COMS 4771
Support Vector Machines

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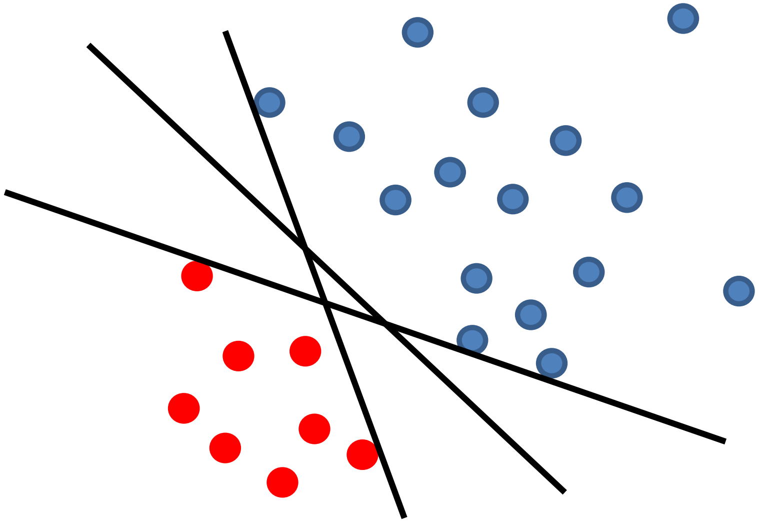
Last time...

- Decision boundaries for classification
- Linear decision boundary (linear classification)
- The Perceptron algorithm
- Mistake bound for the perceptron
- Generalizing to non-linear boundaries (via Kernel space)
- Problems become linear in Kernel space
- The Kernel trick to speed up computation

Perceptron and Linear Separablity

Say there is a **linear** decision boundary which can **perfectly separate** the training data

Which linear separator will the Perceptron algorithm return?



*The separator with a **large margin** γ is better for generalization*

How can we incorporate the margin in finding the linear boundary?

Solution: Support Vector Machines (SVMs)

Motivation:

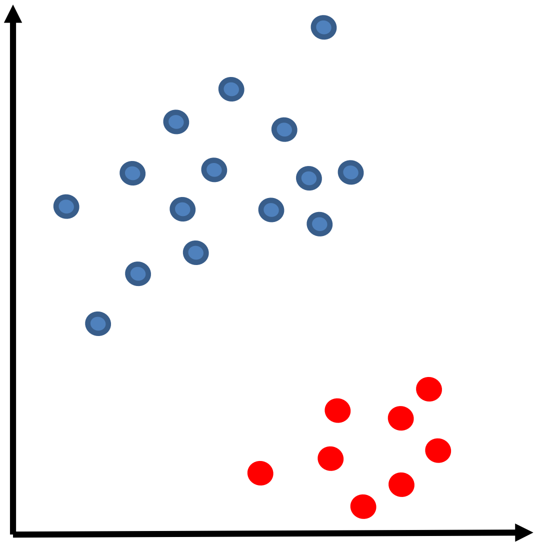
- It returns a linear classifier that is **stable** solution by giving a maximum margin solution

- Slight modification to the problem provides a way to deal with **non-separable** cases

- It is **kernelizable**, so gives an implicit way of yielding non-linear classification.

SVM Formulation

Say the training data *S* is linearly separable by some margin (but the linear separator does not necessarily passes through the origin).



Then:

decision boundary: $g(\vec{x}) = \vec{w} \cdot \vec{x} - b = 0$

Linear classifier:
$$f(\vec{x}) = \mathrm{sign}\big(g(\vec{x})\big) = \mathrm{sign}\big(\vec{w} \cdot \vec{x} - b\big)$$

*Idea: we can try finding **two** parallel hyperplanes that correctly classify all the points, and **maximize** the distance between them!*

SVM Formulation (contd. 1)

