Lecture 9

Kernel Methods

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December 29, 2016

Outline

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   - Why Kernels?
   - Kernel Characterization
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   - Kernelized 1NN Classification
   - Kernelized Ridge Regression
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   - Loss Functions
   - SVM for Regression
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   - Large Margin Principle

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Kernels

Why?

- so far, we have been assuming that each **object** that we wish to classify or cluster or process in anyway can be **represented** as a **fixed-size feature vector** $\mathbf{x}_i \in \mathbb{R}^D$
- this may require to **preprocess** raw data in order to obtain fixed-size feature vectors
- for certain kinds of objects, it is not clear how to best represent them as fixed-sized feature vectors
- for example, how do we represent
  1. a text document or protein sequence, which can be of **variable length**?
  2. a molecular structure, which has **complex 3d geometry**?
  3. an evolutionary tree, which has **variable size** and **shape**?

Kernels

Why?

- common approach: assume that we have some way of measuring the **similarity between objects**, that **doesn't require preprocessing** them into feature vector format
- for example, when comparing strings, we can compute the edit **distance** between them.
- let $\kappa(\mathbf{x}, \mathbf{x}') \geq 0$ be some **measure of similarity** between objects $\mathbf{x}, \mathbf{x}' \in \chi$, where χ is some **abstract space**; we will call κ a **kernel function**
- we will now see together some algorithms that can be written purely in terms of kernel function computations
- we can use such algorithms when we don't have access to (or choose not to look at) the **"inside" of the objects $\mathbf{x}_i$** that we are processing

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Kernels

General Characterization

- we define a **kernel function** to be a **real-valued function** of **two arguments**, $\kappa(\mathbf{x}, \mathbf{x}') \in \mathbb{R}$, for $\mathbf{x}, \mathbf{x}' \in \chi$
- typically the function is **symmetric**, i.e.

$$\kappa(\mathbf{x}, \mathbf{x}') = \kappa(\mathbf{x}', \mathbf{x})$$

  and **non-negative**, i.e.

$$\kappa(\mathbf{x}, \mathbf{x}') \geq 0$$

- in general $\kappa(\mathbf{x}, \mathbf{x}')$ can be interpreted as a **measure of similarity** (but this may also **not be required**)

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Kernels

RBF

- a **radial basis function** or **RBF kernel** $\kappa(\mathbf{x}, \mathbf{x}') \in \mathbb{R}$ is only a function of $\|\mathbf{x} - \mathbf{x}'\|$

$$\kappa(\mathbf{x}, \mathbf{x}') = \varphi(\|\mathbf{x} - \mathbf{x}'\|)$$

- a typical example is the **Squared Exponential kernel** (SE kernel) or **Gaussian Kernel**

$$\kappa(\mathbf{x}, \mathbf{x}') = \exp(-\frac{1}{2}(\mathbf{x} - \mathbf{x}')^T \mathbf{\Sigma}^{-1}(\mathbf{x} - \mathbf{x}')) = \exp(-\frac{1}{2}\|\mathbf{x} - \mathbf{x}'\|^2_{\mathbf{\Sigma}})$$

- if $\mathbf{\Sigma} = \text{diag}(\sigma_1, ..., \sigma_D)$ we obtain the **ARD kernel** (Automatic Relevance Determination)

$$\kappa(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{1}{2}\sum_{j=1}^{D}\frac{(x_j - x'_j)^2}{\sigma_j^2}\right)$$

  σ_j can be interpreted as defining the **characteristic length scale** of dimension j

- if $\mathbf{\Sigma} = \sigma\mathbf{I}$ we obtain the **isotropic kernel**

$$\kappa(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2\sigma^2}\right)$$

  where σ is called the bandwidth

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- when performing document classification or retrieval, it is useful to have a way of **comparing two documents** $\mathbf{x}_i$ and $\mathbf{x}_{i'}$
- if we use a **bag of words representation**, where x_{ij} is the number of times words j occurs in document i, we can use the **cosine similarity**

$$\kappa(\mathbf{x}_i, \mathbf{x}_{i'}) = \frac{\mathbf{x}_i^T \mathbf{x}_{i'}}{\|\mathbf{x}_i\|_2 \|\mathbf{x}_{i'}\|_2}$$

  this quantity measures the cosine of the angle between $\mathbf{x}_i$ and $\mathbf{x}_{i'}$ when interpreted as vectors
- since $\mathbf{x}_i$ is a count vector ($x_{ij} \geq 0$), the cosine similarity $\kappa(\mathbf{x}_i, \mathbf{x}_{i'}) \in [0, 1]$
- $\kappa(\mathbf{x}_i, \mathbf{x}_{i'}) = 0$ means the vectors are orthogonal and therefore have no words in common

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Mercer (Positive Definite) Kernels

- some methods require that the kernel function satisfies the **requirement** that the **Gram matrix**

$$\mathbf{K} = \begin{bmatrix} \kappa(\mathbf{x}_1, \mathbf{x}_1) & \dots & \kappa(\mathbf{x}_1, \mathbf{x}_N) \\ \vdots & \ddots & \vdots \\ \kappa(\mathbf{x}_N, \mathbf{x}_1) & \dots & \kappa(\mathbf{x}_N, \mathbf{x}_N) \end{bmatrix}$$

  is **positive definite** for any set of inputs $\{\mathbf{x}_i\}_{i=1}^N$
- **Mercel kernels** or **positive definite kernels** satisfy the requirement $\mathbf{K} > 0$
- it can be shown that the Gaussian kernel and the cosine similarity kernel are Mercer kernels

Mercer (Positive Definite) Kernels

- the importance of Mercer kernels is the following result, known as **Mercer's theorem**
- if the Gram matrix is positive definite, i.e. $\mathbf{K} > 0$ for any set of inputs $\{\mathbf{x}_i\}_{i=1}^N$, we can compute an eigenvector decomposition

$$\mathbf{K} = \begin{bmatrix} \kappa(\mathbf{x}_1, \mathbf{x}_1) & \dots & \kappa(\mathbf{x}_1, \mathbf{x}_N) \\ \vdots & \ddots & \vdots \\ \kappa(\mathbf{x}_N, \mathbf{x}_1) & \dots & \kappa(\mathbf{x}_N, \mathbf{x}_N) \end{bmatrix} = \mathbf{U}^T \mathbf{\Lambda} \mathbf{U}$$

  where $\mathbf{\Lambda}$ is a diagonal matrix of eigenvalues $\lambda_i > 0$
- now consider an element of $\mathbf{K}$

$$k_{ij} = (\mathbf{\Lambda}^{1/2} \mathbf{U}_{:i})^T (\mathbf{\Lambda}^{1/2} \mathbf{U}_{:j}) = (\mathbf{\Lambda}^{1/2} \mathbf{u}_i)^T (\mathbf{\Lambda}^{1/2} \mathbf{u}_j)$$

- let us define $\phi(\mathbf{x}_i) \triangleq \mathbf{\Lambda}^{1/2} \mathbf{U}_{:i}$, then we can write

$$k_{ij} = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$$

- hence the entries k_{ij} can be computed by performing an inner product of some **new feature vectors** $\phi(\mathbf{x})$ that are implicitly defined by the eigenvectors in $\mathbf{U}$

