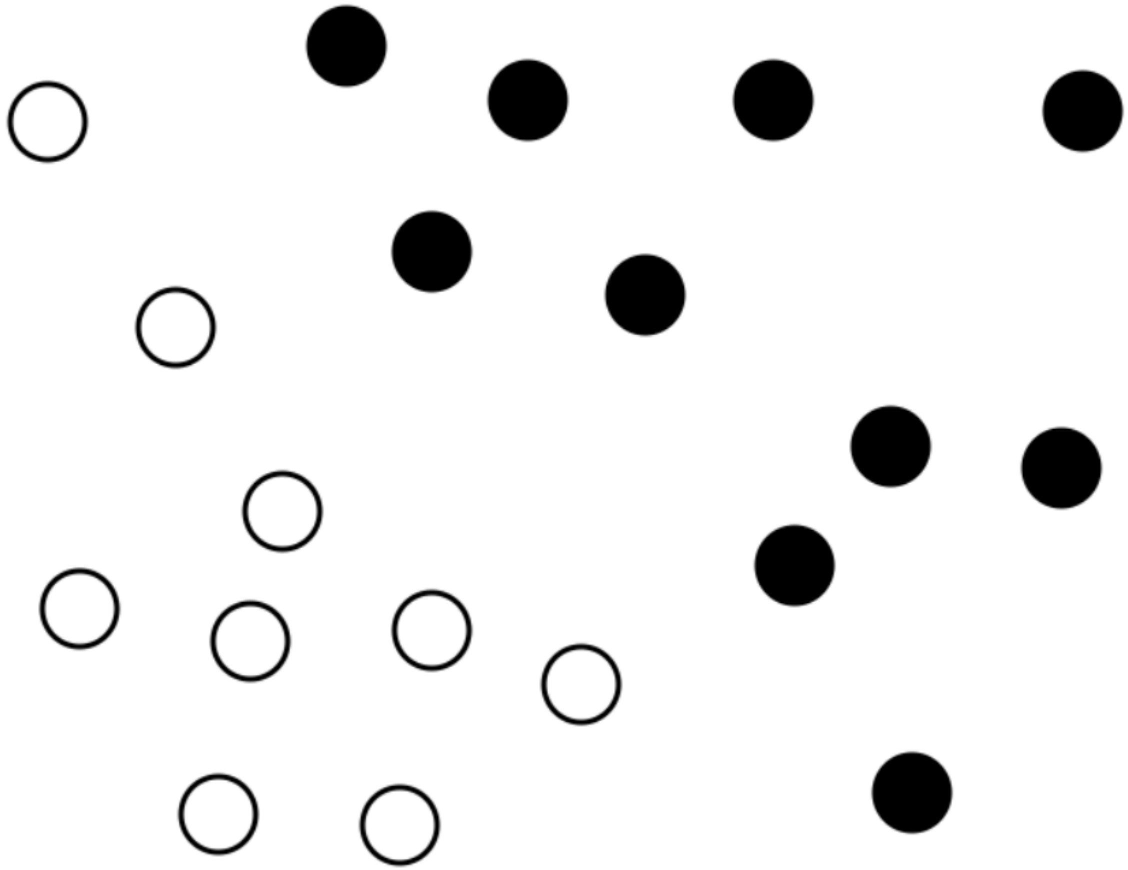
Course content

- Extend well understood linear statistical learning techniques to real-world complicated, structured and high-dimensional data (images, text, time series, graphs, distributions, permutations, …)
- Kernels: basic theory and kernel design
- Neural networks: learning convolutional and recurrent architectures



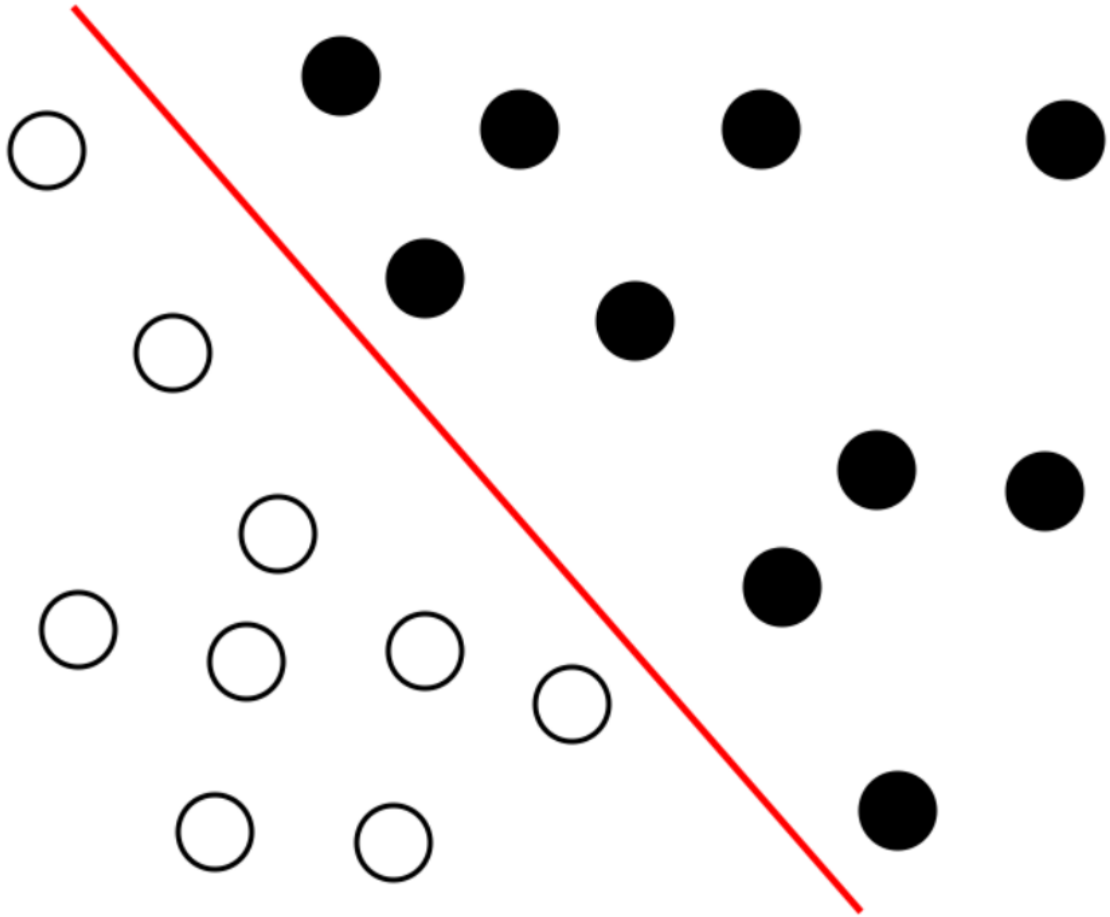
Learning predictive models from data

- Given training data labeled for two or more classes



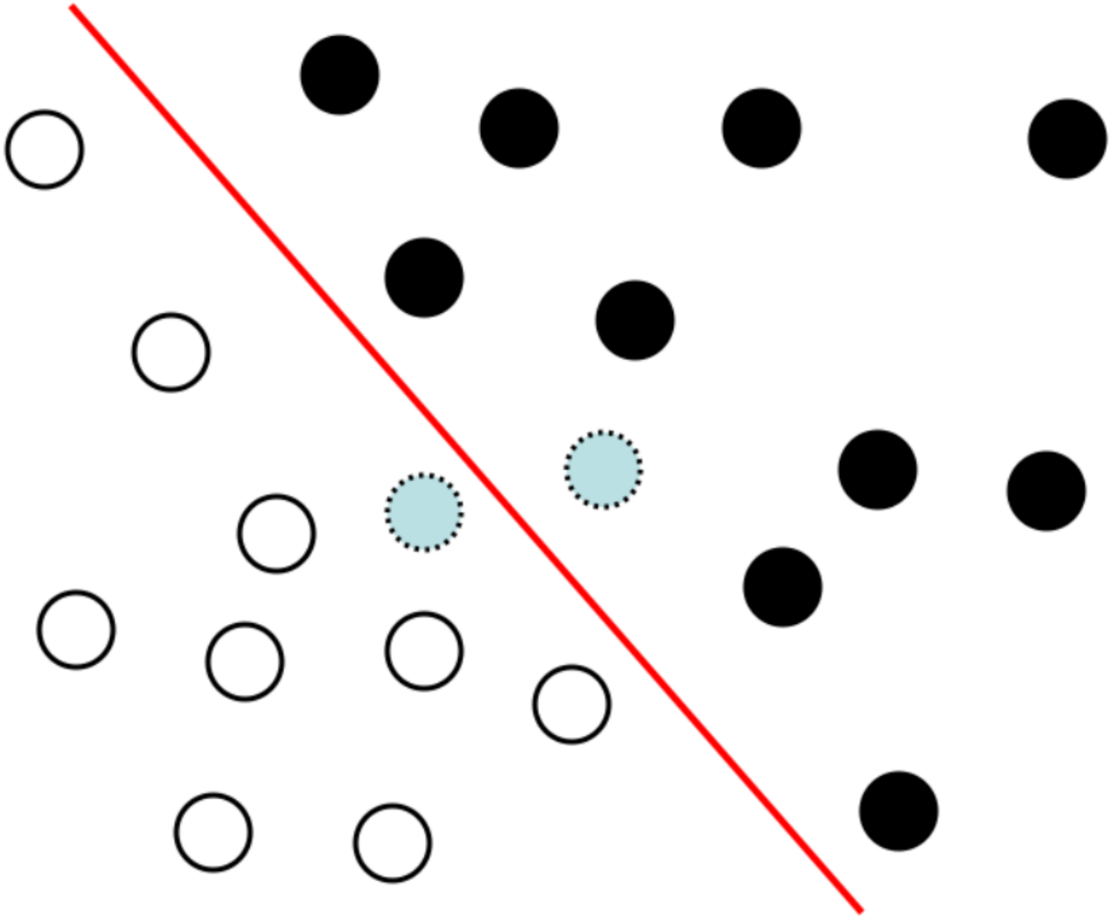
Learning predictive models from data

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



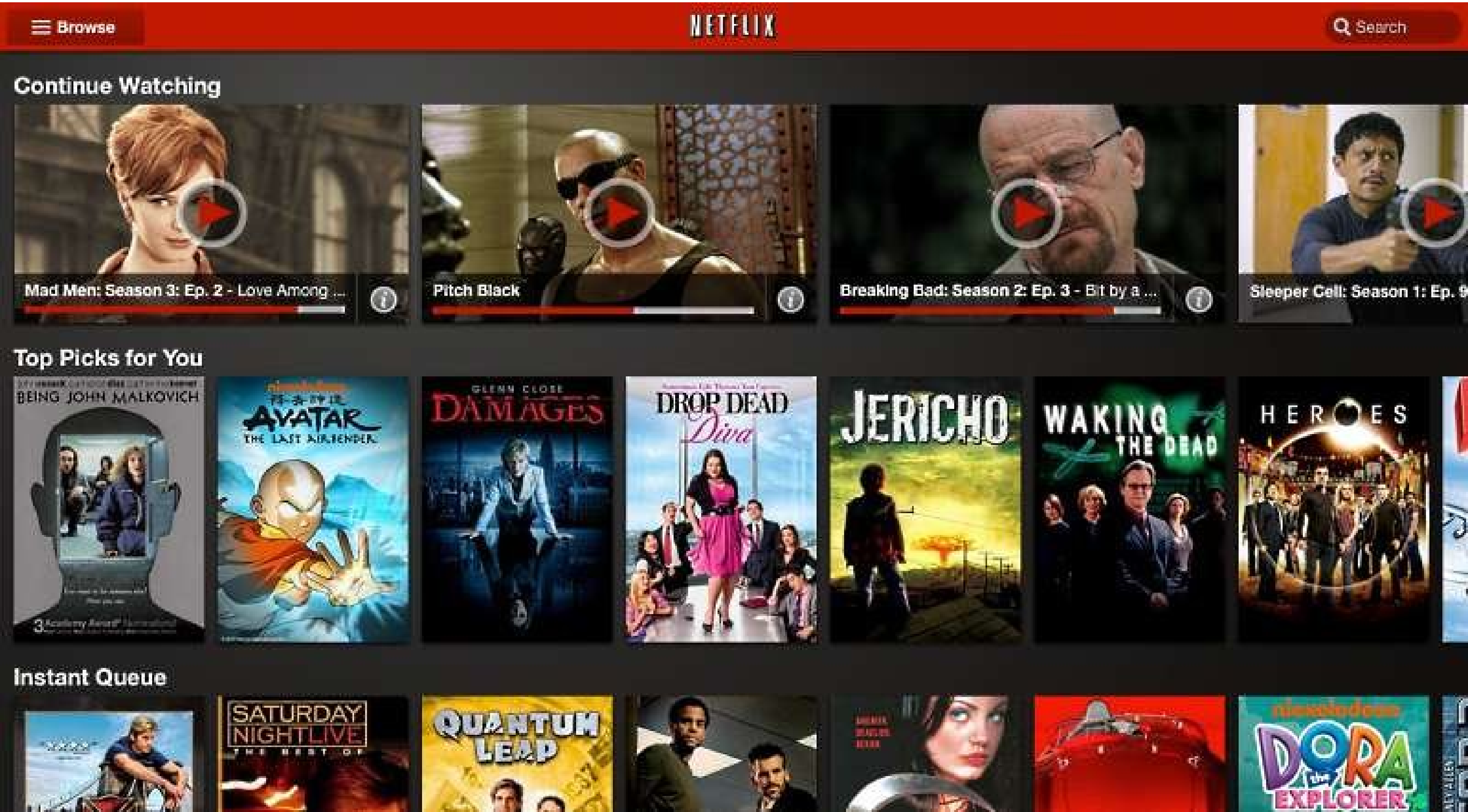
Learning predictive models from data

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



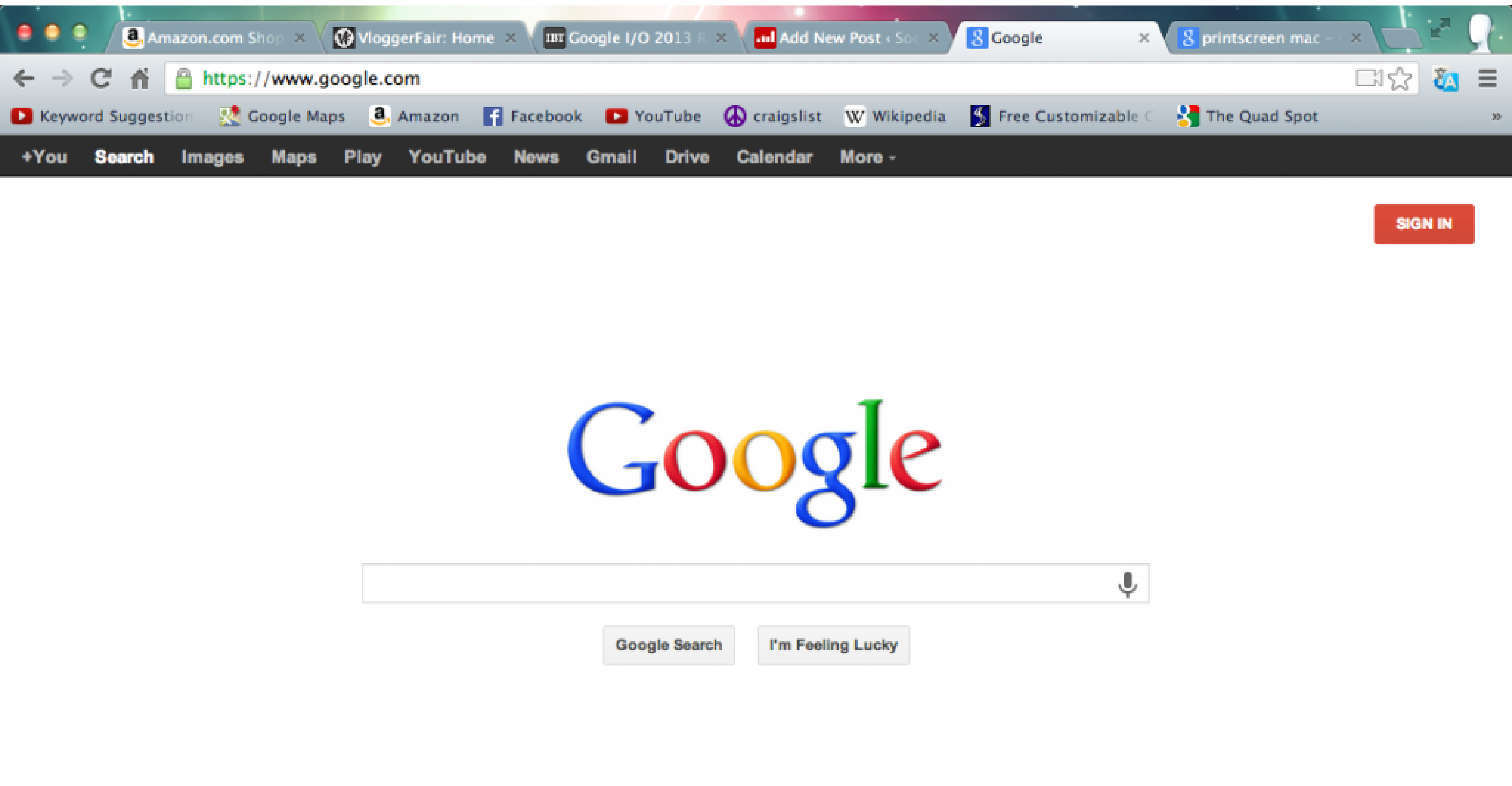
Recommender systems

- Given a dataset of users and the movies they liked
- Predict which other movies a given user would also like