Decision boundary for the two hyperpanes:

$$\vec{w} \cdot \vec{x} - b = +1$$
$$\vec{w} \cdot \vec{x} - b = -1$$

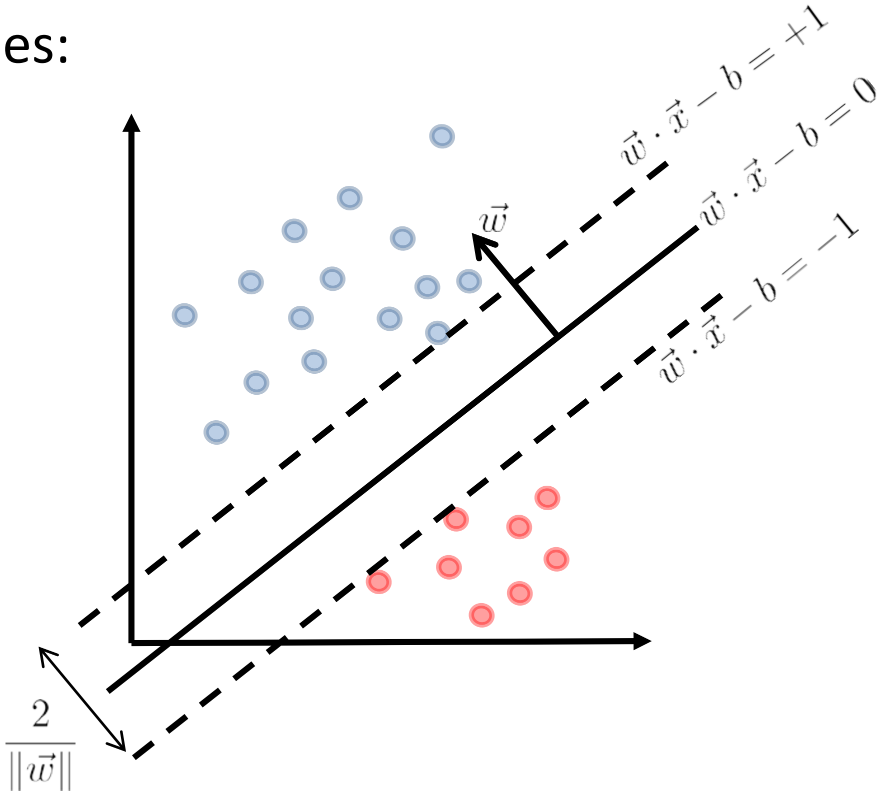
Distance between the two hyperplanes:

$$\frac{2}{||\vec{w}||}$$ *why?*

Training data is correctly classified if:

$$\vec{w} \cdot \vec{x}_i - b \geq +1 \qquad \textit{if } y_i = +1$$
$$\vec{w} \cdot \vec{x}_i - b \leq -1 \qquad \textit{if } y_i = -1$$

Together: $y_i(\vec{w} \cdot \vec{x}_i - b) \geq +1$ for all *i*



SVM Formulation (contd. 2)

Distance between the hyperplanes: $\dfrac{2}{\|\vec{w}\|}$

Training data is correctly classified if:

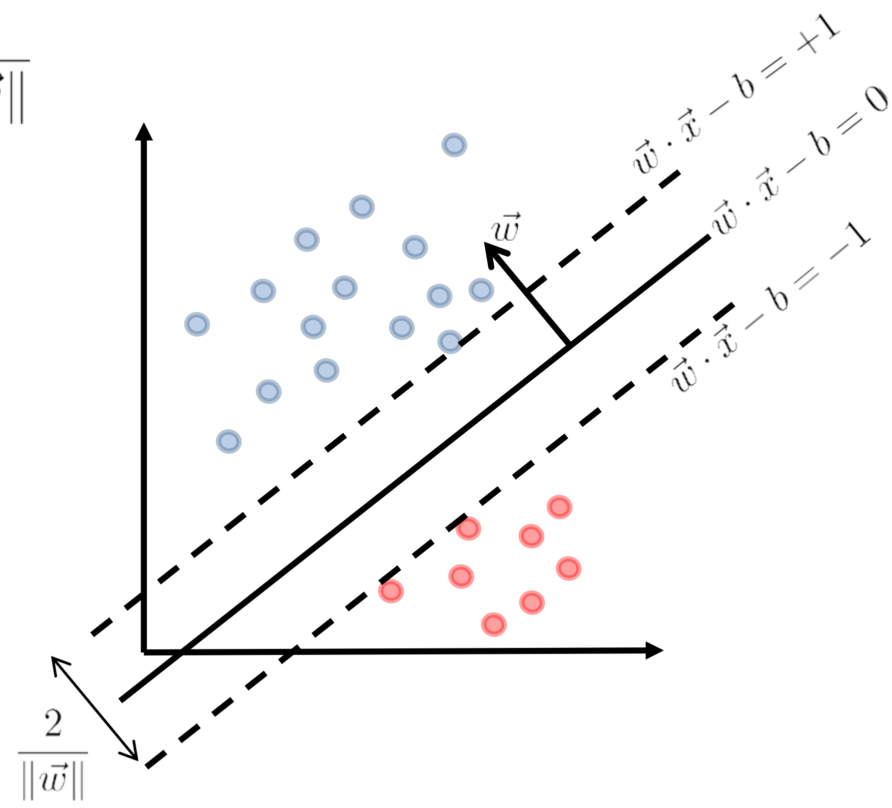
$$y_i(\vec{w} \cdot \vec{x}_i - b) \geq +1 \qquad \textit{(for all i)}$$