Mercer (Positive Definite) Kernels

- in general, if the **kernel is Mercer** then there exists a function ϕ mapping $\mathbf{x} \in \chi$ to $\phi(\mathbf{x}) \in \mathbb{R}^D$ such that

$$\kappa(\mathbf{x}, \mathbf{x}') = \phi(\mathbf{x})^T \phi(\mathbf{x}')$$

  where ϕ depends on the **eigen functions** of κ (where D is potentially infinite)

- **conclusion**: since we are able to define a similarity distance $\kappa(\mathbf{x}, \mathbf{x}')$ in terms of an inner product, i.e. $\kappa(\mathbf{x}, \mathbf{x}') = \phi(\mathbf{x})^T \phi(\mathbf{x}')$, the result is that we are **implicitly transforming** each **raw data sample** $\mathbf{x} \in \chi$ into a new **feature vector** $\phi(\mathbf{x})$ without any need to explicitly represent it

Mercer (Positive Definite) Kernels

- for example, the **polynomial kernel** $\kappa(\mathbf{x}, \mathbf{x}') = (\gamma \mathbf{x}^T \mathbf{x}' + r)^M$, where $r > 0$ is a Mercel kernel
- in this case one can show that $\phi(\mathbf{x})$ contains all the terms up to degree M
- for example with $M = 2$ and $\gamma = r = 1$, we have

$$(\mathbf{x}^T \mathbf{x}' + 1)^2 = \phi(\mathbf{x})^T \phi(\mathbf{x}')$$

with $\phi(\mathbf{x}) = [1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, x_2^2, \sqrt{2}x_1 x_2]^T \in \mathbb{R}^6$

- the **Gaussian kernel** is also a Mercel kernel
- the feature map ϕ of a **Gaussian kernel** lives in an **infinite dimensional space**: in such a case, it is clearly infeasible to explicitly represent the feature vectors
- recall that

$$\exp(x) = \sum_{k=0}^{\infty} \frac{x^k}{k!}$$

which means that we are dealing with a "polynomial degree" $M \to \infty$

Mercer Kernels

- an example of non-Mercer kernel is the **sigmoid kernel**

$$\kappa(\mathbf{x}, \mathbf{x}') = \tanh(\gamma \mathbf{x}^T \mathbf{x}' + r)$$

- in general, **verifying that a kernel is a Mercer kernel** is difficult, and requires techniques from functional analysis
- however, one can show that it is possible to **build up new Mercer kernels** from simpler ones using a set of **standard rules**
- for example, if κ_1 and κ_2 are both Mercer, so is

$$\kappa(\mathbf{x}, \mathbf{x}') = \kappa_1(\mathbf{x}, \mathbf{x}') + \kappa_2(\mathbf{x}, \mathbf{x}')$$

Linear Kernel

- deriving the feature vector ϕ implied by a kernel is in general quite difficult, and only possible if the kernel is Mercer
- however, deriving a kernel from a feature vector ϕ is easy

$$\kappa(\mathbf{x}, \mathbf{x}') = \phi(\mathbf{x})^T \phi(\mathbf{x}') = \langle \phi(\mathbf{x}), \phi(\mathbf{x}') \rangle$$

- if $\phi(\mathbf{x}) = x$, we get the **linear kernel**, defined by

$$\kappa(\mathbf{x}, \mathbf{x}') = \mathbf{x}^T \mathbf{x}'$$

- this is useful if the original features are individually informative and the decision boundary is likely to be representable as a linear combination of the original features
- of course, when data is not linearly separable, non-linear kernels are required

Matern Kernel

- the **Matern kernel** is commonly used in Gaussian process regression and has the following form

$$\kappa(r) = \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{\sqrt{2\nu} r}{l} \right)^{\nu} K_{\nu} \left(\frac{\sqrt{2\nu} r}{l} \right)$$

where $r \triangleq \|\mathbf{x} - \mathbf{x}'\|$ with $\nu > 0$, $l > 0$ and K_{ν} is a modified Bessel function

String Kernel

- the real power of kernels arises when the inputs are structured objects
- we now describe one way of comparing two strings $\mathbf{x}$ and $\mathbf{x}'$ of lengths D, D' using a string kernel
- the two strings are defined over the 20 letter alphabet $\mathcal{A} = \{A, R, N, D, C, E, Q, G, H, I, L, K, M, F, P, S, T, W, Y, V\}$
- let $\mathbf{x}$ be the following sequence of length 110

$$IPTSALVKETLALLSTHRTLLIANETLRIPVPVHKNHQLCTEEIFQGIGTLESQ$$
$$TVQGGTVERLFKNLSLIKKYIDGQKKKCGEERRRVNQFLDYLQEFLGVMNTEWI$$

and let $\mathbf{x}'$ be the following sequence of length 153

$$PHRRDLCSRSIWLARKIRSDLTALTESYVKHQGLWSELTEAERLQENLQAYRTFHV$$
$$LLARLLEDQQVHFTPTEGDFHQAIHTLLLQVAAFAYQIEELMILLEYKIPRNEADG$$
$$MLFEKKLWGLKVLQELSQWTVRSIHDLRFISSHQTGIP$$

- these strings have the substring LQE in common
- we can define the **similarity of two strings** to be the number of substrings they have in common

String Kernel

- more formally and more generally, let us say that s is a substring of $\mathbf{x}$ if we can write $\mathbf{x} = usv$ for some (possibly empty) strings u, s and v
- now let $\phi_s(x)$ denote the number of times that substring s appears in string $\mathbf{x}$
- we define the kernel between two strings $\mathbf{x}$ and $\mathbf{x}'$ as

$$\kappa(\mathbf{x}, \mathbf{x}') = \sum_{s \in \mathcal{A}^*} w_s \phi_s(x) \phi_s(x')$$

  where $w_s \geq 0$ and $\mathcal{A}^*$ is the set of all strings (of any length) from the alphabet $\mathcal{A}$
- this is a Mercer kernel

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Kernel Machines

- we define a **kernel machine** to be a Generalized Linear Model (GLM) where the input feature vector has the form

$$\phi(\mathbf{x}) = \left[\kappa(\mathbf{x}, \boldsymbol{\mu}_1), ..., \kappa(\mathbf{x}, \boldsymbol{\mu}_K)\right]$$