Recommender systems

- Given a dataset of queries and click-through data
- Predict which are the most relevant pages for a given query

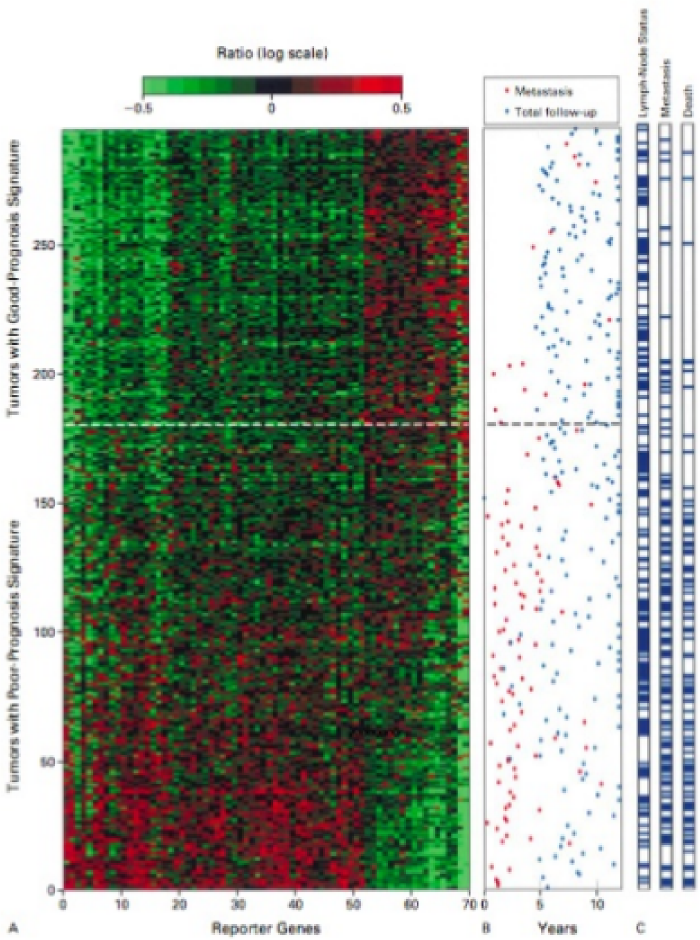


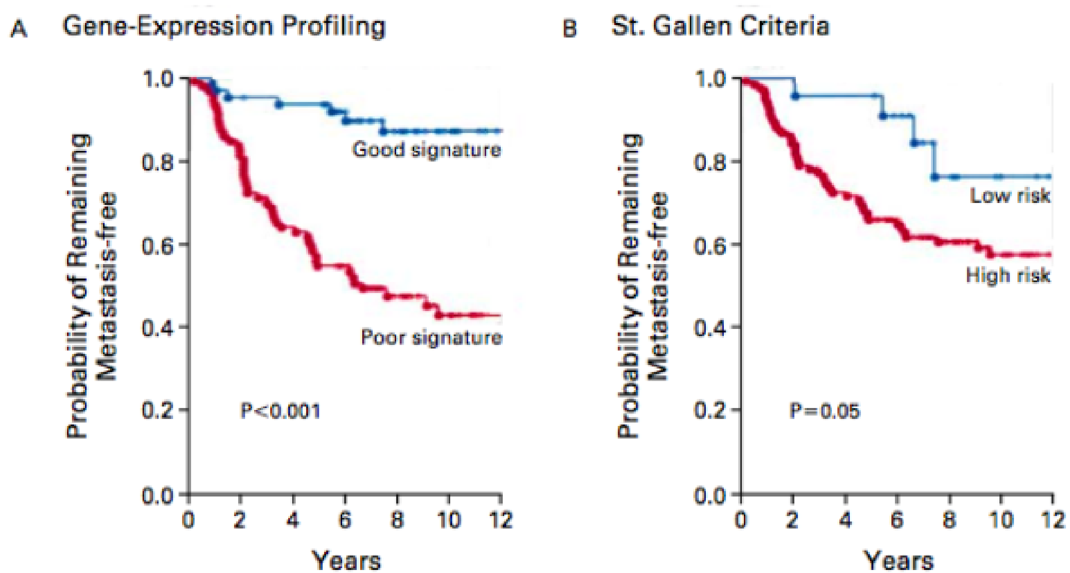
Natural Language Processing

- Given a text, predict its topic
- Given an email, predict whether it is spam
- Given a text, predict its translation in another language
- Etc.

Tumor classification for prognosis

- Given the expression of genes in a new tumor, predict the development over the next 5 years





No. at Risk

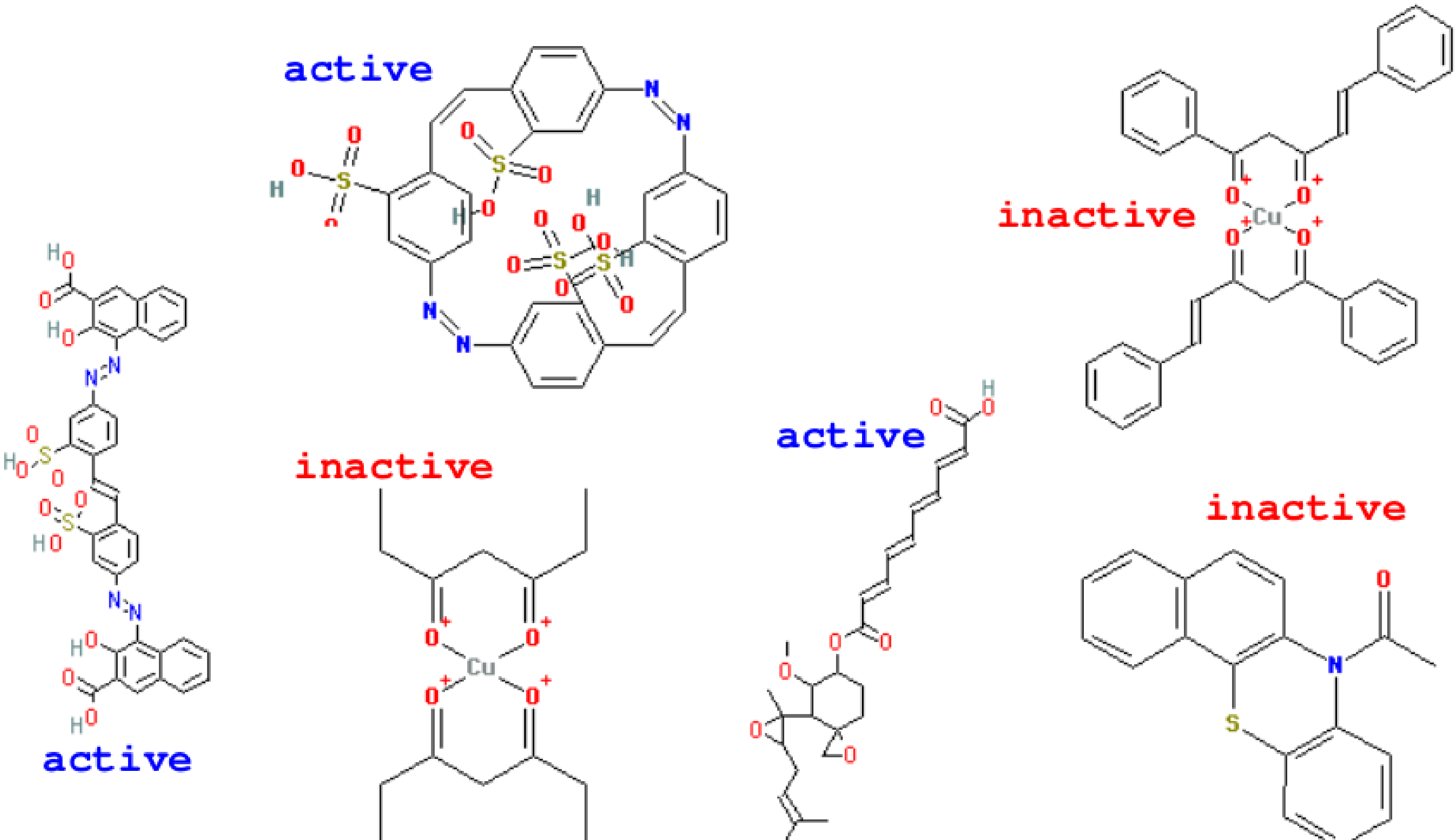
	0	2	4	6	8	10	12
Good signature	60	57	54	45	31	22	12
Poor signature	91	72	55	41	26	17	9

No. at Risk

	0	2	4	6	8	10	12
Low risk	22	22	21	17	9	5	2
High risk	129	107	88	69	48	34	19

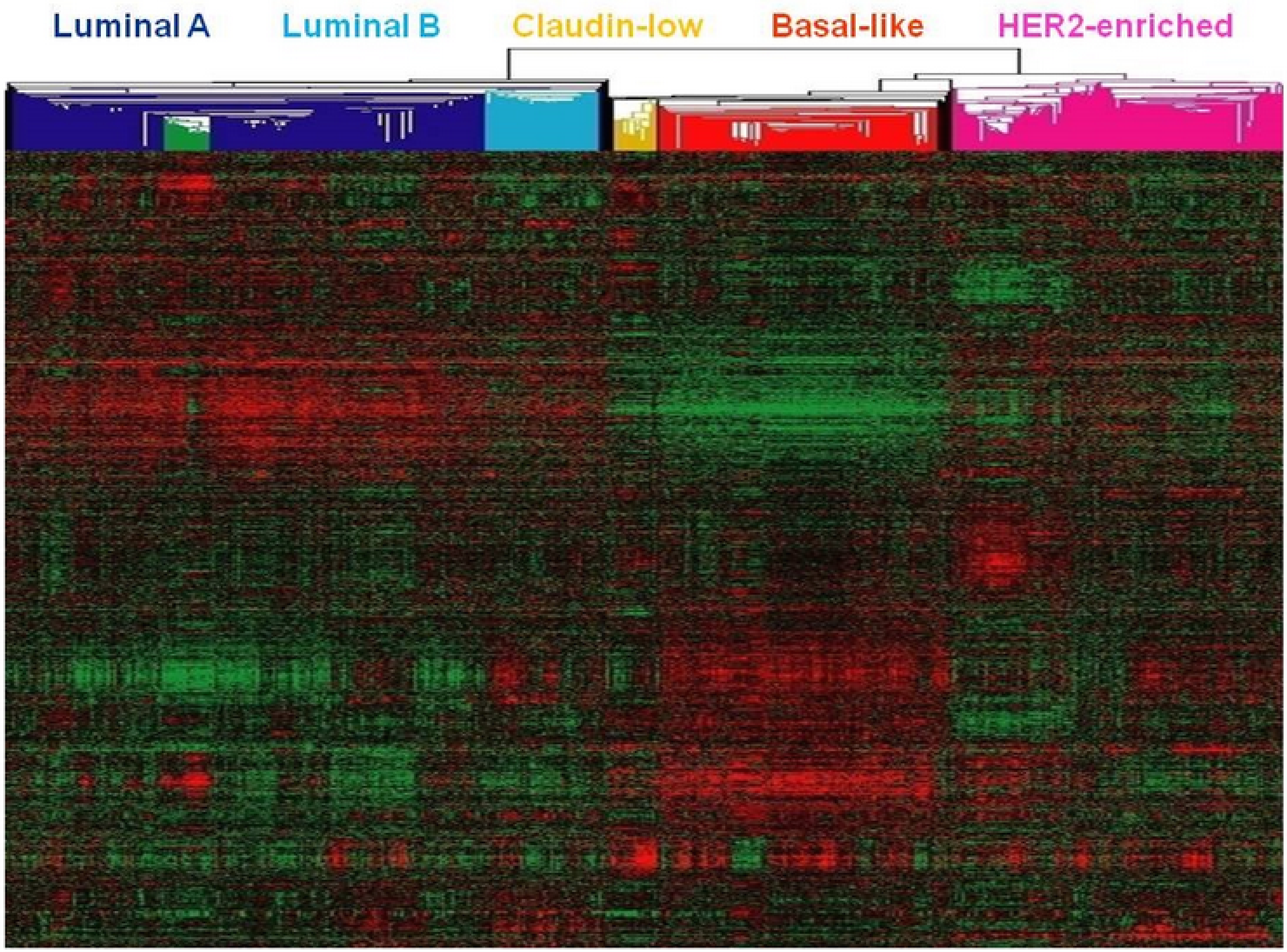
Molecule classification for drug design

- Given a candidate molecule, predict whether it is active against a certain condition