Therefore, want:

Maximize the distance: $\dfrac{2}{\|\vec{w}\|}$

Such that: $y_i(\vec{w} \cdot \vec{x}_i - b) \geq +1$

(for all i)



Let's put it in the standard form…

SVM Formulation (finally!)

Maximize: $\frac{2}{\|\vec{w}\|}$

Such that: $y_i(\vec{w} \cdot \vec{x}_i - b) \geq +1$

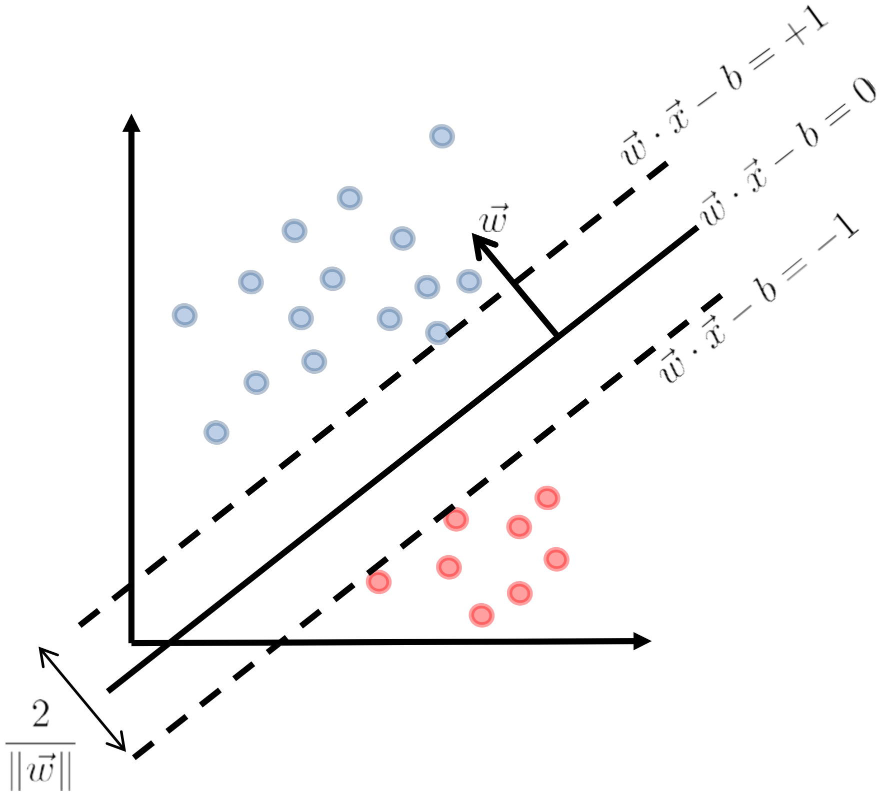
(for all i)

SVM standard (primal) form:

Minimize: $\frac{1}{2}\|\vec{w}\|^2$

Such that: $y_i(\vec{w} \cdot \vec{x}_i - b) \geq +1$

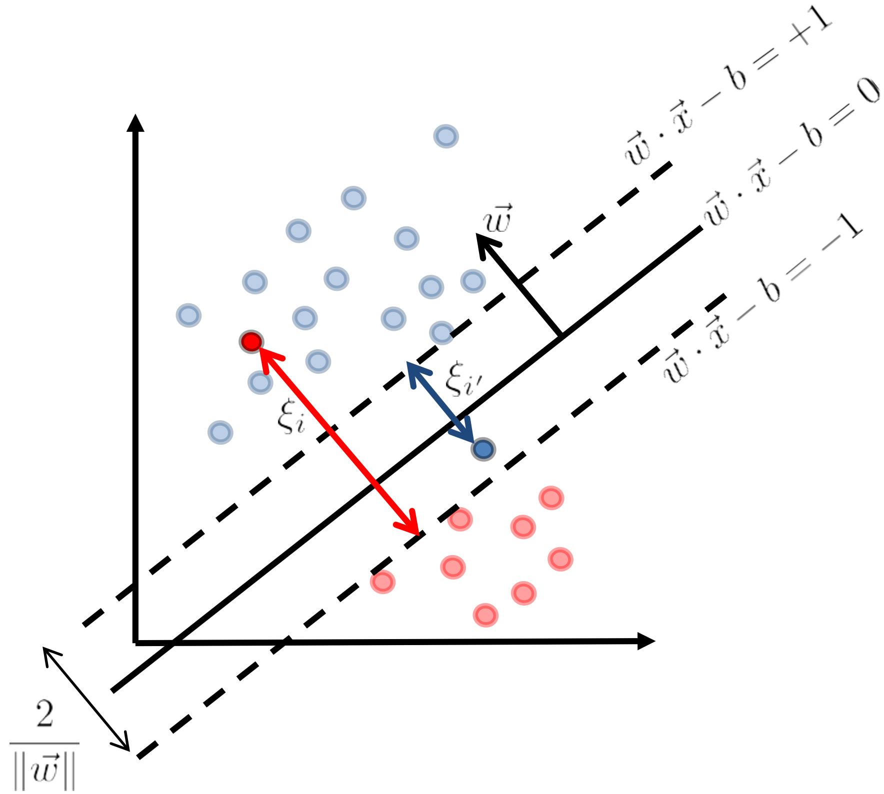
(for all i)



What can we do if the problem is not-linearly separable?

SVM Formulation (non-separable case)

*Idea: introduce a **slack** for the mis-classified points, and **minimize** the slack!*



SVM standard (primal) form (with slack):

Minimize: $\frac{1}{2}\|\vec{w}\|^2 \; + \; C\sum_{i=1}^{n}\xi_i$

Such that: $y_i(\vec{w}\cdot\vec{x}_i - b) \geq 1 - \xi_i$

(for all i)

$\xi_i \geq 0$

SVM: Question

SVM standard (primal) form (with slack):

Minimize: $$\frac{1}{2}\|\vec{w}\|^2 + C\sum_{i=1}^{n}\xi_i$$

Such that: $$y_i(\vec{w}\cdot\vec{x}_i - b) \geq 1 - \xi_i$$

(for all i)

$$\xi_i \geq 0$$

Questions:

1. *How do we find the optimal w, b and ξ?*
2. *Why is it called "Support Vector Machine"?*

How to Find the Solution?

SVM standard (primal) form:

Minimize: $\frac{1}{2}\|\vec{w}\|^2 + C\sum_{i=1}^{n}\xi_i$

Such that: $y_i(\vec{w}\cdot\vec{x}_i - b) \geq 1 - \xi_i$

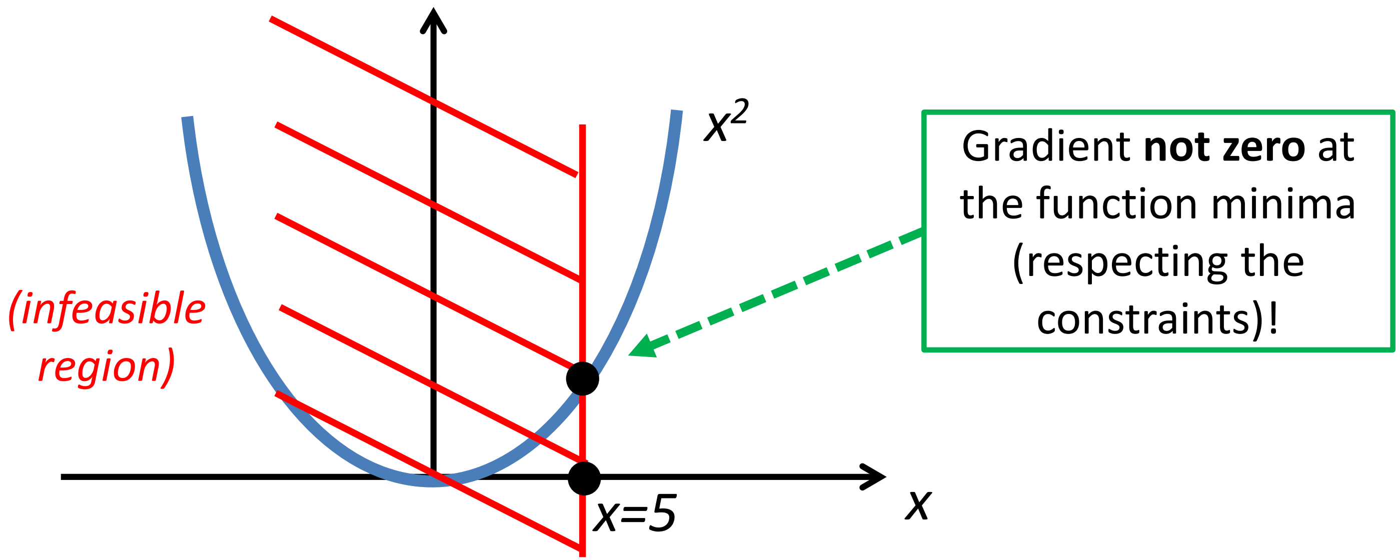
(for all i) $\xi_i \geq 0$

Cannot simply take the derivative (wrt *w*, *b* and ξ) and examine the stationary points…

Why?

Minimize: x^2

Such that: $x \geq 5$



Need a way to do optimization with constraints

Detour: Constrained Optimization

Constrained optimization (standard form):

$$\underset{\vec{x} \in \mathbf{R}^d}{\text{minimize}} \quad f(\vec{x}) \qquad \textit{(objective)}$$

$$\text{subject to:} \quad g_i(\vec{x}) \leq 0 \quad \text{for } 1 \leq i \leq n \qquad \textit{(constraints)}$$

What to do?

We'll assume that the problem is feasible

- Projection methods

  start with a feasible solution x_0,

  find x_1 that has slightly lower objective value,

  if x_1 violates the constraints, **project back** to the constraints.

  iterate.

- Penalty methods

  use a **penalty function** to incorporate the constraints into the objective

- …

The Lagrange (Penalty) Method

Optimization problem:

Minimize: $f(\vec{x})$

Such that: $g_i(\vec{x}) \leq 0$
(for all i)

Consider the augmented function:

$$L(\vec{x}, \vec{\lambda}) \quad := \quad f(\vec{x}) + \sum_{i=1}^{n} \lambda_i g(\vec{x})$$

(Lagrange function)

(Lagrange variables, or dual variables)

Observation:

For ***any*** feasible *x* and ***all*** $\lambda_i \geq 0$, we have $L(\vec{x}, \vec{\lambda}) \leq f(\vec{x})$

$$\implies \max_{\lambda_i \geq 0} L(\vec{x}, \vec{\lambda}) \leq f(\vec{x})$$

So, the optimal value to the constrained optimization:

$$p^* := \min_{\vec{x}} \max_{\lambda_i \geq 0} L(\vec{x}, \vec{\lambda})$$

The problem becomes unconstrained in x!