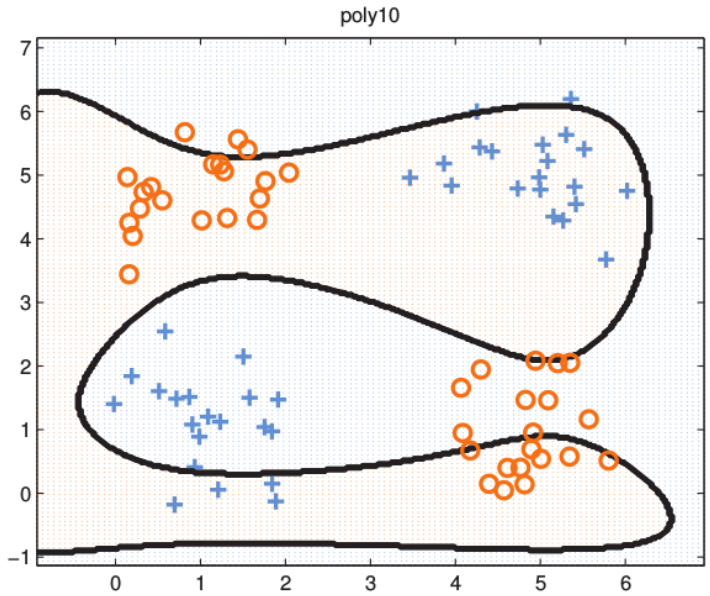
  where $\boldsymbol{\mu}_k \in \chi$ are the set of K **centroids**
- open question: how to choose the centroids $\boldsymbol{\mu}_k$?
- the above vector $\phi(\mathbf{x})$ is called **kernelized feature vector**
- kernel machines do not require that the kernel are Mercel
- if κ is an RBF kernel, the corresponding kernel machine is called a **RBF network**

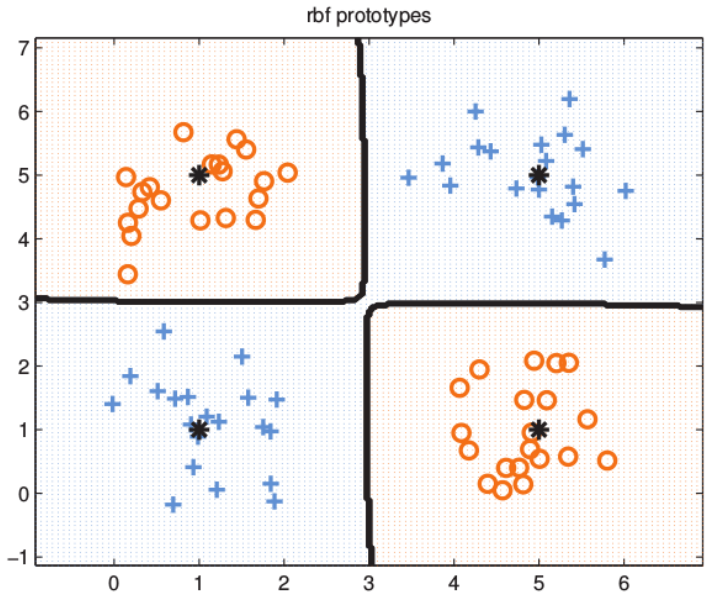
Kernel Machines

- we can use the **kernelized feature vector for logistic regression** by defining

$$p(y|\mathbf{x}, \boldsymbol{\theta}) = \text{Ber}(y|\text{sigm}(\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x})))$$

this provides a simple way to define a **non-linear decision boundary**





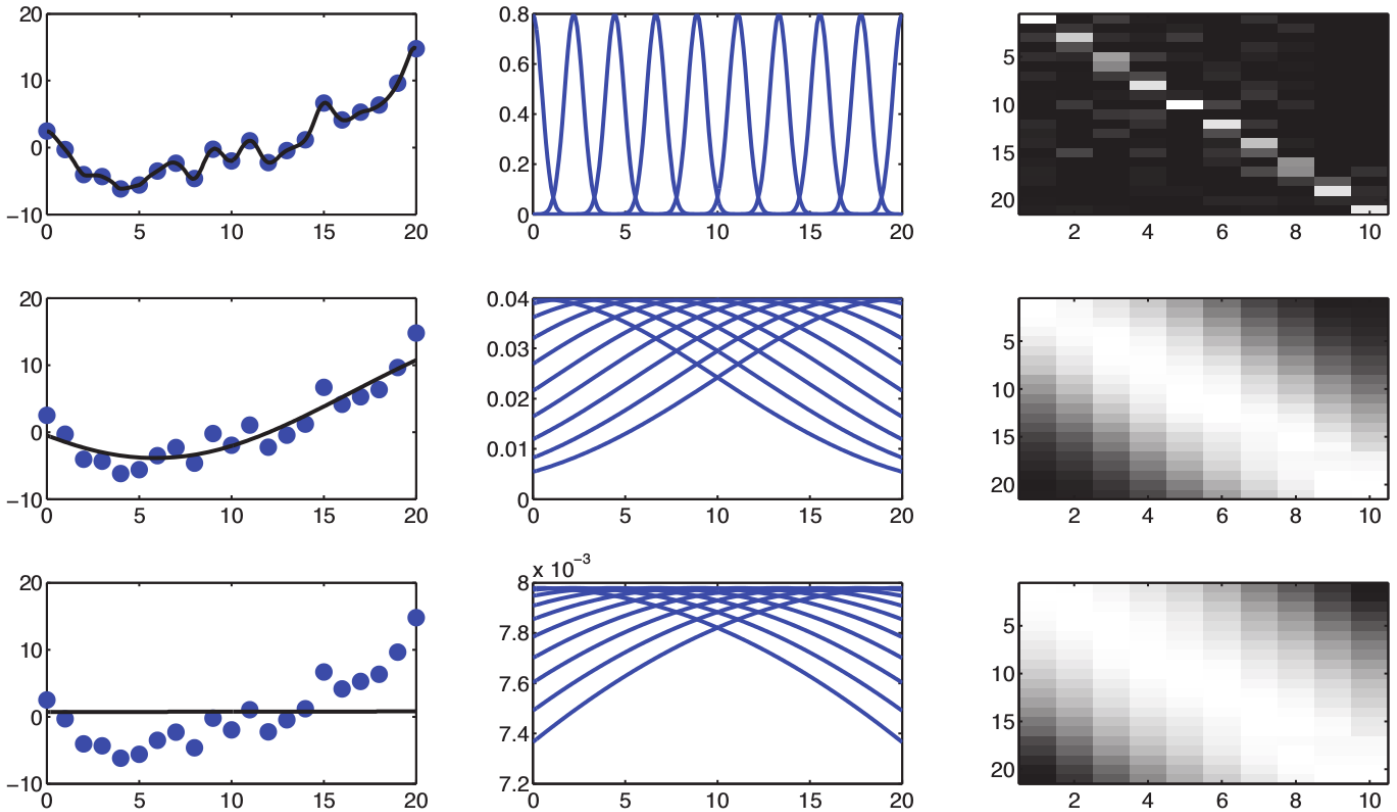
- *left*: fitting a linear logistic regression classifier using degree 10 polynomial expansion.
- *right*: same model, but using an RBF kernel with centroids specified by the 4 black crosses

Kernel Machines

- we can also use the **kernelized feature vector inside a linear regression model** by defining

$$p(y|\mathbf{x}, \boldsymbol{\theta}) = \mathcal{N}(y|\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}), \sigma^2)$$

Kernel Machines



- left column: fitted function where $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^{N}$ and $y_i, x_i \in \mathbb{R}$
- middle column: RBF basis functions $\kappa(x, \mu_i)$ evaluated on a grid ($K = 10$ functions uniformly spaced)
- right column: design matrix
- top to bottom we show different bandwidths: $\sigma = 0.1$, $\sigma = 0.5$, $\sigma = 50$

how to choose the centroids $\boldsymbol{\mu}_k$?