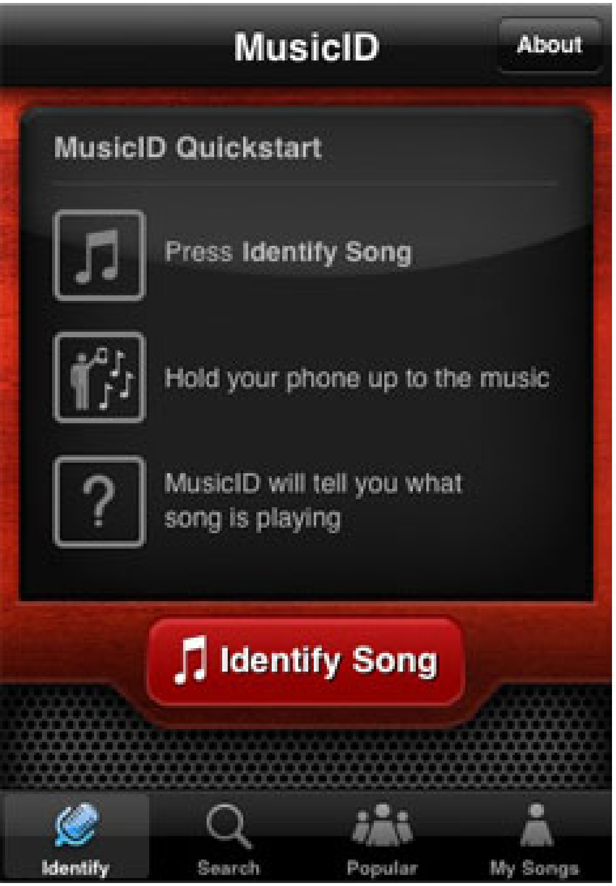
Gene expression clustering

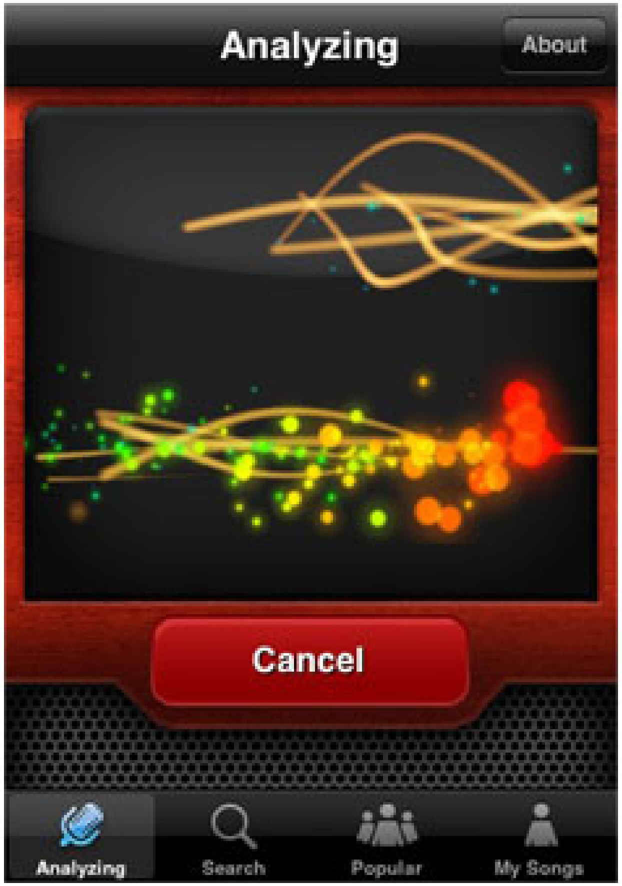
- Are there groups of breast tumors with similar gene expression profile?



Audio understaning

- Given an audio stream, predict which song is played





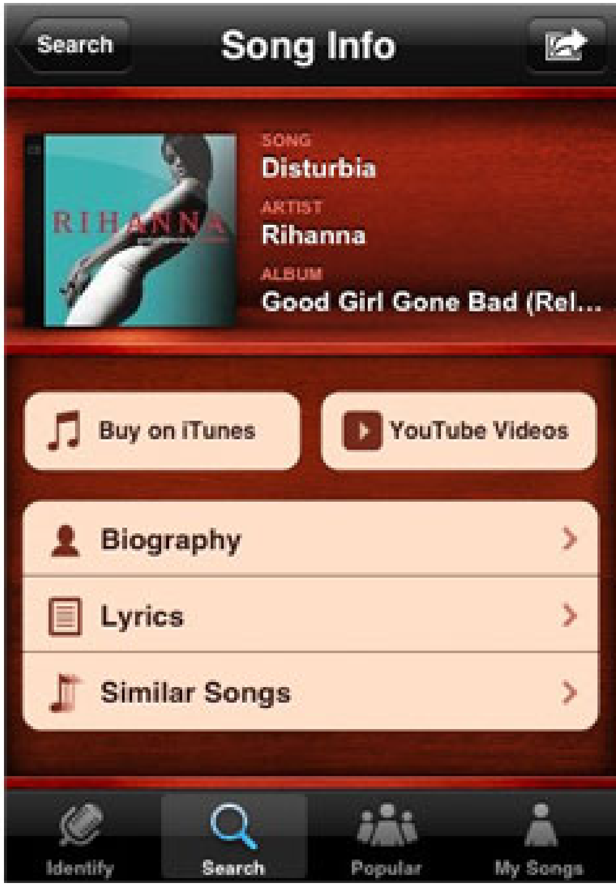


Image Inpainting

- Complete an image with missing parts
- predict each image patch, as a linear combination of dictionary elements

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Image Inpainting

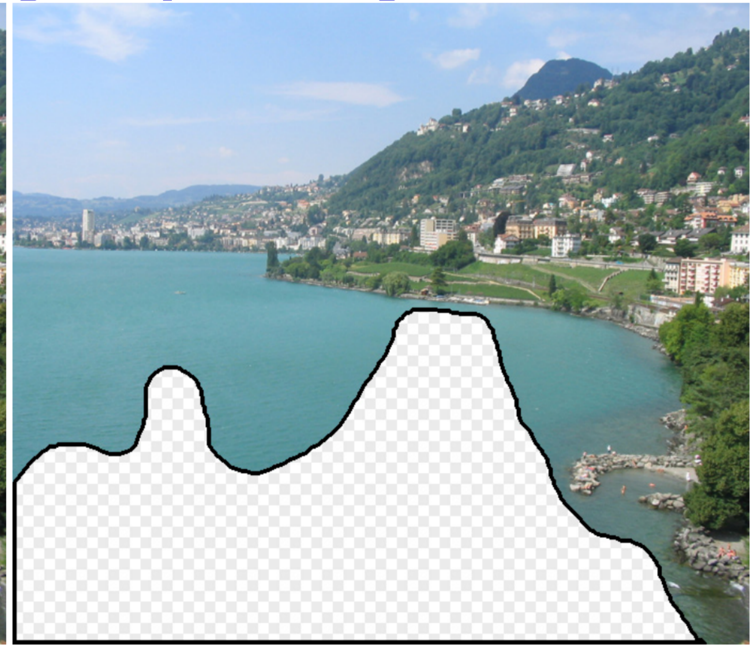
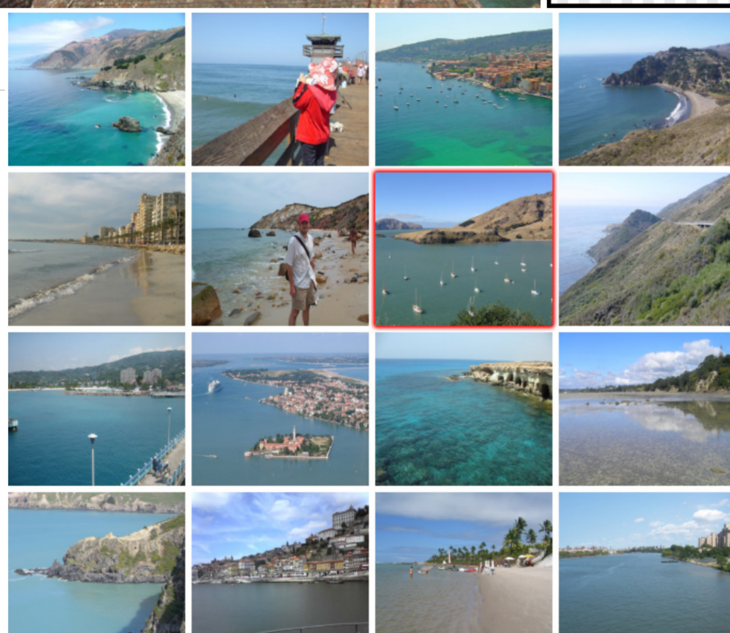





Image super resolution

- Given an image, predict a high-resolution version of it
- Predictions per-patch, ensure spatial consistency

Classification examples in category-level recognition

- Given an image, predict if labels are relevant or not
- For example: Person = yes, TV = yes, car = no, ...

Classification examples in category-level recognition

- Category localization: predict bounding box coordinates for each object

Classification examples in category-level recognition

- Semantic segmentation: classify pixels to categories (multi-class)
- Impose spatial smoothness by Markov random field models.



Video understanding

- Given a video: predict the type of event that is shown: birthday party

Video understanding

- Given a video: predict spatio-temporal location of an action, eg drinking

Image captioning

- Given an image: predict a natural language description

a brown dog is running through the grass

Advanced learning models

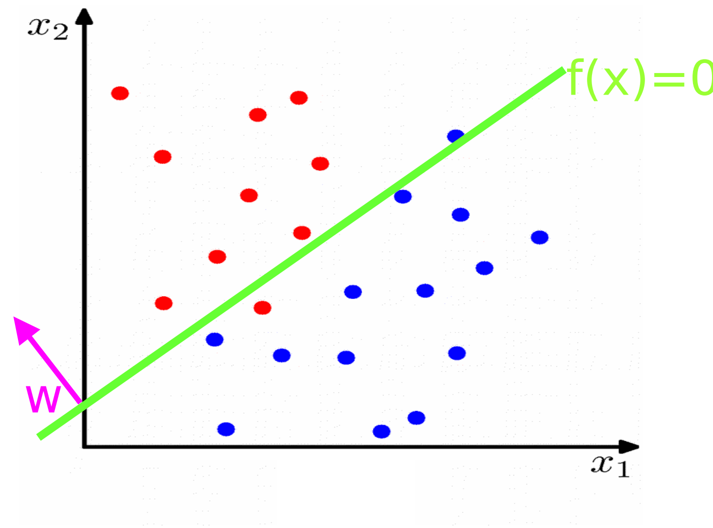
- Each of these examples involves complex objects/large numbers of features for a restricted number of samples
- Intuitively, observing all these characteristics should allow us to predict or understand complex mechanisms
- But it also means that we should use very **rich model classes** that can capture a wealth of complex dependencies
- Introduces a **risk of overfitting**: modeling co-incidental structure in the data
- However, this wealth of features can cause trouble in statistical learning
- This course
  - Modeling complex data structures with **kernels** and **neural networks**
  - **Regularization** to avoid overfitting

Course content

- Introduction
- **Linear classification**
- Non-linear classification with kernels
- Kernel-trick more generally
- Bias-variance decomposition

Binary linear classifier

- Decision function is linear in the features: $f(x) = w^T x + b$
- Classification based on the sign of f(x)



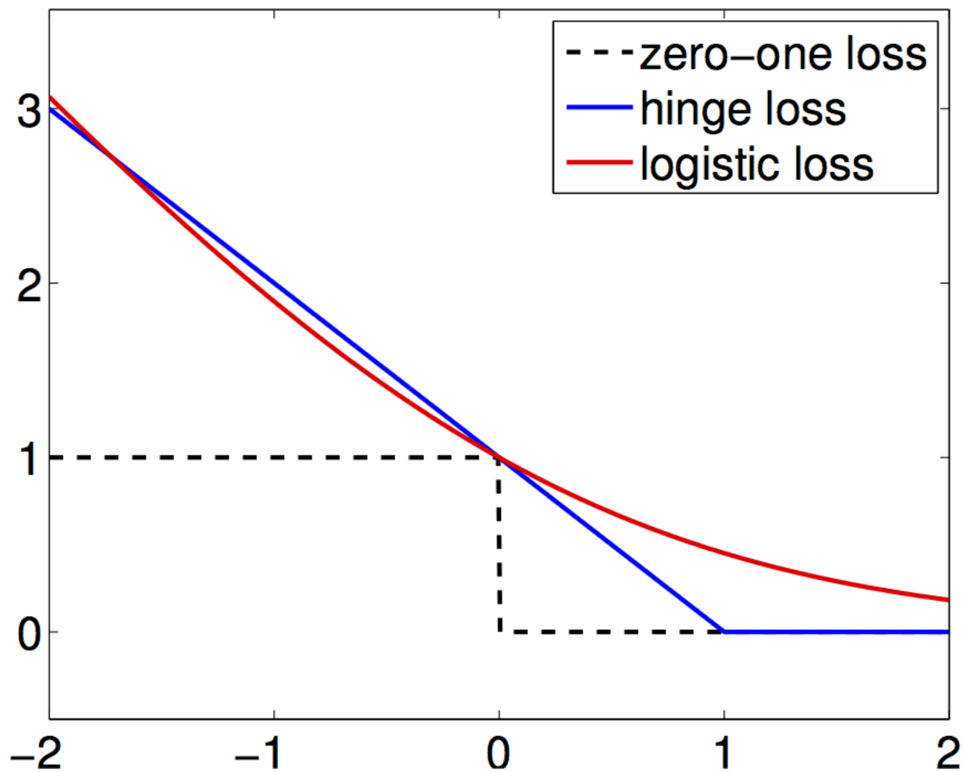
- Decision surface is (d-1) dimensional hyper-plane orthogonal to **w**
- Offset from origin is determined by *b*

- We drop offset b, absorb it in x and w
  $x \leftarrow (x^T 1)^T$
  $w \leftarrow (w^T b)^T$

- We will now consider the two most commonly used linear classifiers
  - Logistic discriminant
  - Support vector machines

Common loss functions for classification

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



Common loss functions for classification

- Assign class label using $y = sign(f(x))$
  - Zero-One loss: $L(y_i, f(x_i)) = [y_i f(x_i) \le 0]$
  - Hinge loss: $L(y_i, f(x_i)) = max(0, 1 - y_i f(x_i))$
  - Logistic loss: $L(y_i, f(x_i)) = \log_2 \left(1 + e^{-y_i f(x_i)}\right)$
- 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
- Combined with convex penalties to prevent overfitting this leads to convex objective functions, for which global optima can be found.