The Dual Problem

Optimal value: $p^* = \min_{\vec{x}} \max_{\lambda_i \geq 0} L(\vec{x}, \vec{\lambda})$

(also called the primal)

Now, consider the function: $\min_{\vec{x}} L(\vec{x}, \vec{\lambda})$

Observation:

Since, for ***any*** feasible *x* and ***all*** $\lambda_i \geq 0$:

$$p^* \geq \min_{\vec{x}} L(\vec{x}, \vec{\lambda})$$

Thus:

$$\boxed{d^* := \max_{\lambda_i \geq 0} \min_{\vec{x}'} L(\vec{x}', \vec{\lambda})} \leq p^*$$

(also called the dual)

Optimization problem:

Minimize: $f(\vec{x})$

Such that: $g_i(\vec{x}) \leq 0$
(for all i)

Lagrange function:

$$L(\vec{x}, \vec{\lambda}) := f(\vec{x}) + \sum_{i=1}^{n} \lambda_i g_i(\vec{x})$$

(Weak) Duality Theorem

Theorem (weak Lagrangian duality):

$$d^* \leq p^*$$

(also called the minimax inequality)

$p^* - d^*$ *(called the duality gap)*

Under what conditions can we achieve equality?

Optimization problem:

Minimize:	$f(\vec{x})$
Such that: *(for all i)*	$g_i(\vec{x}) \leq 0$

Lagrange function:

$$L(\vec{x}, \vec{\lambda}) := f(\vec{x}) + \sum_{i=1}^{n} \lambda_i g_i(\vec{x})$$

Primal:

$$p^* = \min_{\vec{x}} \max_{\lambda_i \geq 0} L(\vec{x}, \vec{\lambda})$$

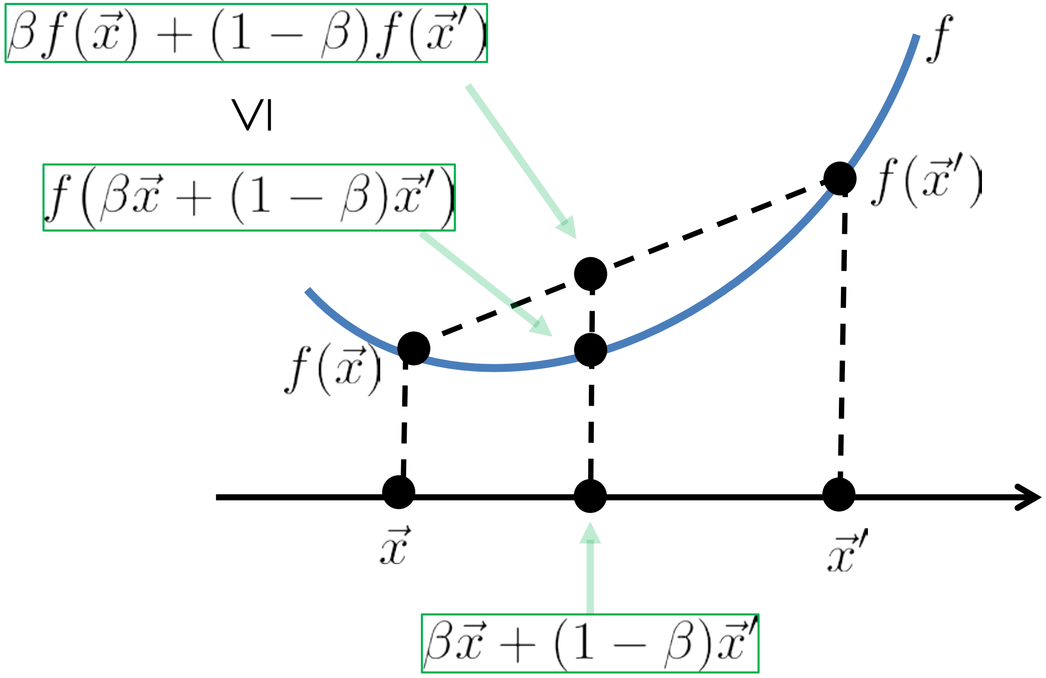
Dual:

$$d^* := \max_{\lambda_i \geq 0} \min_{\vec{x}} L(\vec{x}, \vec{\lambda})$$

Convexity

A function f: $\mathbf{R}^d \rightarrow \mathbf{R}$ is called convex iff for any two points x, x' and $\beta \in [0,1]$

$$f\left(\beta\vec{x} + (1-\beta)\vec{x}'\right) \leq \beta f(\vec{x}) + (1-\beta) f(\vec{x}')$$