$$\boldsymbol{\phi}(\mathbf{x}) = \left[\kappa(\mathbf{x}, \boldsymbol{\mu}_1), ..., \kappa(\mathbf{x}, \boldsymbol{\mu}_K)\right]$$

- if D is small, a simple solution is to **uniformly tile**/grid the space occupied by the data (recall the curse of dimensionality)
- another approach is to **find clusters** in the data (but how to pick the number of clusters)
- a simpler approach is to make **each sample $\mathbf{x}_i$ a prototype**

  $$\boldsymbol{\phi}(\mathbf{x}) = \left[\kappa(\mathbf{x}, \mathbf{x}_1), ..., \kappa(\mathbf{x}, \mathbf{x}_N)\right]$$

  and use a sparse-promoting prior for $\mathbf{w}$ to efficiently select subset of training exemplars $\mathbf{x}_i$
- another very popular approach is the **Support Vector Machine** (SVM) which modify the likelihood term instead of using a sparsity-promoting prior

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Kernel Trick

- rather than defining our feature vector in terms of kernels

$$\phi(\mathbf{x}) = \left[\kappa(\mathbf{x}, \mathbf{x}_1), ..., \kappa(\mathbf{x}, \mathbf{x}_N)\right]$$

  we can instead **work with the original feature vectors x**, but modify the algorithm so that it **replaces all inner products** of the form $\langle \mathbf{x}, \mathbf{x}' \rangle = \mathbf{x}^T \mathbf{x}'$ with a call to the kernel function, $\kappa(\mathbf{x}, \mathbf{x}')$
- this is called the **kernel trick**
- it turns out that many algorithms can be kernelized in this way
- the use of Mercer kernel is required for this trick to work

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Kernelized 1NN Classification

- a 1NN classifier computes the Euclidean distance of a test vector to all the training points, find the closest one, and look up its label
- this can be kernelized by observing that

$$\|\mathbf{x} - \mathbf{x}'\|_2^2 = \langle \mathbf{x} - \mathbf{x}', \mathbf{x} - \mathbf{x}' \rangle = \langle \mathbf{x}, \mathbf{x} \rangle + \langle \mathbf{x}', \mathbf{x}' \rangle - 2\langle \mathbf{x}, \mathbf{x}' \rangle$$

- in this way we can redefine the distance by using the chosen kernel

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Kernelized Ridge Regression

The Primal Problem

- $\mathbf{x} \in \mathbb{R}^D$ and $\mathbf{X} \in \mathbb{R}^{N \times D}$
- minimization problem

$$J(\mathbf{w}) = \frac{1}{N} \sum_{i=1}^{N} (y_i - (w_0 + \mathbf{w}^T \mathbf{x}_i)^2) + \lambda \|\mathbf{w}\|_2^2 = \|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2 + \lambda \|\mathbf{w}\|_2^2$$

- the solution is

$$\mathbf{w} = (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_D)^{-1} \mathbf{X}^T \mathbf{y}$$

- but here we do not have yet inner products to replace with kernel functions

- by using the matrix inversion lemma

$$(\mathbf{E} - \mathbf{F}\mathbf{H}^{-1}\mathbf{G})^{-1}\mathbf{F}\mathbf{H}^{-1} = \mathbf{E}^{-1}\mathbf{F}(\mathbf{H} - \mathbf{G}\mathbf{E}^{-1}\mathbf{F})^{-1}$$

and setting $\mathbf{E} = \mathbf{I}_D$, $\mathbf{H} = \mathbf{I}_N$, $\mathbf{F} = -\mathbf{X}^T$ and $\mathbf{G} = \mathbf{X}$ we can pass from

$$\mathbf{w} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I}_D)^{-1}\mathbf{X}^T\mathbf{y}$$

to

$$\mathbf{w} = \mathbf{X}^T(\mathbf{X}\mathbf{X}^T + \lambda\mathbf{I}_N)^{-1}\mathbf{y}$$

Kernelized Ridge Regression

The Dual Problem

- given
$$\mathbf{w} = \mathbf{X}^T(\mathbf{X}\mathbf{X}^T + \lambda \mathbf{I}_N)^{-1}\mathbf{y}$$
- we can replace $\mathbf{X}\mathbf{X}^T$ with $\mathbf{K}$ since $k_{ij} = \mathbf{x}_i^T\mathbf{x}_j$
- we can define the **dual variables**
$$\boldsymbol{\alpha} \triangleq (\mathbf{X}\mathbf{X}^T + \lambda \mathbf{I}_N)^{-1}$$
- hence, one has
$$\mathbf{w} = \mathbf{X}^T\boldsymbol{\alpha} = \sum_{i=1}^{N} \alpha_i \mathbf{x}_i$$
the solution vector $\mathbf{w}$ is just a linear sum of the N training vectors
- if we plug this in at test time to compute the predictive mean
$$\hat{f}(\mathbf{x}) = \mathbf{w}^T\mathbf{x} = \sum_{i=1}^{N} \alpha_i \mathbf{x}_i^T\mathbf{x} = \sum_{i=1}^{N} \alpha_i \kappa(\mathbf{x}, \mathbf{x}_i)$$
- this kind of technique can be used to kernelize many other linear models such as logistic regression

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- consider the regularized **empirical risk function**

$$J(\mathbf{w}, \lambda) = \sum_{i=1}^{N} L(y_i, \hat{y}_i) + \lambda \|\mathbf{w}\|^2$$

  where $\hat{y}_i = \mathbf{w}^T \mathbf{x} + w_0$
- if $L(y_i, \hat{y}_i) = (y_i - \hat{y}_i)^2$ we have a **quadratic loss** and the problem becomes a **ridge regression**
- if $L(y_i, \hat{y}_i) = -\log p(y_i|\mathbf{x}_i, \mathbf{w}_i) = -\log(\text{sigm}(y_i \eta_i)) = \log(1 + e^{-y_i \eta_i})$ with $y_i \in \{-1, 1\}$ and $\eta_i = \mathbf{w}^T \mathbf{x}_i + w_0$, we have a **log-loss** and the problem becomes a **logistic regression**
- we have seen how to kernelize a model but we want also a sparse solution for efficiency reasons
- if we replace the quadratic/log-loss with some other loss function, we can ensure that the **solution is sparse**, so that predictions only depend on a subset of the training data, known as **support vectors**
- this combination of the kernel trick plus a modified loss function is known as a **support vector machine** or SVM