Logistic discriminant classifier

- Map linear score function to class probabilities with sigmoid

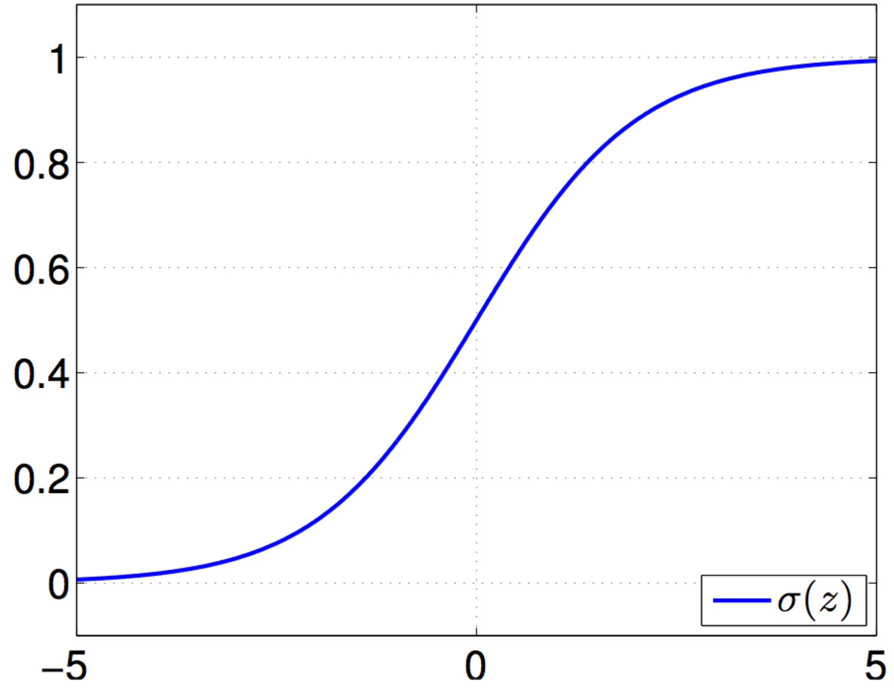
$$p(y=+1|x)=\sigma(w^T x)$$

- For binary classification problem, we have by definition

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

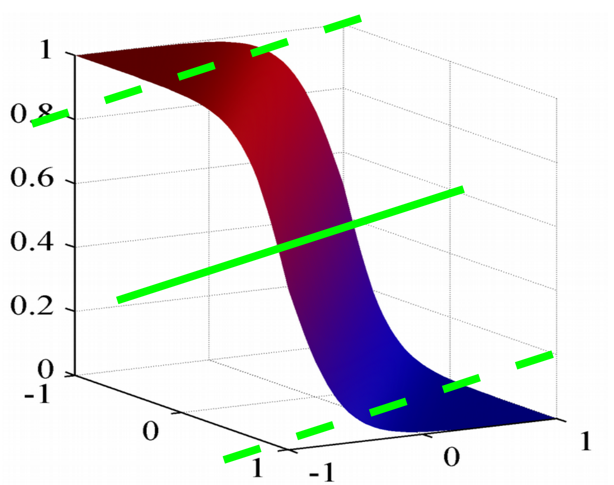
  - Exercise: show that $p(y=-1|x)=\sigma(-w^T x)$

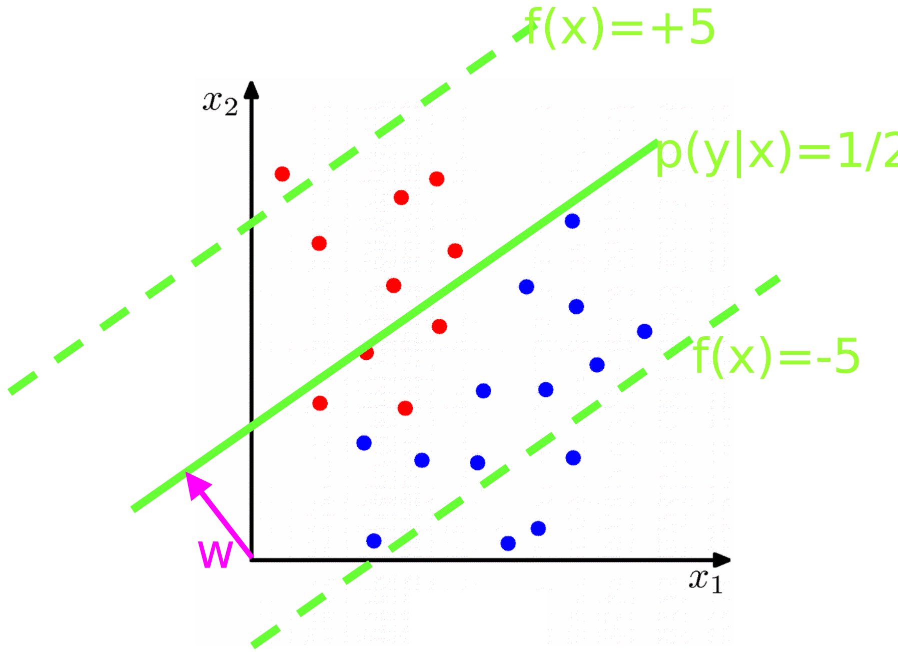
$$\sigma(z)=\frac{1}{1+\exp(-z)}$$



Logistic discriminant classifier

- Map linear score function to class probabilities with sigmoid.
- The class boundary at f(x)=0, or equivalently p(y|x)=1/2.
- Soft transition between class assignment along decision boundary.





Logistic discriminant classifier

- Probability of class *y* given by sigmoid of score function times label

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

- Log-likelihood of correct classification of i.i.d. data in training set

$$\log \prod_{i=1}^{n} p(y_i|x_i) = \sum_{i=1}^{n} \log p(y_i|x_i)$$

$$= \sum_{i=1}^{n} \log \sigma(y_i w^T x_i)$$

$$= -\sum_{i=1}^{n} \log\left(1 + \exp(-y_i w^T x_i)\right)$$

$$= -\sum_{i=1}^{n} L_{\text{logistic}}(y_i, w^T x_i)$$

- We have obtained the logistic loss as negative log-likelihood

Logistic discriminant estimation

- Estimate classifier from data by minimizing, e.g. L2, penalized loss:
  - Penalty reduces risk of overfitting

$$min_w \sum_{i=1}^{n} L(y_i, w^T x_i) + \lambda \frac{1}{2} w^T w$$

$$= min_w \sum_{i=1}^{n} \log\left(1 + \exp(-y_i w^T x_i)\right) + \lambda \frac{1}{2} w^T w$$

- Exercise 1: derive the gradient of the loss

$$\frac{\partial L(y_i, w^T x_i)}{\partial w} = -y_i \left(1 - p(y_i | x_i)\right) x_i$$

- Exercise 2: Show that this is a convex optimization problem

Logistic discriminant estimation

- Estimate classifier from data by minimizing, e.g. L2, penalized loss:

$$min_w \sum_{i=1}^{n} L\left(y_i, w^T x_i\right) + \lambda \frac{1}{2} w^T w$$

$$= min_w \sum_{i=1}^{n} \log\left(1 + \exp\left(-y_i w^T x_i\right)\right) + \lambda \frac{1}{2} w^T w$$

- Exercise: Show that this is a convex optimization problem
  - Calculate gradient of loss w.r.t. w

$$\frac{\partial L\left(y, w^T x\right)}{\partial w} = -yx \frac{1}{1+\exp\left(y w^T x\right)}$$

  - Calculate Hessian of Loss w.r.t. w

$$H(L) = yx \left(\frac{1}{1+\exp\left(y w^T x\right)}\right)^2 \exp\left(y w^T x\right) y x^T$$

$$= \sigma\left(y w^T x\right) \sigma\left(-y w^T x\right) x x^T$$

Logistic discriminant estimation

- Consider arbitrary w with non-zero norm

$$w^T H(L) w = w^T \left(\sigma(yw^T x)\sigma(-yw^T x) xx^T \right) w$$

$$= \sigma(yw^T x)\sigma(-yw^T x)(w^T x)^2 \geq 0$$

- Hessian is semi-positive definite, thus L is convex in w.
- Squared L2 norm also convex in w.

Logistic discriminant estimation

- Solve objective function using first or second order methods

$$min_w \sum_{i=1}^{n} \log\left(1+\exp\left(-y_{iw}^{T} x_i\right)\right)+\lambda \frac{1}{2} w^T w$$

  - E.g. using gradient descent, conjugate gradient descent,...
  - Stochastic gradient descent for large-scale problems

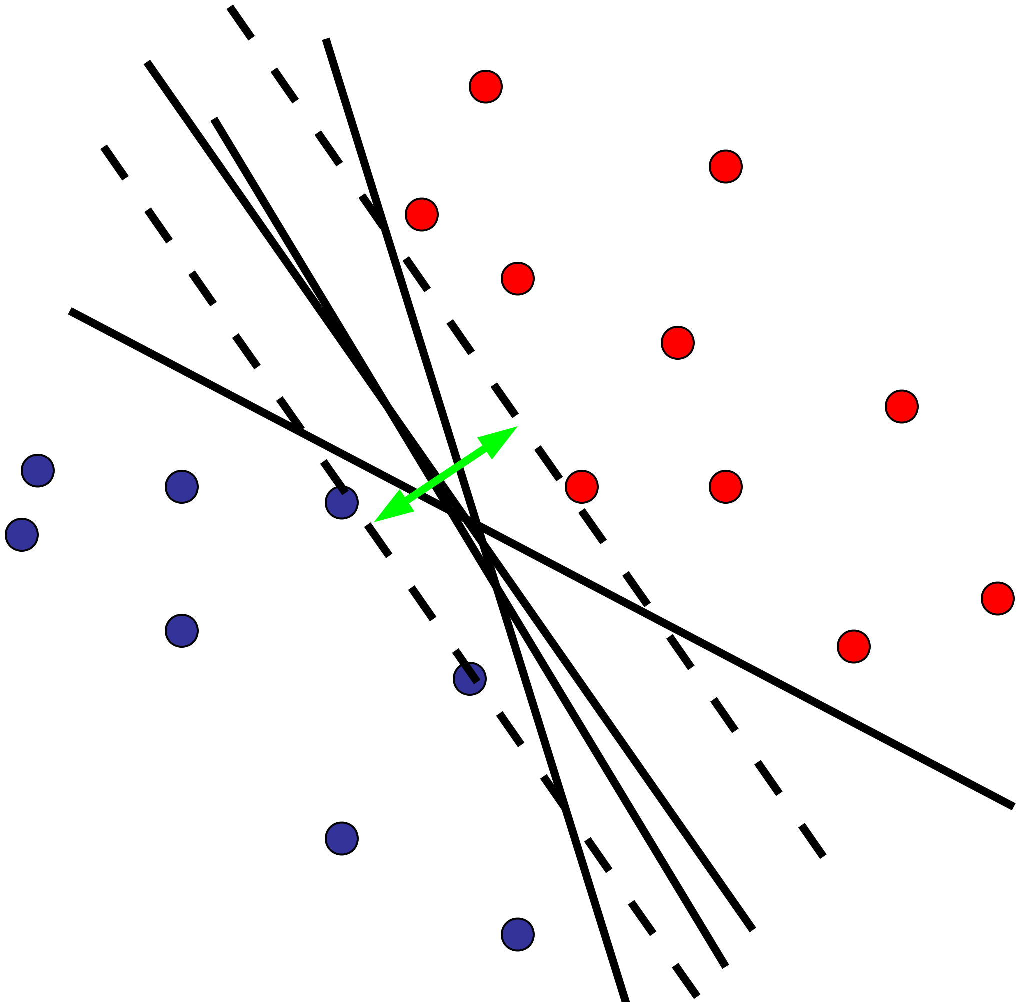
- Recall the gradient $$\frac{\partial L(y_i, w^T x_i)}{\partial w} = -y_i(1-p(y_i|x_i))x_i$$

- Consider gradient descent, starting from w=0
  - Each step we add to w a linear combination of the data points
  - Magnitude of weight given by probability of misclassification
  - Sign of weight given by the label

- The optimal w is a linear combination of the data samples
  - L2 regularization term does not change this property

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

- Without loss of generality, define function value at margin as +/- 1
- Now constrain w to that all points fall on correct side of the margin:

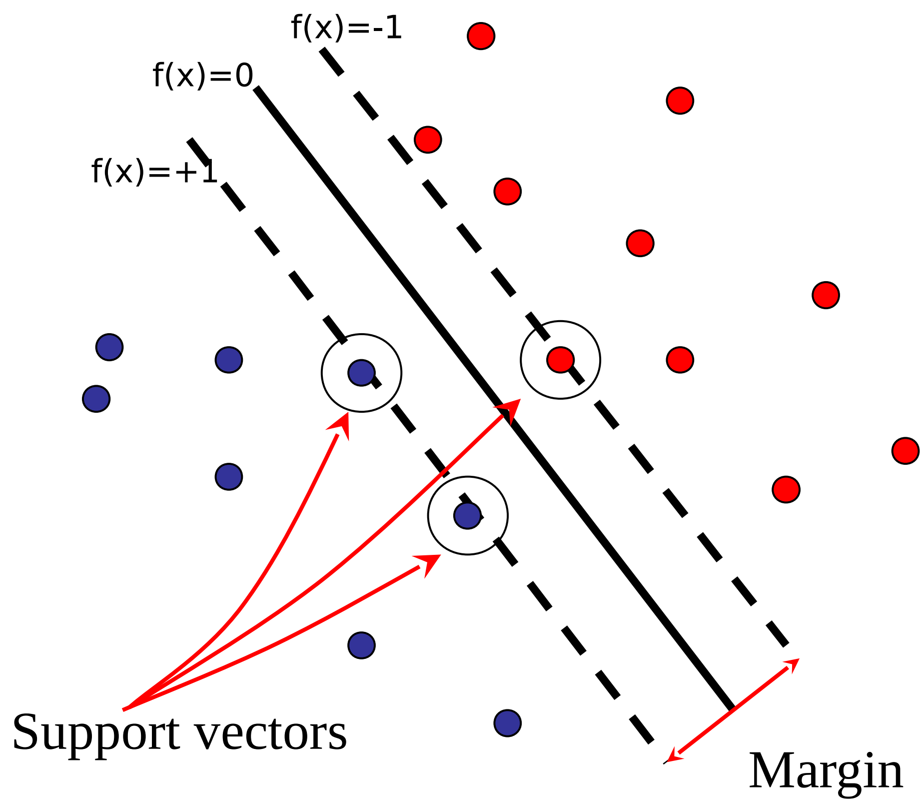
$$y_i\left(w^T x_i + b\right) \geq 1$$

- 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.