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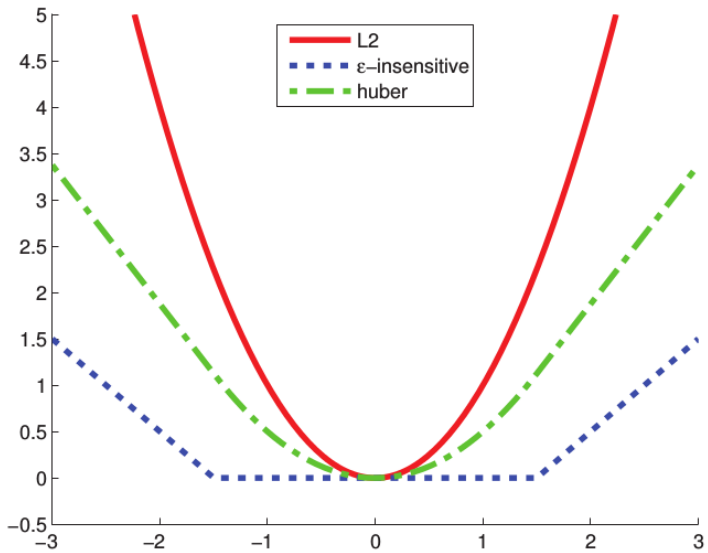
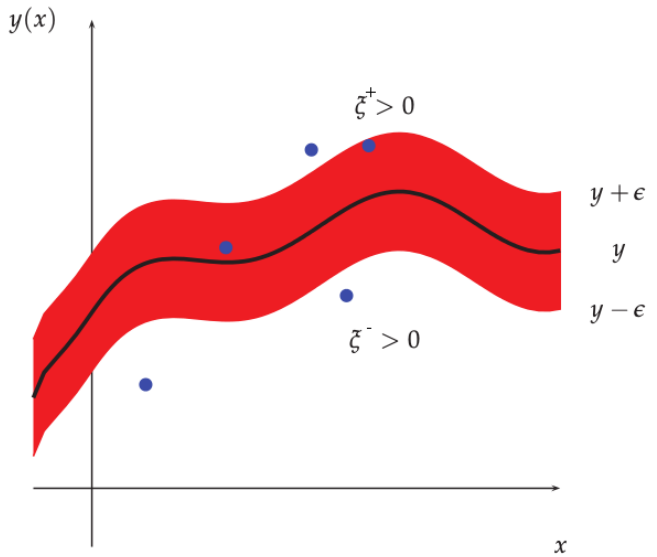
- let's consider a regression problem $J(\mathbf{w}, \lambda) = \sum_{i=1}^{N} L(y_i, \hat{y}_i) + \lambda \|\mathbf{w}\|^2$ with $\hat{y}_i = \mathbf{w}^T \mathbf{x} + w_0$
- if we use the **epsilon insensitive loss function**

$$L_\epsilon(y, \hat{y}) \triangleq \begin{cases} 0 & \text{if } \|y - \hat{y}\| < \epsilon \\ \|y - \hat{y}\| - \epsilon & \text{otherwise} \end{cases}$$

it means that any point lying inside an ϵ-tube around the prediction is not penalized



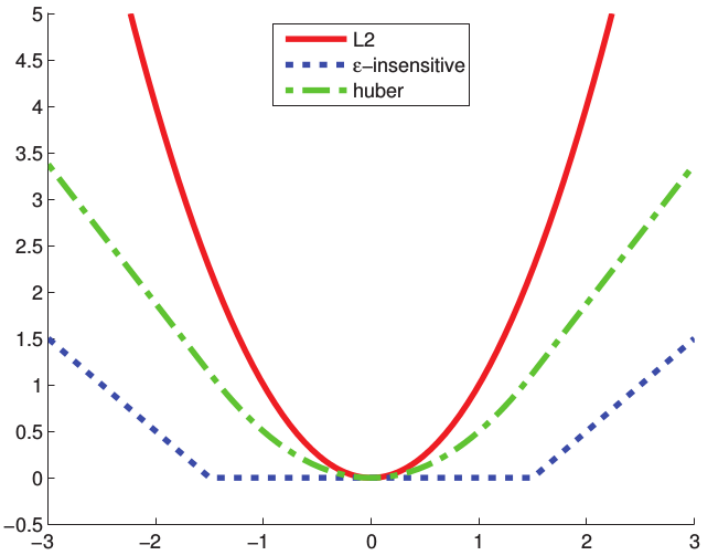


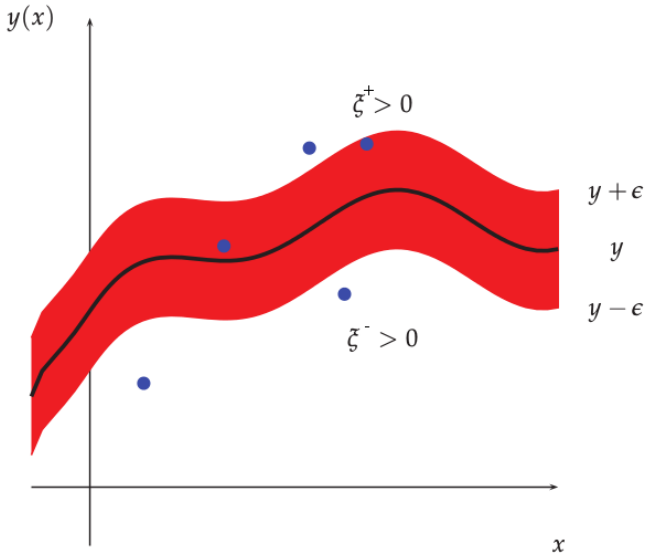
- the objective function is usually written as

$$J = C \sum_{i=1}^{N} L_\epsilon(y_i, \hat{y}_i) + \frac{1}{2}\|\mathbf{w}\|^2$$

with $\hat{y}_i = f(\mathbf{x}_i) = \mathbf{w}^T \mathbf{x}_i + w_0$ and $C = \frac{1}{\lambda}$ is regularization constant

- this objective function is **convex** and **unconstrained** but **not differentiable**



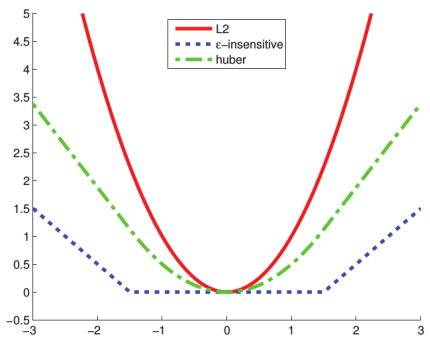


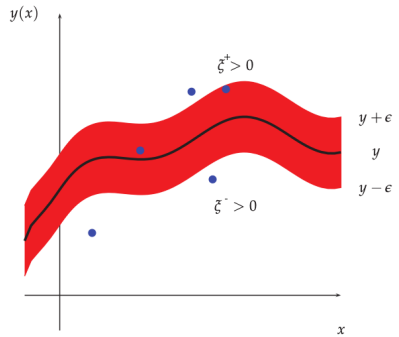
- one popular approach is to formulate the problem as a **constrained optimization problem**
- in particular, we can introduce the **slack variables** $\xi_i^+ \geq 0$ and $\xi_i^- \geq 0$ to represent the degree to which each point $\mathbf{x}_i$ lies outside the tube

$$y_i \leq f(\mathbf{x}_i) + \epsilon + \xi_i^+$$
$$y_i \geq f(\mathbf{x}_i) - \epsilon - \xi_i^+$$

- the problem can be restated as a standard quadratic program in $2N + D + 1$ variables

$$J = C \sum_{i=1}^{N} (\xi_i^+ + \xi_i^-) + \frac{1}{2}\|\mathbf{w}\|^2 \qquad \text{s.t.} \quad \xi_i^+ \geq 0 \text{ and } \xi_i^- \geq 0$$





- the problem

$$J = C\sum_{i=1}^{N}(\xi_i^+ + \xi_i^-) + \frac{1}{2}\|\mathbf{w}\|^2 \qquad \text{s.t.} \quad \xi_i^+ \geq 0 \ \textit{and} \ \xi_i^- \geq 0$$