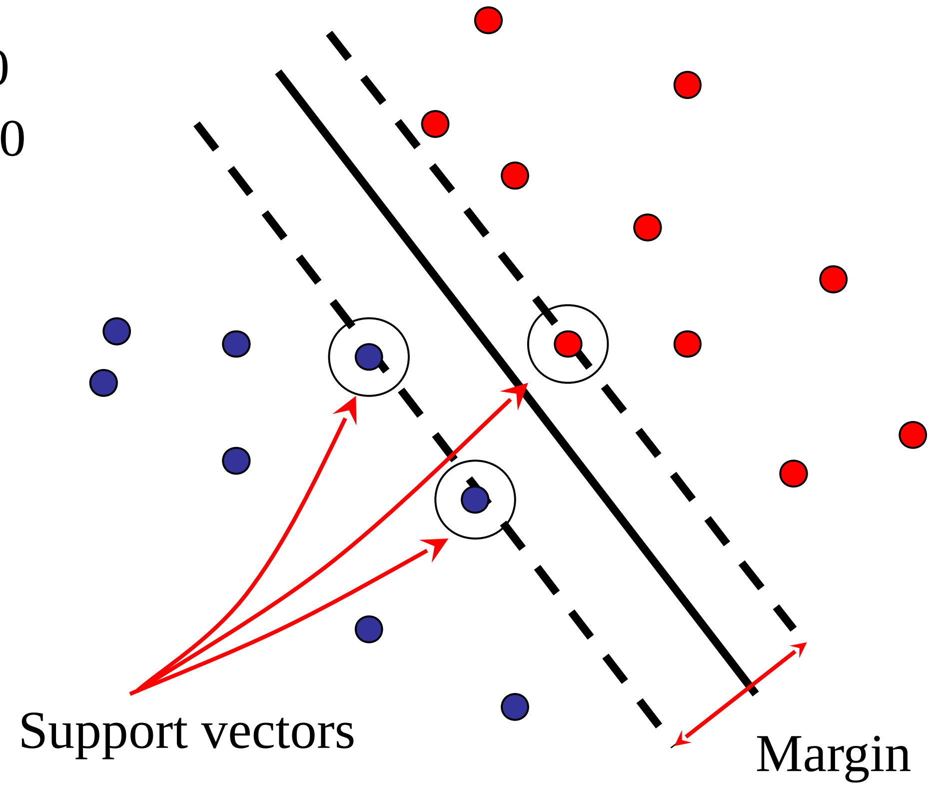
Support vector machines

- 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

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

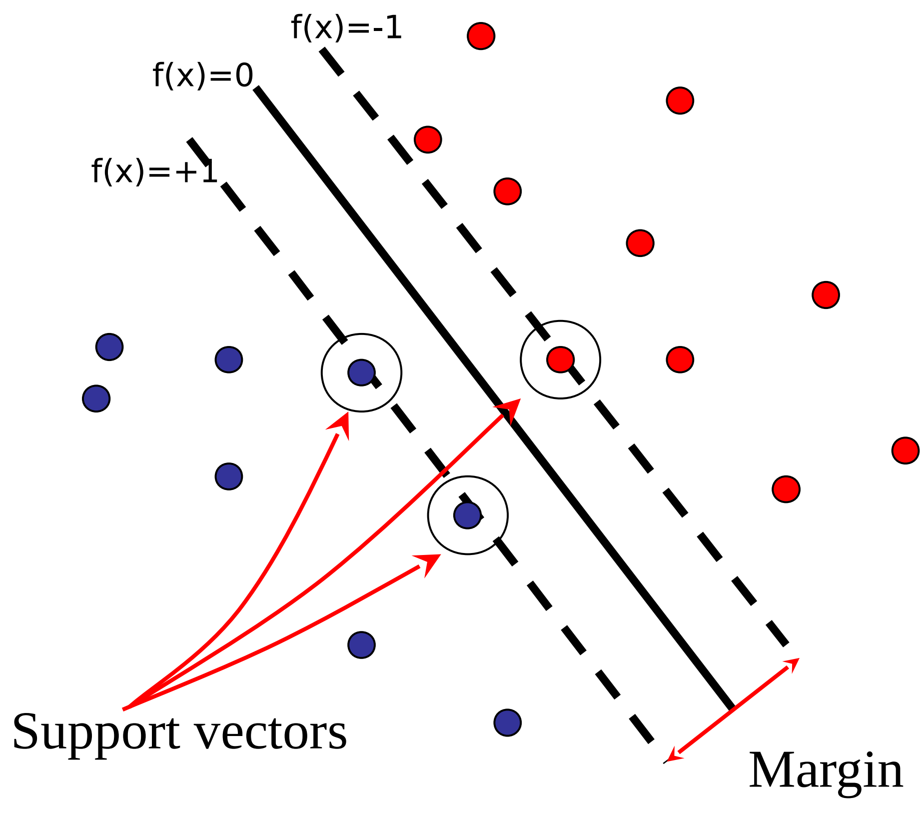


Support vector machines

- 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

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

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

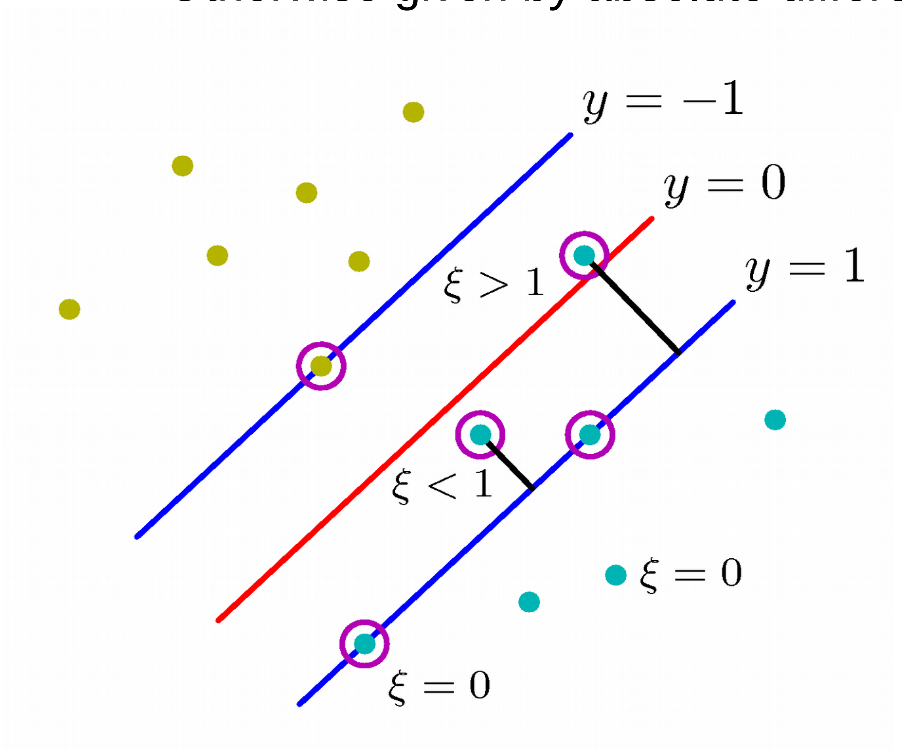


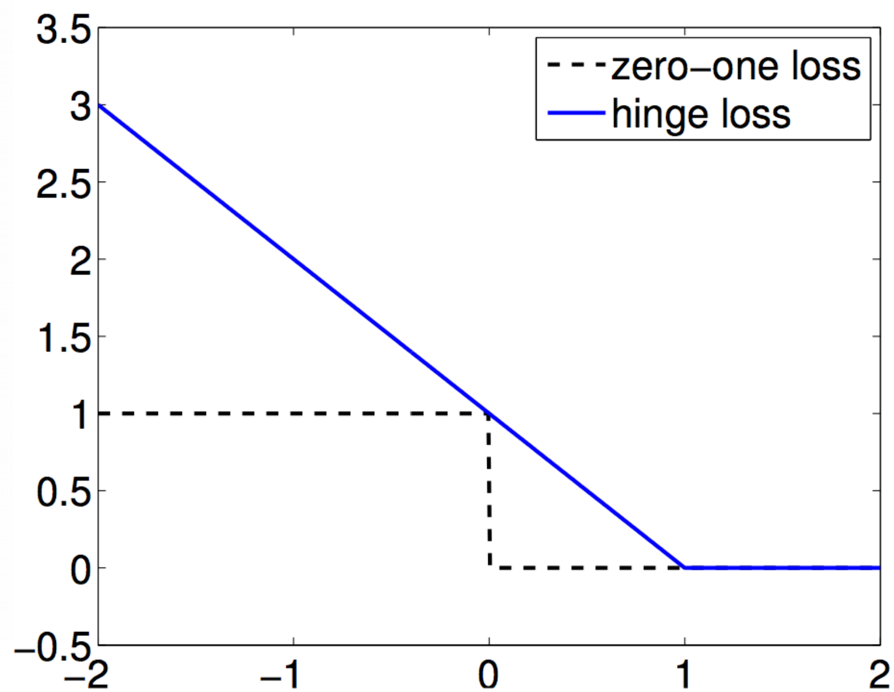
Support vector machines: inseperable classes

- 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**.

- Can again be transformed to 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

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

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

Support vector machines: solution

- Minimize penalized loss function

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

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

- Solution for w will be a linear combination of the input data
  - Split w into a part inside and outside the span of the data

$$w = w_p + w_o \qquad \forall_i : w_o^T x_i = 0 \qquad w_p = \sum_i \alpha_i x_i$$

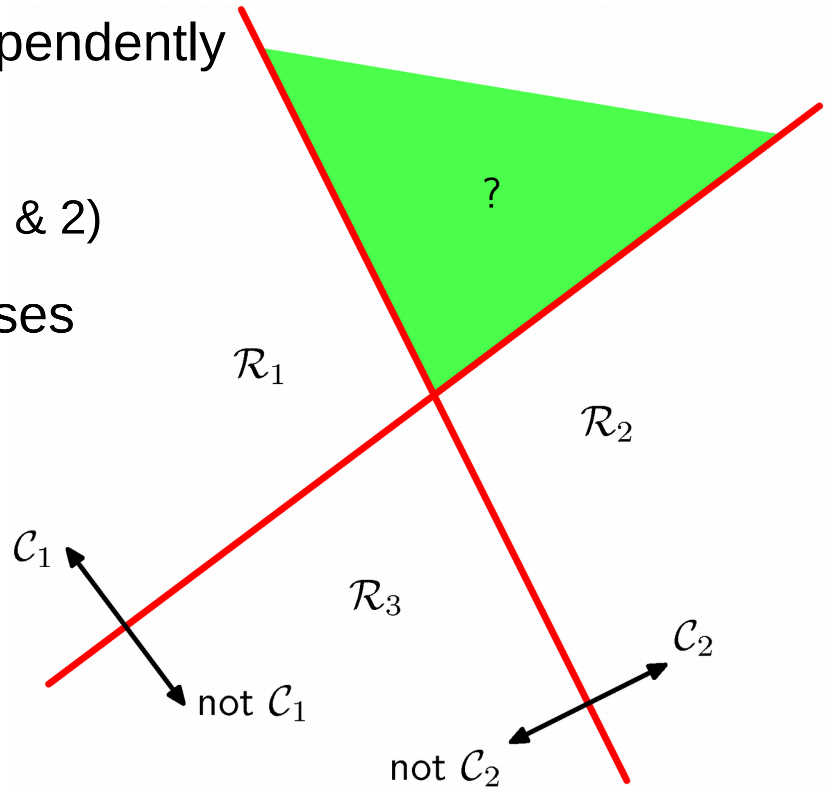
  - Only norm of w depends on part of w outside the data span
  - Note that

$$w^T w = w_p^T w_p + w_o^T w_o \geq w_p^T w_p$$

  - Therefore optimal w is a linear combination of the data
- This is a special case of the more general “representer theorem”

Dealing with more than two classes

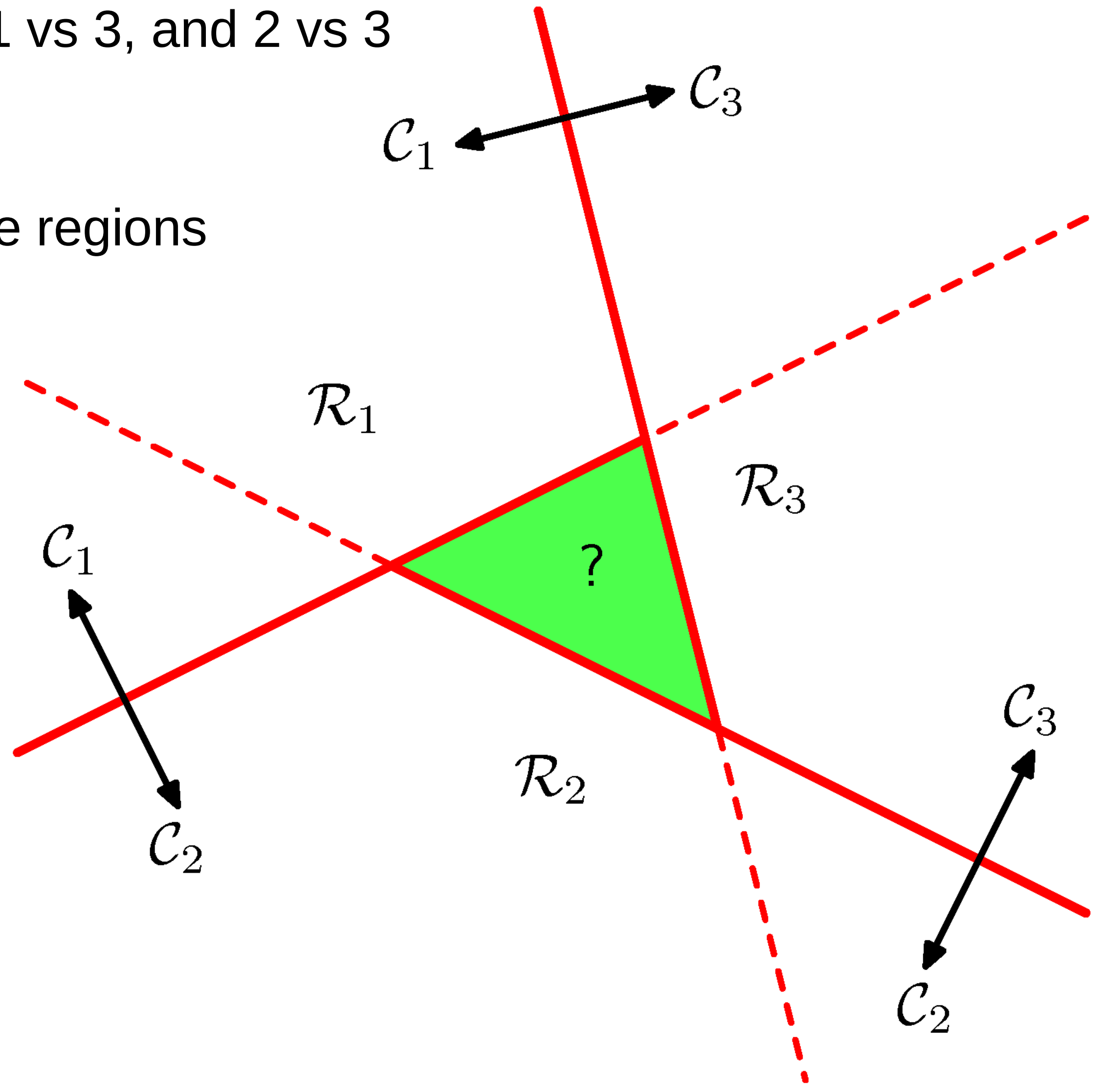
- So far, we have only considered the, useful, case for two classes
  - E.g., is this email spam or not ?
- Many practical problems have more classes
  - E.g., which fruit is placed on the supermarket weight scale: apple, orange, or banana ?
- First idea: construction from multiple binary classifiers
  - Learn binary “base” classifiers independently
- One vs rest approach:
  - Train: 1 vs (2 & 3), 2 vs (1 & 3), 3 vs (1 & 2)
- Issue: regions claimed by several classes



Dealing with more than two classes

- One vs one approach:
  - Train: 1 vs 2, and 1 vs 3, and 2 vs 3

- Issue: conflicts in some regions



Dealing with more than two classes

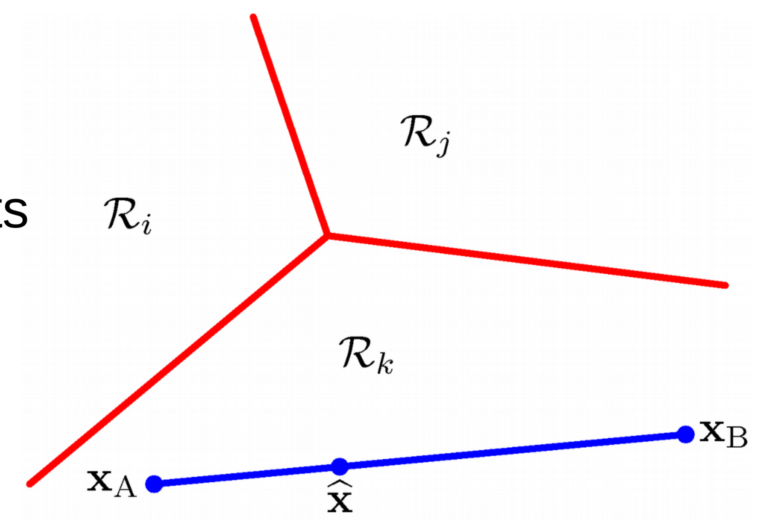
- Instead: define a separate linear score function for each class

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

- 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 are assigned to a class, then all points on connecting line are also assigned to that class.