- it is possible to show that the optimal solution has the form

$$\hat{\mathbf{w}} = \sum_i \alpha_i \mathbf{x}_i \qquad \text{with} \quad \alpha_i \geq 0$$

- it turns out that in the solution the vector $\boldsymbol{\alpha}$ is **sparse**, because we don't care about errors which are smaller than ϵ
- the $\mathbf{x}_i$ for which $\alpha_i > 0$ are called the **support vectors**: these are points for which the errors lie on or outside the tube
- all other vectors can be neglected when computing $\hat{\mathbf{w}}$

- at test time we evaluate the y function as

$$\hat{y}(\mathbf{x}) = \hat{w}_0 + \hat{\mathbf{w}}^T \mathbf{x}$$

- once we plug in the definition of $\hat{\mathbf{w}}$ we have

$$\hat{y}(\mathbf{x}) = \hat{w}_0 + \sum_i \alpha_i \mathbf{x}_i^T \mathbf{x}$$

and we can **kernelize** it by replacing the inner product with the kernel function

$$\hat{y}(\mathbf{x}) = \hat{w}_0 + \sum_i \alpha_i \kappa(\mathbf{x}, \mathbf{x}_i)$$

Outline

1. Intro
   - Why Kernels?
   - Kernel Characterization
2. Kernels Functions
   - RBF Kernels
   - Kernels for Comparing Documents
   - Mercer Kernels
3. Kernel-based Models
   - Kernel Machines
   - Kernel Trick
   - Kernelized 1NN Classification
   - Kernelized Ridge Regression
4. Support Vector Machine (SVM)
   - Loss Functions
   - SVM for Regression
   - SVM for Classification
   - Large Margin Principle

- let's consider a logistic regression problem where $y_i \in \{-1, +1\}$
- the objective function is

$$J(\mathbf{w}, \lambda) = \sum_{i=1}^{N} L(y_i, \hat{y}_i) + \lambda \|\mathbf{w}\|^2$$

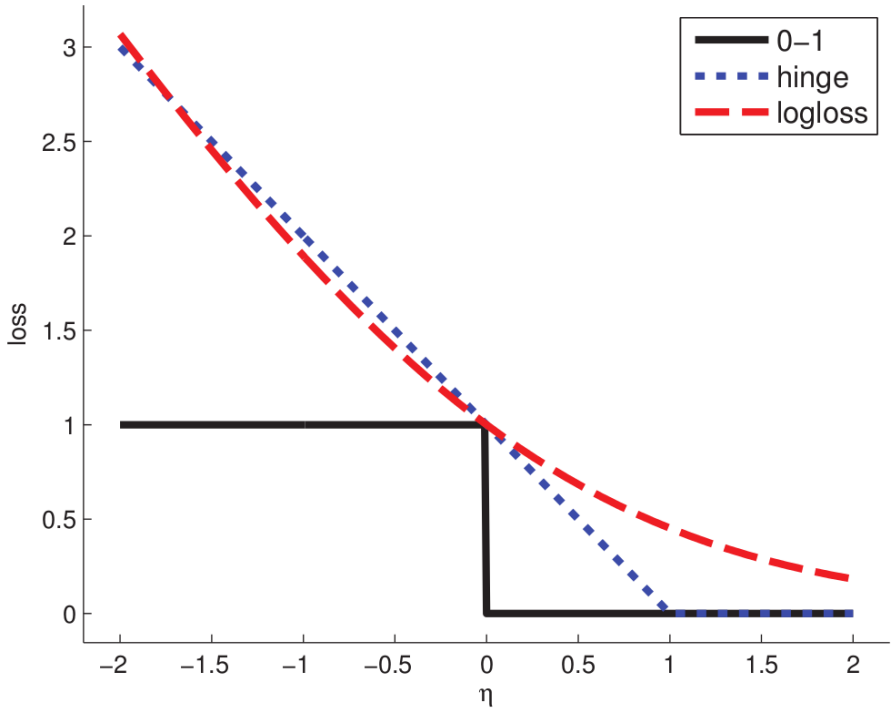
with a **log-loss** $L(y_i, \eta_i) = -\log p(y_i|\mathbf{x}_i, \mathbf{w}_i) = -\log(\text{sigm}(y_i \eta_i)) = \log(1 + e^{-y_i \eta_i})$ where $\eta_i = f(\mathbf{x}_i) = \mathbf{w}^T \mathbf{x}_i + w_0$ represents our "confidence" in choosing label $\hat{y}_i = 1$

- in principle, we could use the **0-1 loss** $L(y_i, \eta_i) = \mathbb{I}(y_i \neq \eta_i) = \mathbb{I}(y_i \eta_i < 0)$ so as to minimize the **misclassification error**
- unfortunately, the 0-1 risk is a very non-smooth objective and hence is hard to optimize
- the SVM algorithm replaces the log-loss with the **hinge loss**

$$L_{hinge}(y_i, \eta_i) \triangleq \max(0, 1 - y_i \eta_i) = (1 - y_i \eta_i)_+$$

where $(v)_+ \triangleq \max(0, v)$

- $\eta = f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + w_0$ represents our "confidence" in choosing label $y = 1$
- **log-loss** $L(y, \eta) = -\log p(y|\mathbf{x}, \mathbf{w}) = \log(1 + e^{-y\eta})$
- **0-1 loss** $L(y, \eta) = \mathbb{I}(y \neq \eta) = \mathbb{I}(y\eta < 0)$
- **hinge loss** $L_{hinge}(y, \eta) \triangleq \max(0, 1 - y\eta) = (1 - y\eta)_+$
- the hinge loss and log-loss represent smooth convex upper bounds on the 0-1 loss
- in the figure below, the horizontal axis is the margin $y\eta$, the vertical axis is the loss



- the objective function is

$$J = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{N}(1 - y_i\eta_i)_+$$

with $\eta_i = f(\mathbf{x}_i) = \mathbf{w}^T\mathbf{x}_i + w_0$

- since the function $(1 - y_i\eta_i)_+$ is not differentiable we can introduce the **slack variable** $\xi_i \geq 0$ and rewrite the objective as

$$J = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{N}\xi_i \quad \text{s.t.} \quad \xi_i \geq 0, \quad y_i(\mathbf{w}^T\mathbf{x}_i + w_0) \geq 1 - \xi, \quad i = 1 : N$$

- the objective

$$J = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{N}\xi_i \quad \text{s.t.} \quad \xi_i \geq 0, \quad y_i(\mathbf{w}^T\mathbf{x}_i + w_0) \geq 1 - \xi, \quad i = 1 : N$$

- it is possible to show that the **optimal solution** has the form

$$\hat{\mathbf{w}} = \sum_i \alpha_i \mathbf{x}_i \qquad \text{with} \quad \alpha_i = \lambda_i y_i$$

  and where $\boldsymbol{\alpha}$ is sparse (because of the hinge loss)

- the $\mathbf{x}_i$ for which $\alpha_i > 0$ are called **support vectors**: these are points which are either incorrectly classified, or are classified correctly but are on or inside the margin