Multi-class logistic discriminant classifier

- Map score functions to class probabilities with "soft-max"

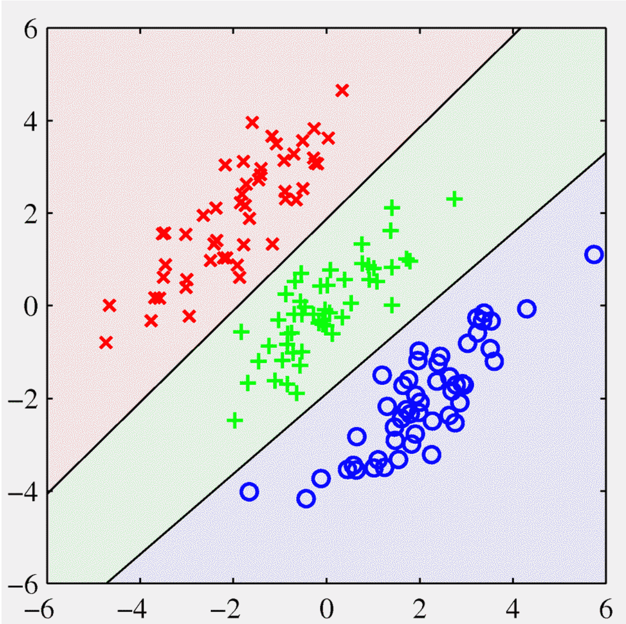
$$f_k(x) = w_k^T x \qquad\qquad p(y=c|x) = \frac{\exp(f_c(x))}{\sum_{k=1}^{K} \exp(f_k(x))}$$

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

- Relative probability of classes changes 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, they are equally likely on a hyperplane in the feature space



Multi-class logistic discriminant: estimation

- Consider the likelihood of correct classification of i.i.d. data in training set

$$\log \prod_{i=1}^{n} p(y_i|x_i) = \sum_{i=1}^{n} \log p(y_i|x_i)$$
$$= \sum_{i=1}^{n} \left(f_{y_i}(x_i) - \log \sum_{k=1}^{K} \exp(f_k(x_i)) \right)$$

- As before, we define loss function as negative log-likelihood

$$L(y, \{f_k(x)\}) = -f_y(x) + \log \sum_{k=1}^{K} \exp(f_k(x))$$

- Estimate model by means of penalized empirical risk

$$min_w \sum_{i=1}^{n} L(y_i, \{f_k(x_i)\}) + \lambda \frac{1}{2} \sum_{k=1}^{K} w_k^T w_k$$

Multi-class logistic discriminant: estimation

- Derivative of loss function has an intuitive interpretation
  - Focus on points with poor classification, w is linear combination of x's

$$L = \sum_{i=1}^{n} L\left(y_i, \{f_k(x_i)\}\right)$$

$$\frac{\partial L}{\partial w_k} = \sum_{i=1}^{n} \left([y_i = k] - p(y_i = k | x_i) \right) x_i$$

- Gradient is zero when $\sum_{i=1}^{n} [y_i = k] x_i = \sum_{i=1}^{n} p(y_i = k | x_i) x_i$
  - If x also contains the constant 1 as last element then empirical count of each class matches expected count.

$$\sum_{i=1}^{n} [y_i = k] = \sum_{i=1}^{n} p(y_i = k | x_i)$$

  - Therefore, for each class 1st order moment matches for empirical distribution and the model's class conditional distribution.

$$\frac{\sum_{i=1}^{n} [y_i = k] x_i}{\sum_{i=1}^{n} [y_i = k]} = \frac{\sum_{i=1}^{n} p(y_i = k | x_i) x_i}{\sum_{i=1}^{n} p(y_i = k | x_i)}$$

Summary of linear classifiers

- Two most widely used binary linear classifiers:
  - Logistic discriminant, also considered the extension to >2 classes.
  - Support vector machines, similar multi-class extensions exist.

- Both minimize convex upper bounds on the 0/1 loss
- In both cases the optimal weight vector w is a linear combination of the data points

$$w = \sum_{i=1}^{n} \alpha_i x_i$$

- Therefore, **we only need the inner-products between data points to use linear classifiers**. This also holds for the optimization of w.

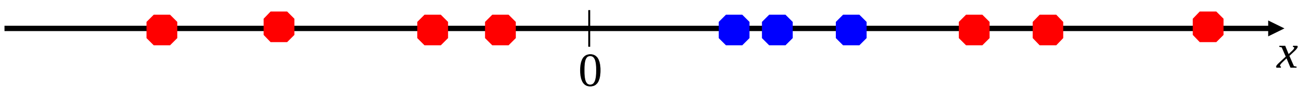
$$f(x) = w^T x + b$$
$$= \sum_{i=1}^{n} \alpha_i \left(x_i^T x \right) + b$$

Course content

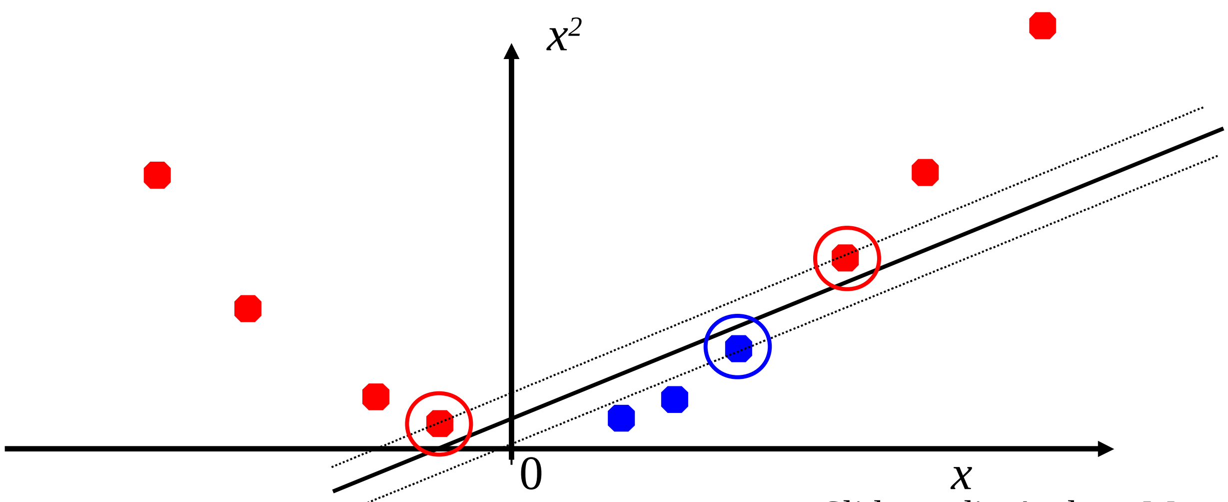
- Introduction
- Linear classification
- **Non-linear classification with kernels**
- Kernel-trick more generally
- Bias-variance decomposition

Nonlinear Classification

- So far we just considered linear classifiers.
- Obviously limits the problems that can be addressed.
- What to do it the data is not linearly separable?



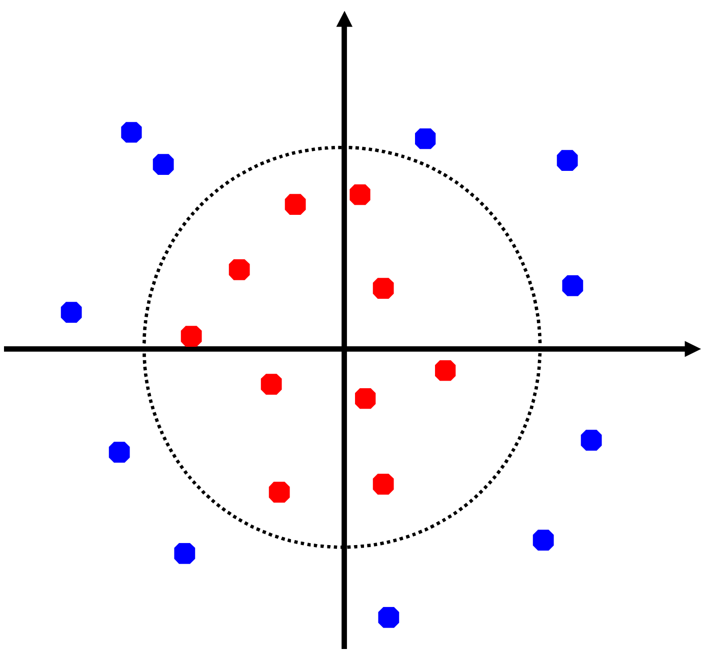
- Similar to what we considered last week for regression with higher-order polynomials, we can do linear classification on non-linear features. For example augment map the data to R^2 by adding x^2.



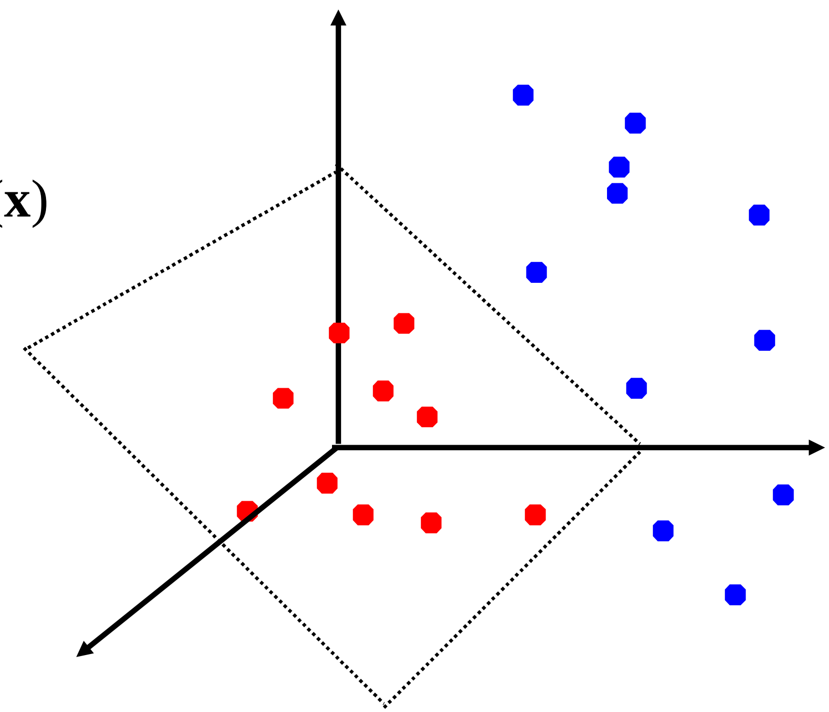
Slide credit: Andrew Moore

Non-linear feature mappings for classification

- Map the original input space to some higher-dimensional feature space where the training set is separable
- Data occupies a (non-linear) subspace of dimension equal to the original space.
- Which features could separate this 2dimensional data linearly ?



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



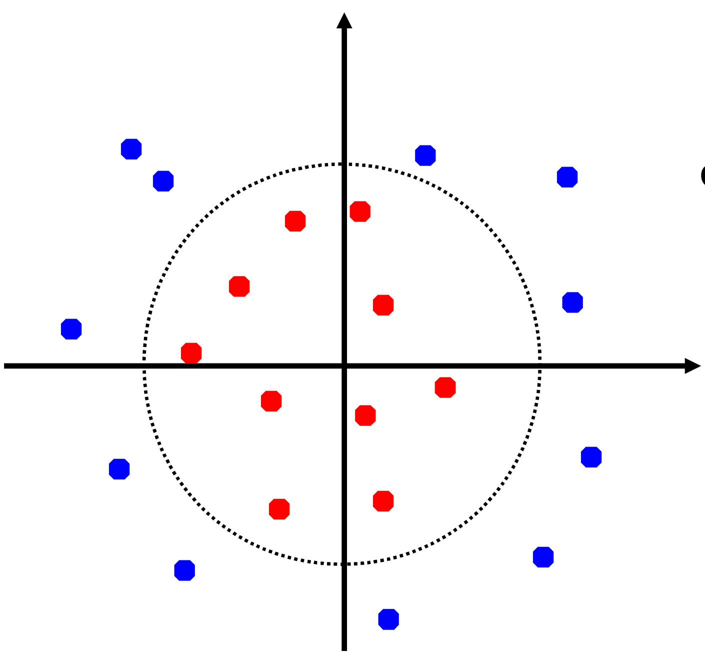
Slide credit: Andrew Moore

Non-linear feature mappings for classification

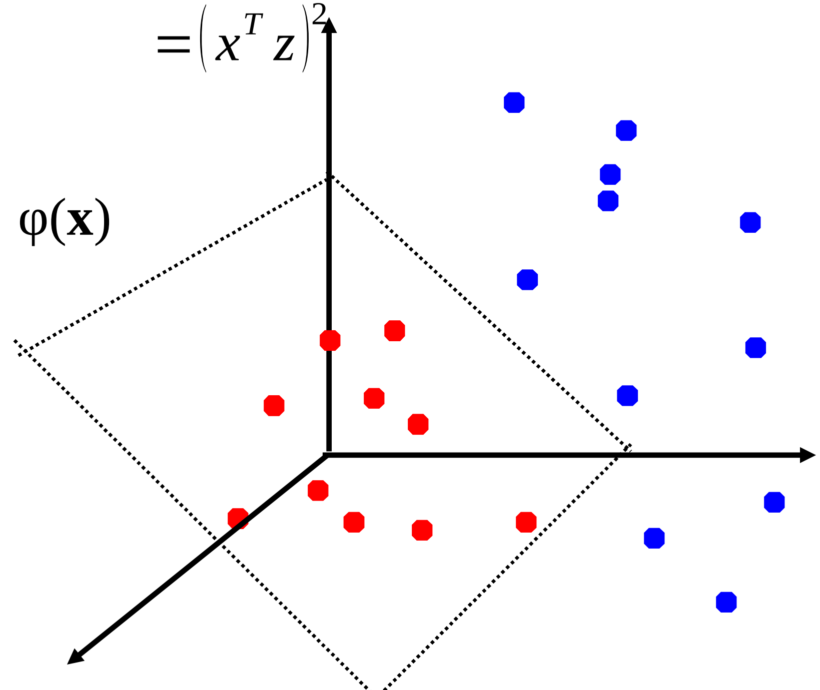
- Remember that for classification we only need dot-products.
- Let's calculate the dot-product explicitly for our example.
  - New dot-product easily computed from the original one.