- at test time we evaluate the y function as

$$\hat{y}(\mathbf{x}) = \text{sign}(f(\mathbf{x})) = \text{sign}(\hat{w}_0 + \hat{\mathbf{w}}^T \mathbf{x})$$

- once we plug in the definition of $\hat{\mathbf{w}}$ we have

$$\hat{y}(\mathbf{x}) = \text{sign}(\hat{w}_0 + \sum_{i=1}^{N} \alpha_i \mathbf{x}_i^T \mathbf{x})$$

and we can **kernelize** by replacing the inner product with the kernel function

$$\hat{y}(\mathbf{x}) = \text{sign}(\hat{w}_0 + \sum_{i=1}^{N} \alpha_i \kappa(\mathbf{x}, \mathbf{x}_i))$$

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SVM Classification

Large Margin Principle

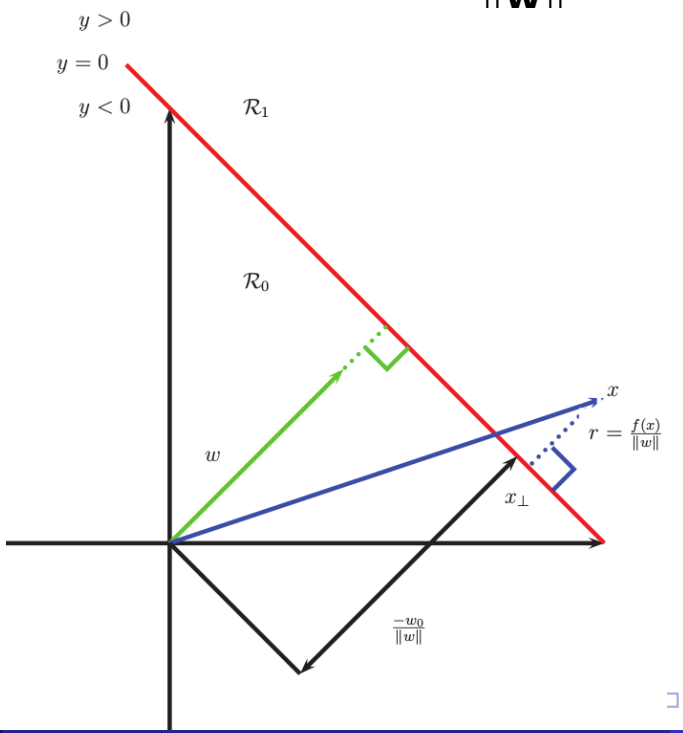
- now let's revise the previous concepts under a geometrical point of view
- $f(\mathbf{x})$ is the **discriminant function** which will be **linear** in the **feature space implied by the choice of the kernel**
- $f(\mathbf{x}) = 0$ is the **decision boundary**
- now, for simplicity, let's assume that $\mathbf{x}$ belongs to the kernel induced space $\phi(\chi)$

SVM Classification

Large Margin Principle

- for each point we have $\mathbf{x} = \mathbf{x}_\perp + r\frac{\mathbf{w}}{\|\mathbf{w}\|}$ where r is the distance of $\mathbf{x}$ from the decision boundary $f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + w_0 = 0$ (which is an hyperplane whose normal vector is $\mathbf{w}$), and $\mathbf{x}_\perp$ is the orthogonal projection of $\mathbf{x}$ onto this boundary (hence $\mathbf{w}^T\mathbf{x}_\perp + w_0 = 0$)
- if we plug the decomposition of $\mathbf{x}$ in $f(\mathbf{x})$, we have

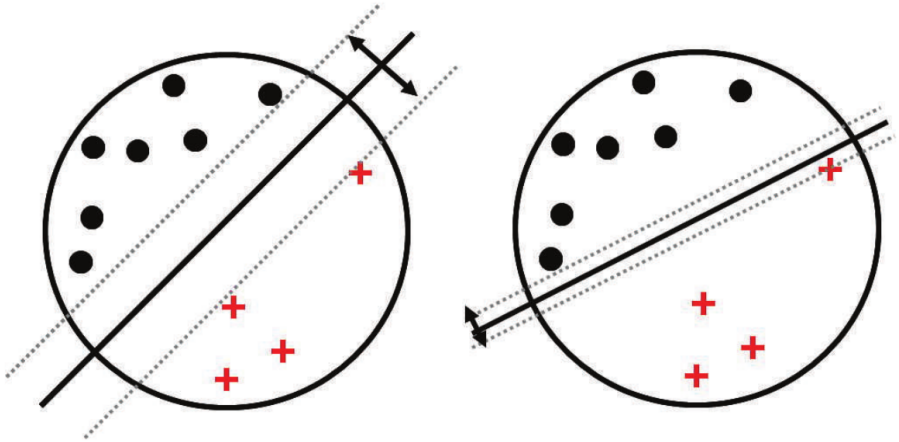
$$f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + w_0 = (\mathbf{w}^T\mathbf{x}_\perp + w_0) + r\frac{\mathbf{w}^T\mathbf{w}}{\|\mathbf{w}\|} = r\|\mathbf{w}\| \implies r = \frac{f(\mathbf{x})}{\|\mathbf{w}\|}$$



SVM Classification

Large Margin Principle

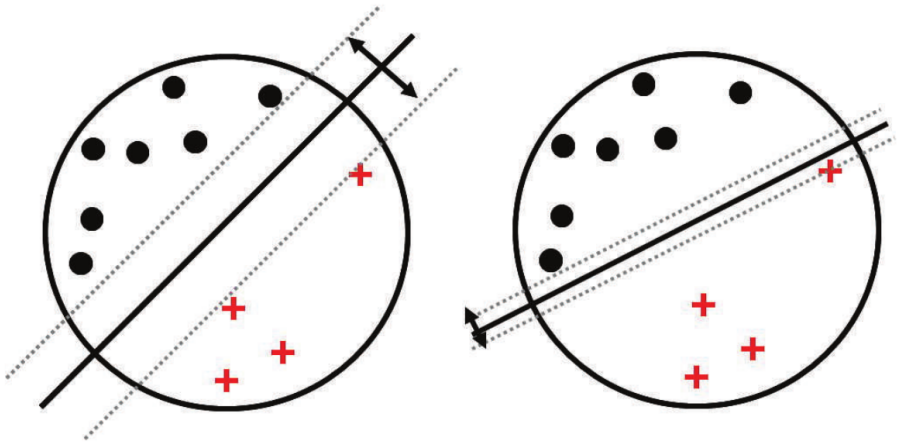
- for each point $\mathbf{x}_i$ we would like to make this perpendicular distance $r = \frac{f(\mathbf{x}_i)}{\|\mathbf{w}\|}$ as large as possible
- in particular, there might be many lines that perfectly separate the training data
- the best one to pick is the one that **maximizes the margin**, i.e., the **perpendicular distance to the closest point**
- in addition, we want to ensure each point is on the correct side of the boundary, hence we want $f(\mathbf{x}_i)y_i > 0$



- our objective becomes

$$\max_{\mathbf{w}, w_0} \min_{i=1}^{N} \frac{y_i(\mathbf{w}^T \mathbf{x}_i + w_0)}{\|\mathbf{w}\|}$$

- rescaling the parameters using $\mathbf{w} \rightarrow k\mathbf{w}$ and $w_0 \rightarrow kw_0$, we do not change the distance of any point to the boundary, since the k factor cancels out when we divide by $\|\mathbf{w}\|$



SVM Classification

Large Margin Principle

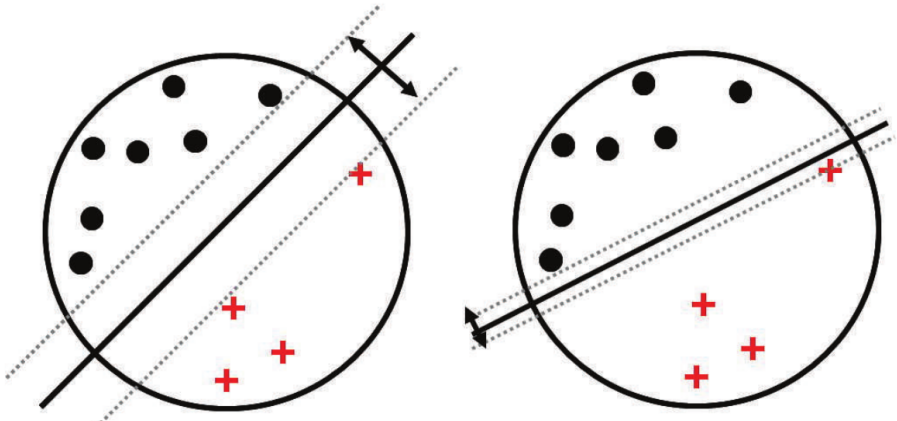
- our objective is

$$\max_{\mathbf{w},w_0} \min_{i=1}^{N} \frac{y_i(\mathbf{w}^T\mathbf{x}_i + w_0)}{\|\mathbf{w}\|}$$

- therefore let us define the scale factor such that $y_i f_i = 1$ for the point that is **closest** to the decision boundary
- note that maximizing $1/\|\mathbf{w}\|$ is equivalent to minimizing $\|\mathbf{w}\|^2$
- thus we get the new objective

$$\min_{\mathbf{w},w_0} \frac{1}{2}\|\mathbf{w}\|^2 \quad \text{s.t} \quad y_i(\mathbf{w}^T\mathbf{x}_i + w_0) \geq 1, \quad i = 1 : N$$

- the constraint says that we want all points to be on the correct side of the decision boundary with a margin of at least 1

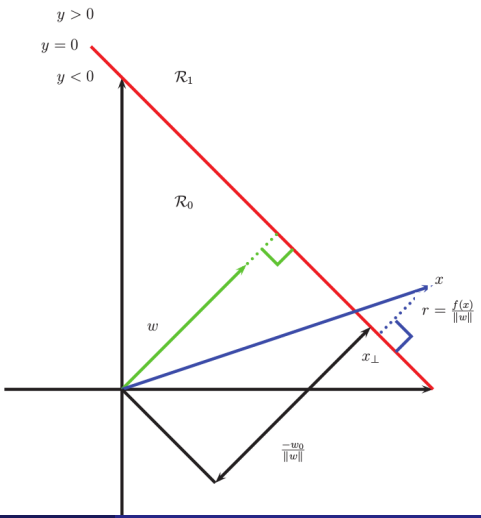


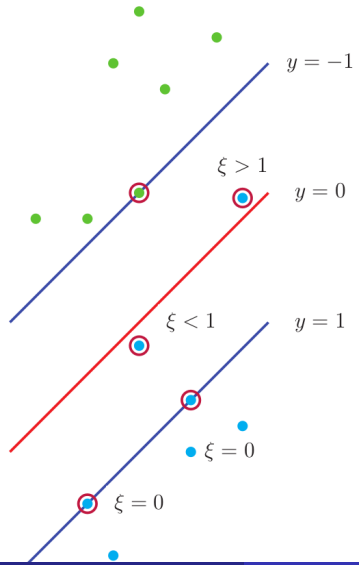
SVM Classification

Large Margin Principle

- if the data is **not linearly separable** (even after using the kernel trick), there will be no feasible solution in which $y_i f_i \geq 1$ for all i
- we therefore introduce **slack variables** $\xi \geq_i 0$ such that $\xi_i = 0$ if the point is on or inside the correct margin boundary, and $\xi_i = |y_i - f_i|$ otherwise
- we replace the **hard constraints** that $y_i f_i \geq 1$ with the **soft margin constraints** that $y_i f_i \geq 1 - \xi_i$
- the new objective becomes

$$\min_{\mathbf{w}, w_0} \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i-1}^{N} \xi_i \quad \text{s.t} \quad \xi_i \geq 0, \; y_i(\mathbf{w}^T \mathbf{x}_i + w_0) \geq 1, \quad i = 1 : N$$





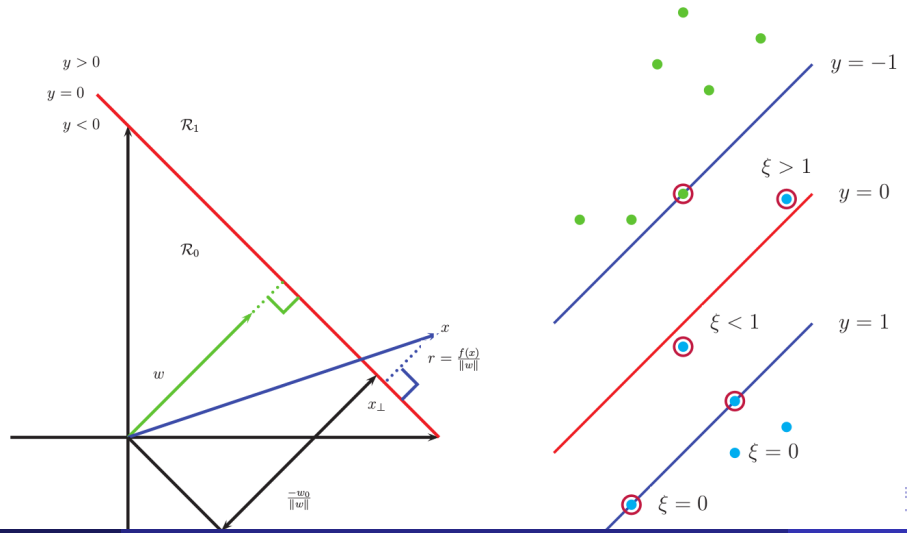
SVM Classification

Large Margin Principle

- the new objective

$$\min_{\mathbf{w},w_0} \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{N}\xi_i \quad \text{s.t} \;\; \xi_i \geq 0, \;\; y_i(\mathbf{w}^T\mathbf{x}_i + w_0) \geq 1, \quad i = 1:N$$

- since $\xi_i > 1$ means point i is misclassified, we can interpret $\sum_i \xi_i$ as an upper bound on the **number of misclassified points**
- the parameter C is a regularization parameter that controls the number of errors we are willing to tolerate on the training set
- it is common to define this using $C = 1/(\nu N)$ where $0 < \nu \leq 1$ controls the fraction of misclassified points that we allow during the training phase



Credits

- Kevin Murphy's book