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

$$\begin{aligned} k(x,z) = \varphi(x)^T \varphi(z) &= ? \\ &= x_1^2 z_1^2 + x_2^2 z_2^2 + 2 x_1 x_2 z_1 z_2 \\ &= (x_1 z_1 + x_2 z_2)^2 \\ &= (x^T z)^2 \end{aligned}$$



$$\Phi\colon\ \mathbf{x} \rightarrow \varphi(\mathbf{x})$$

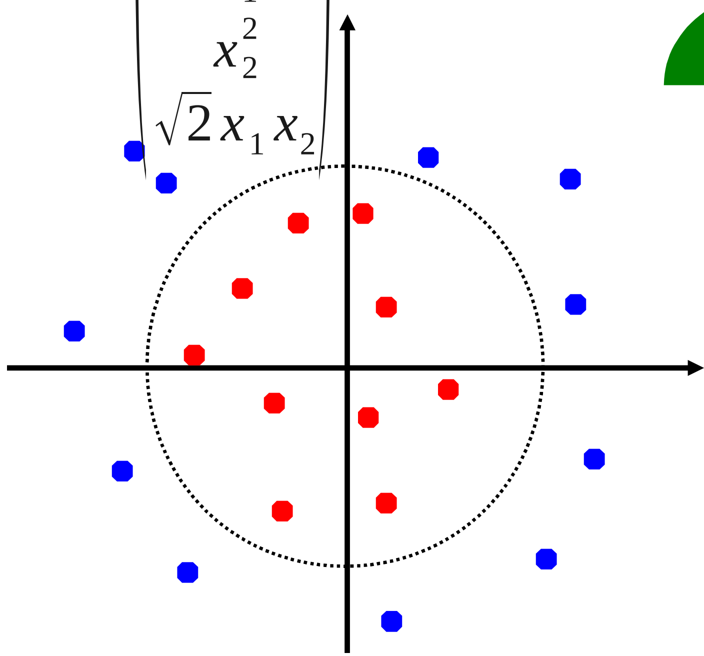


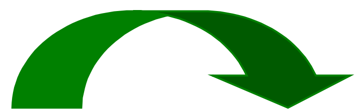
Non-linear feature mappings for classification

- Suppose we also want to keep the original features to still be able to implement linear functions
  - Again efficient computation in 6d, roughly at cost of 2d dot-product

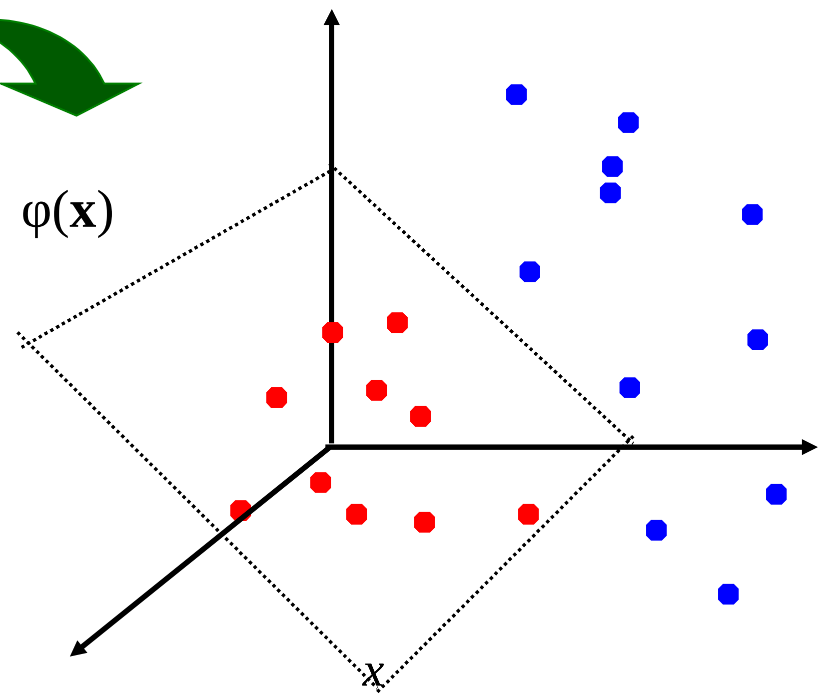
$$\varphi(x) = \begin{pmatrix} 1 \\ \sqrt{2}\,x_1 \\ \sqrt{2}\,x_2 \\ x_1^2 \\ x_2^2 \\ \sqrt{2}\,x_1 x_2 \end{pmatrix}$$

$$\begin{aligned} k(x,y) &= \varphi(x)^T \varphi(y) = ? \\ &= 1 + 2x^T y + (x^T y)^2 \\ &= (x^T y + 1)^2 \end{aligned}$$





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



Slide credit: Andrew Moore

Non-linear feature mappings for classification

- What happens if we do the same for higher dimensional data
  - Which feature vector $\varphi(x)$ 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 $(x^T y)^2=(x_1 y_1+\ldots+x_D y_D)^2$

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

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

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

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

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

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

- This allows us to obtain nonlinear classification in the original space:

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

$$\begin{aligned} w^T w &= \sum_i \sum_j \alpha_i \alpha_j \varphi(x_i)^T \varphi(x_j) \\ &= \sum_i \sum_j \alpha_i \alpha_j k(x_i, x_j) \\ &= \alpha^T K \alpha \end{aligned}$$

Summary of classification

- Linear classifiers learned by minimizing convex cost functions
  - Logistic loss: smooth objective, minimized using gradient descent, etc.
  - Hinge loss: 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.

- Using kernel functions non-linear classification has drawbacks
  - Requires storing the data with non-zero weights, memory cost
  - Kernel evaluations for test point may be computationally expensive

Course content

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- **Kernel-trick more generally**
- Bias-variance decomposition

Representation by pairwise comparisons

- We can think of a kernel function as a pairwise comparison function

$$K: \quad X \times X \rightarrow R$$

- Represent a set of n data points by the n x n matrix $[K]_{ij} = K(x_i, x_j)$

- Always an n x n matrix, whatever the nature of the data
  - Same algorithms will work for any type of data: images, text...

- Modularity between the choice of K and the choice of algorithms.

- Poor scalability with respect to the data size (squared in n).

- We will restrict attention to a specific class of kernels.

Positive definite kernels

- Definition: A positive definite kernel on the set X is a function

$$K: \quad X \times X \rightarrow R$$

which is symmetric:

$$\forall (x, x') \in X^2: \quad K(x, x') = K(x', x)$$

and which satisfies

$$\forall n \in N$$
$$\forall (x_{1,} \ldots, x_n) \in R^n \quad \text{and} \quad (a_{1,} \ldots, a_n) \in R^n$$
$$\sum_{i=1}^{n} \sum_{j=1}^{n} a_i a_j K(x_i, x_j) \geq 0$$

- Equivalently, a kernel K is positive definite if and only if, for any n and any set of n points, the similarity matrix K is positive semidefinite:

$$a^T K a \geq 0$$

The simplest positive definite kernel

- Lemma: The kernel function defined by the inner product over vectors is a positive definite kernel.
  - This kernel is known as the “linear kernel”

$$K: \quad X \times X \rightarrow R$$
$$\forall (x, x') \in X^2: \quad K(x, x') = x^T x'$$

- Proof
  - Symmetry: $K(x, x') = x^T x' = (x')^T x = K(x', x)$
  - Positive definiteness:

$$\sum_{i=1}^{n} \sum_{j=1}^{n} a_i a_j K(x_i, x_j) = \sum_{i=1}^{n} \sum_{j=1}^{n} a_i a_j x_i^T x_j = \| \sum_{i=1}^{n} a_i x_i \|_2^2 \geq 0$$

More generally: for any embedding function

- Lemma: The kernel function defined by the inner product over data points embedded in a vector space by a function φ is a positive definite kernel.

$$K:\ X \times X \rightarrow R$$
$$\forall (x, x') \in X^2: \quad K(x, x') = \langle \varphi(x), \varphi(x') \rangle_H$$

- Proof
  - Symmetry: $K(x, x') = \langle \varphi(x), \varphi(x') \rangle_H = \langle \varphi(x'), \varphi(x) \rangle_H = K(x', x)$
  - Positive definiteness:

$$\sum_{i=1}^{n} \sum_{j=1}^{n} a_i a_j K(x_i, x_j) = \sum_{i=1}^{n} \sum_{j=1}^{n} a_i a_j \langle \varphi(x_i), \varphi(x_j) \rangle_H = \| \sum_{i=1}^{n} a_i \varphi(x_i) \|_H^2 \geq 0$$

Conversely: Kernels as inner products

- Theorem (Aronszajn,1950)

  K is a positive definite kernel on the set X if and only if there exists a Hilbert space H and a mapping

  $$\Phi: \ X \rightarrow H$$

  such that for any x and x' in X

  $$K(x, x') = \langle \varphi(x), \varphi(x') \rangle_H$$

- Establishes the correspondence between kernels and representations.

The kernel trick

- Choosing a p.d. kernel K on a set X amounts to embedding the data in a Hilbert space: there exists a Hilbert space H and a mapping $\Phi \; : \; X \rightarrow H$

  such that for all x and x' in X

  $$k(x, x') = \langle \varphi(x), \varphi(x') \rangle_{H.}$$

- This mapping might not be explicitly given, nor convenient to work with in practice, e.g. for very large or even infinite dimensions.

- The “trick” is to work implicitly in the feature space H by means of kernel evaluations.

The kernel trick

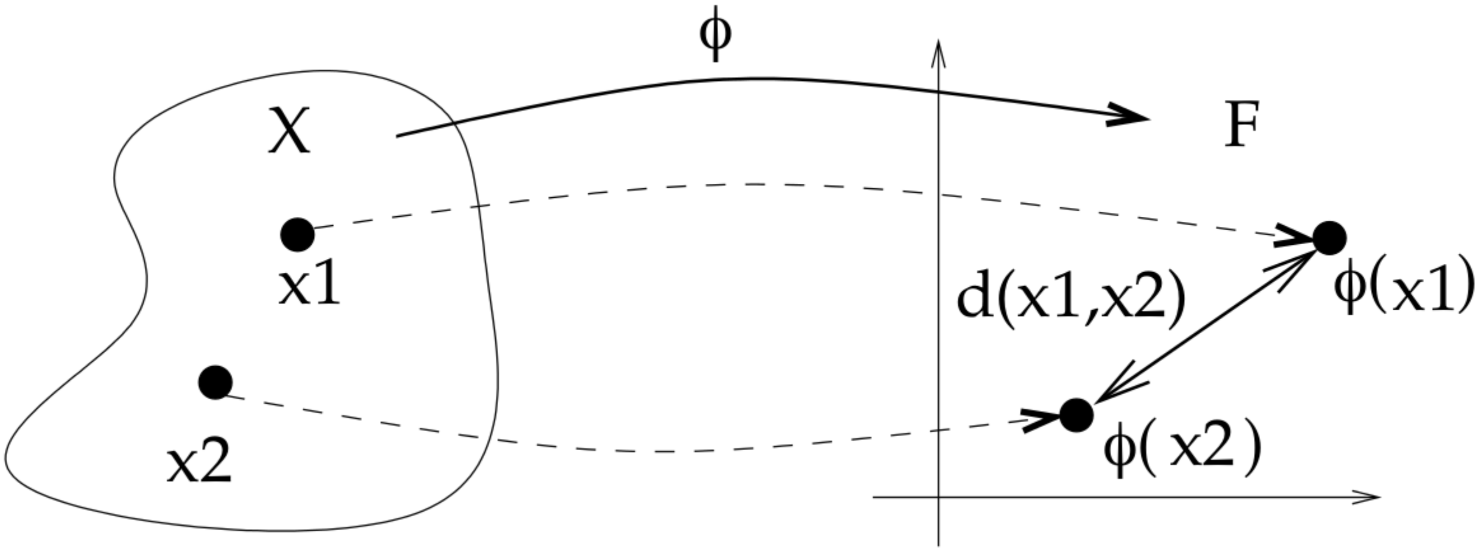
- Any algorithm to process finite dimensional vectors that can be expressed only in terms of pairwise inner products can be applied to potentially infinite-dimensional vectors in the feature space of a p.d. kernel by replacing each inner product evaluation by a kernel evaluation.

- This statement is trivially true, since the kernel computes the inner product in the associated RKHS.

- The practical implications of this “trick” are important.

- Vectors in the feature space are only manipulated implicitly, through pairwise inner products, there is no need to explicitly represent any data in the feature space.

Example 1: computing distances in the feature space



$$
\begin{aligned}
d_k(x, x')^2 &= \|\varphi(x) - \varphi(x')\|_H^2 \\
&= \langle \varphi(x) - \varphi(x'), \varphi(x) - \varphi(x') \rangle_H \\
&= \langle \varphi(x), \varphi(x) \rangle_H + \langle \varphi(x'), \varphi(x') \rangle_H - 2 \langle \varphi(x), \varphi(x') \rangle_H \\
&= k(x, x) + k(x', x') - 2\mathrm{k}(x, x')
\end{aligned}
$$

Distance for the Gaussian kernel

- The Gaussian kernel with bandwidth sigma is given by

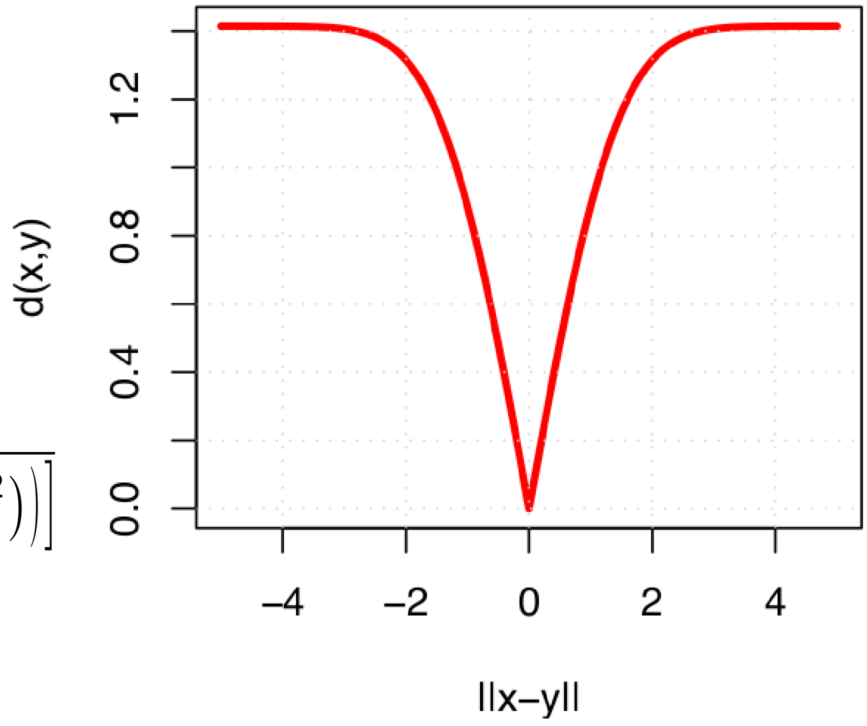
$$k(x,x')=\exp\left(-\|x-x'\|_2/(2\sigma^2)\right)$$

- In the feature space, all points are embedded on the unit sphere since

$$k(x,x)=\|\varphi(x)\|_H^2=1$$

- The distance in the feature space between x and x' is given by

$$d_k(x,x')=\sqrt{2\left[1-\exp\left(-\|x-x'\|^2/(2\sigma^2)\right)\right]}$$



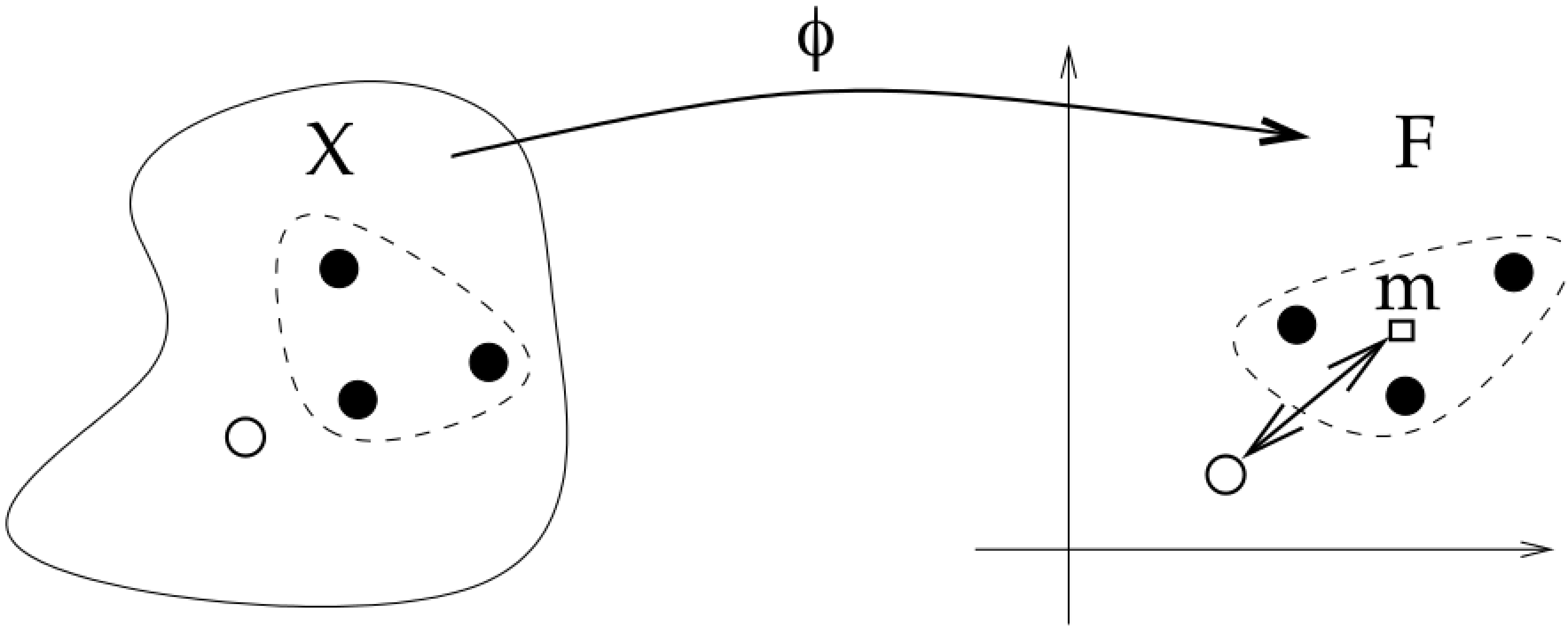
Example 2: distance between a point and a set

- Let S be a finite set of points in X: $S=(x_{1,},\ldots,x_n)$
- How to define and compute the similarity between any point x in X and the set S?

- The following is a simple approach:
  - Map all points to the feature space
  - Summarize S by the barycenter of the points $m=\frac{1}{n}\sum_{i=1}^{n}\varphi(x_i)$
  - Define the distance between x and S as

$$d_k(x,S)=\|\varphi(x)-m\|_H$$

Example 2: distance between a point and a set



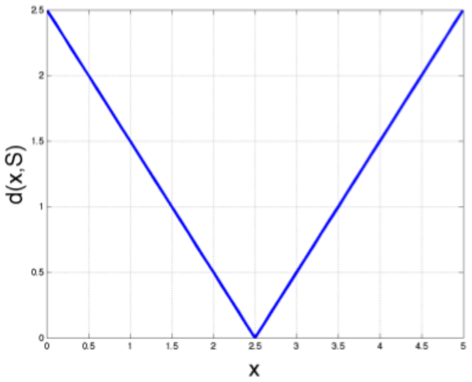
$$d_k(x,S) = \|\varphi(x) - m\|_H$$

$$= \|\varphi(x) - \frac{1}{n}\sum_{i=1}^{n} \varphi(x_i)\|_H$$

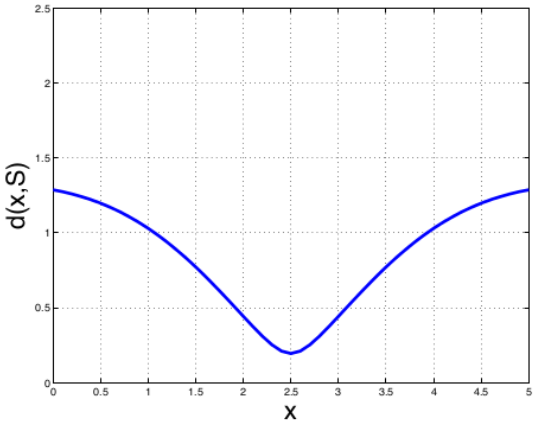
$$= \sqrt{k(x,x) - \frac{2}{n}\sum_{i=1}^{n} k(x,x_i) + \frac{1}{n^2}\sum_{i,j=1}^{n} k(x_i,x_j)}$$

Uni-dimensional illustration

- Let S = {2,3}, plot f(x) = d(x,S).

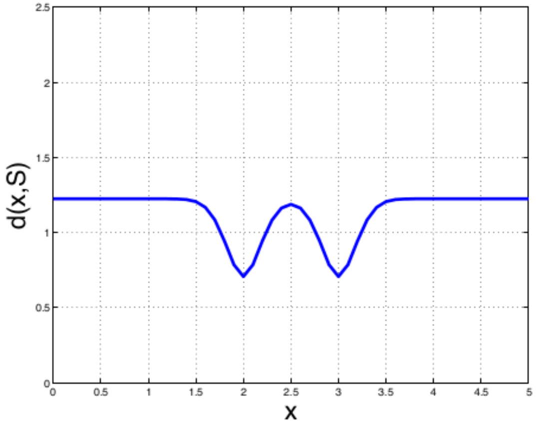


Linear kernel



Gaussian kernel,

with $\sigma = 1$

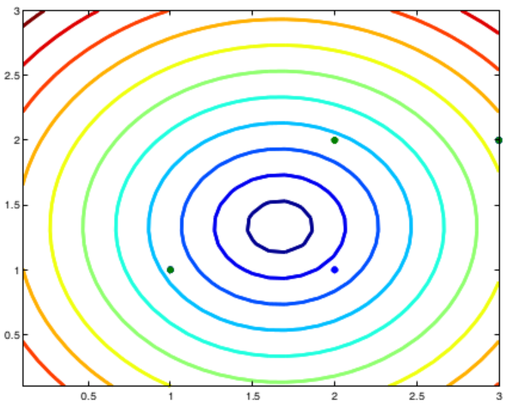


Gaussian kernel,

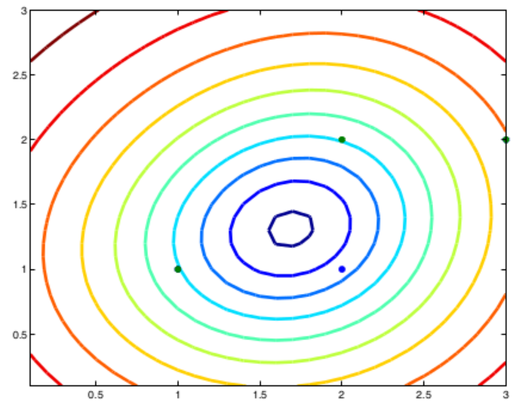
with $\sigma = 0.2$

2D illustration

- Let S = { (1,1)', (1,2)', (2,2)' }, plot f(x) = d(x,S).

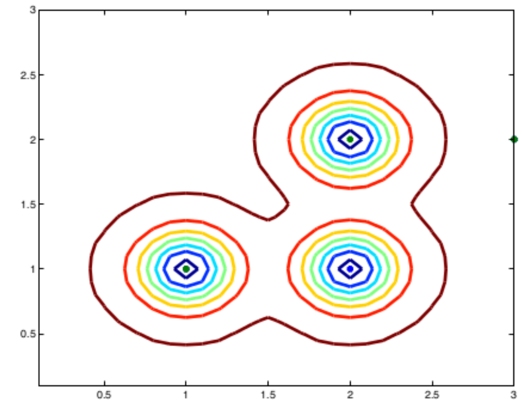


Linear kernel



Gaussian kernel,

with $\sigma = 1$



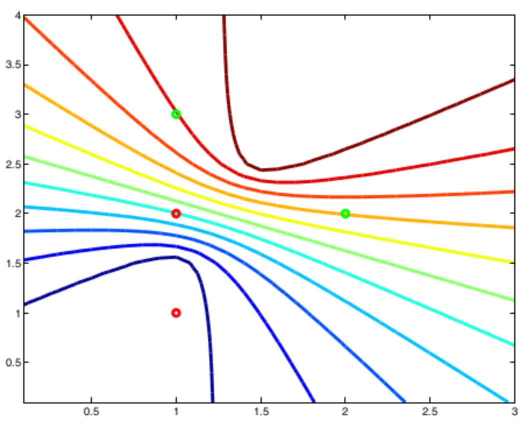
Gaussian kernel,

with $\sigma = 0.2$

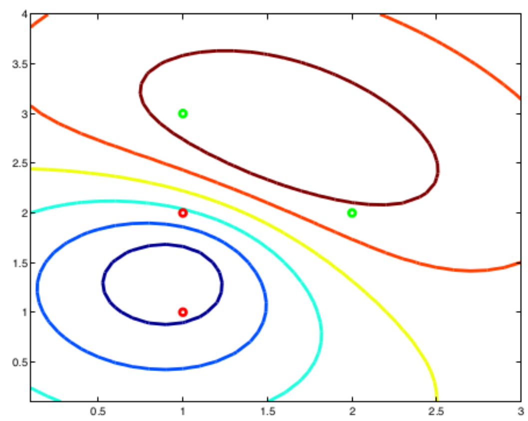
Application to discrimination

- Consider a set of points from positive class P = { (1,1)', (1,2)' }
- And a set of points from the negative class N={ (1,3)', (2,2)' }
- Plot $f(x)=d_k(x,P)^2-d_k(x,N)^2$

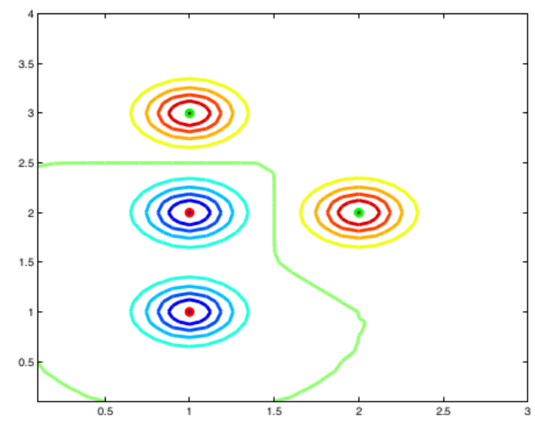
$$
\begin{aligned}
&=\|\varphi(x)-m_P\|_H^2-\|\varphi(x)-m_N\|_H^2\\
&=\frac{2}{n}\sum_{x_i\in N}k(x,x_i)-\frac{2}{n}\sum_{x_i\in P}k(x,x_i)+\text{constant}
\end{aligned}
$$



Linear kernel



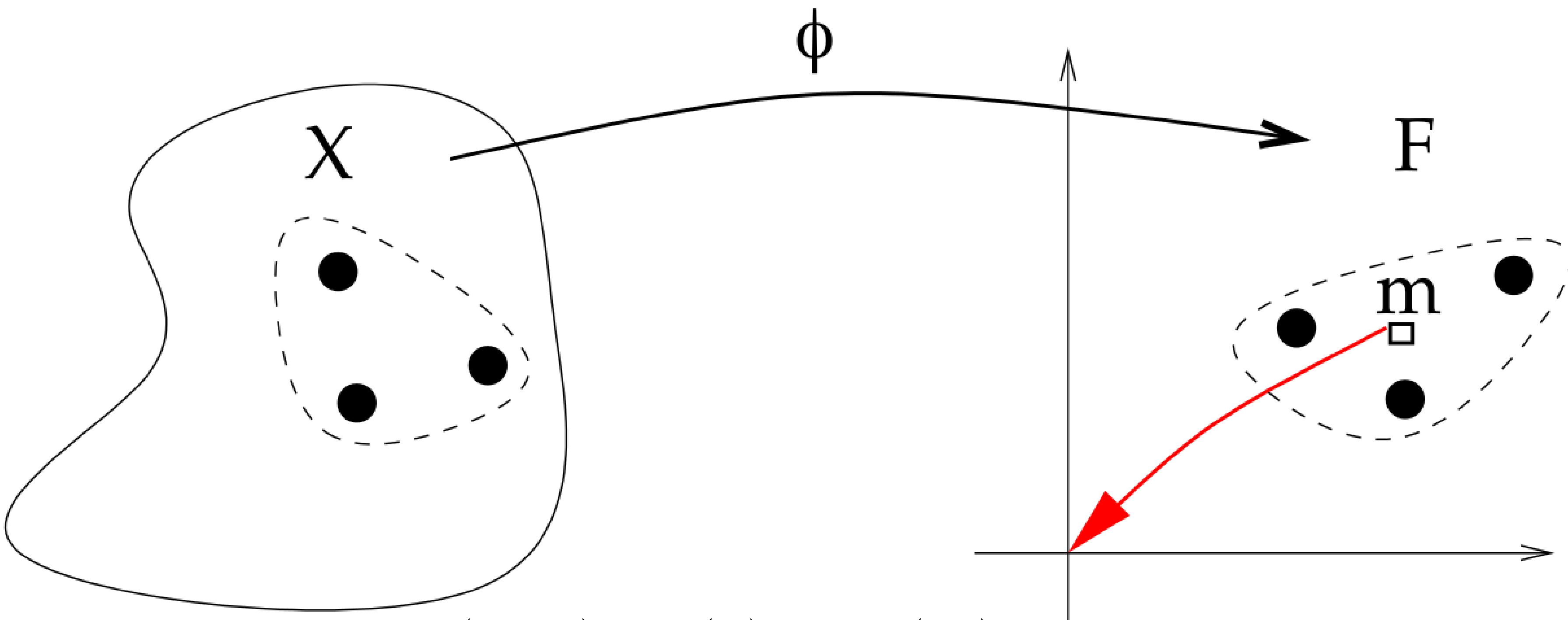
Gaussian kernel, with $\sigma=1$



Gaussian kernel, with $\sigma=0.2$

Example 3: centering data in feature space

- Let S be a set of n points in X.
- Let K be the kernel matrix generated by the p.d. kernel k(.,.).
- Let m be the barycenter in the feature space of the points in S.
- How to compute the kernel matrix when the points are centered on m?



$$h(x,x')=\langle \varphi(x)-m, \varphi(x')-m\rangle_H$$

Example 3: centering data in feature space

- Substitution of the barycenter gives

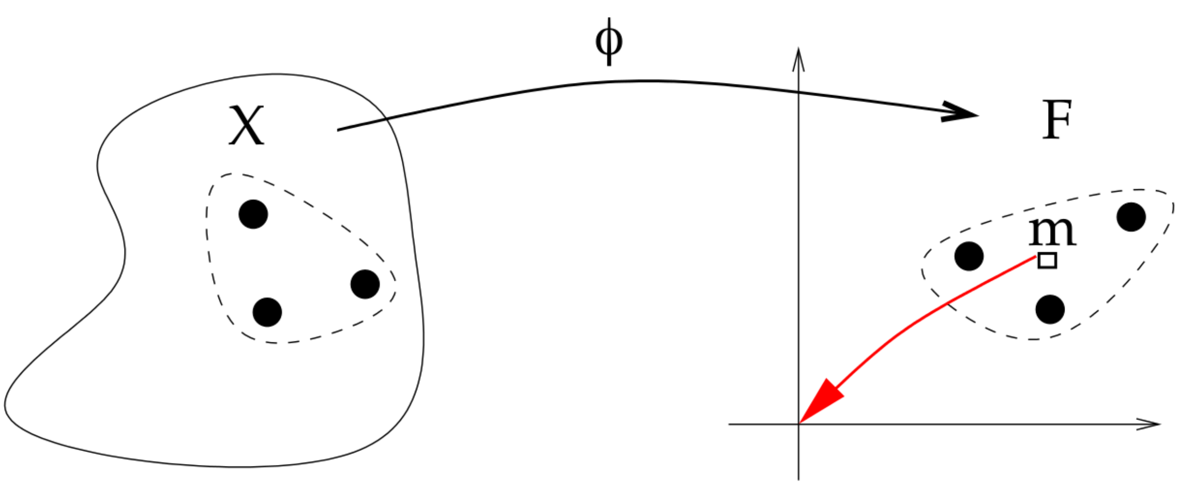
$$h(x_i, x_j) = \langle \varphi(x_i) - m, \varphi(x_j) - m \rangle_H$$
$$= \langle \varphi(x_i), \varphi(x_j) \rangle_H - \langle m, \varphi(x_i) + \varphi(x_j) \rangle_H + \langle m, m \rangle_H$$
$$= k(x_i, x_j) - \frac{1}{n} \sum_{k=1}^{n} \left(k(x_i, x_k) + k(x_k, x_j) \right) + \frac{1}{n^2} \sum_{k,l=1}^{n} k(x_k, x_l)$$

- Or, in matrix notation we get

$$H = K - KU - UK + UKU = (I - U) K (I - U)$$

where for all i,j:

$$U_{i,j} = 1/n$$



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