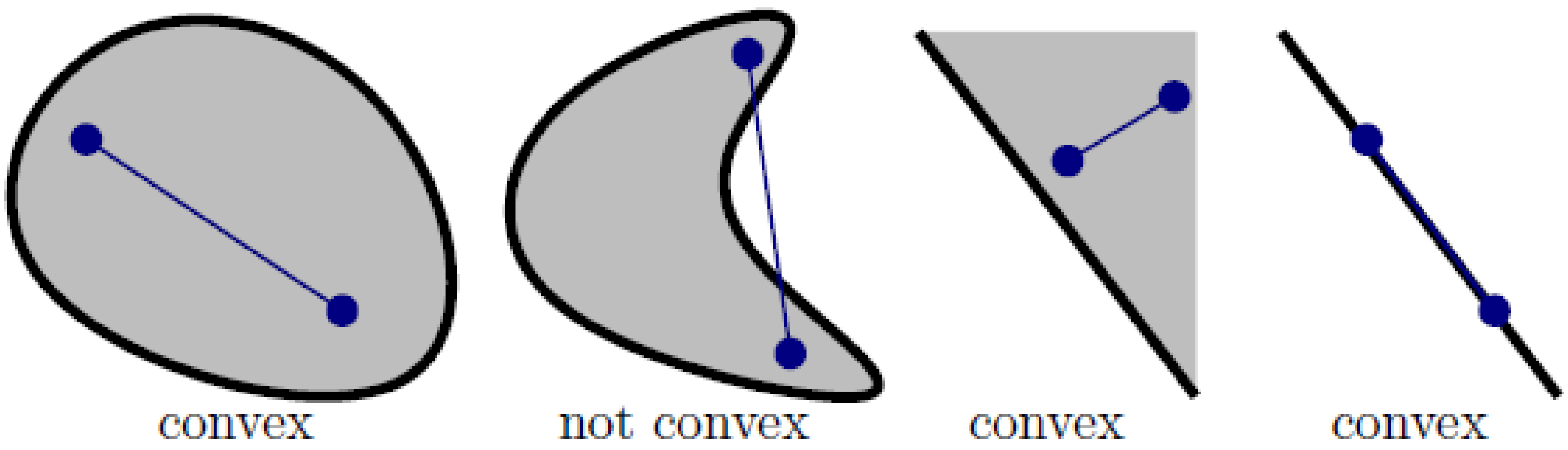


Convexity

A set S $\subset \mathbf{R}^d$ is called convex iff for any two points *x*, *x'* $\in$ S and any $\beta \in [0,1]$

$$\beta\vec{x} + (1-\beta)\vec{x}' \in S$$

Examples:



Convex Optimization

A constrained optimization

$\underset{\vec{x} \in \mathbf{R}^d}{\text{minimize}}$	$f(\vec{x})$		*(objective)*
subject to:	$g_i(\vec{x}) \leq 0$	for $1 \leq i \leq n$	*(constraints)*

is called convex a convex optimization problem

If:

the objective function $f(\vec{x})$ is convex function, and

the feasible set induced by the constraints g_i is a convex set

Why do we care?

*We and find the optimal solution for convex problems **efficiently**!*

Convex Optimization: Niceties

- Every local optima is a **global optima** in a convex optimization problem.

  Example convex problems:

  Linear programs, quadratic programs,

  Conic programs, semi-definite program.

  Several **solvers exist** to find the optima:

  CVX, SeDuMi, C-SALSA, …

- We can use a **simple** ‘descend-type’ algorithm for finding the minima!

Gradient Descent (for finding local minima)

Theorem (Gradient Descent):

Given a smooth function $f : \mathbf{R}^d \to \mathbf{R}$

Then, for any $\vec{x} \in \mathbf{R}^d$ and $\vec{x}' := \vec{x} - \eta \nabla_x f(\vec{x})$

For sufficiently small $\eta > 0$, we have: $f(\vec{x}') \leq f(\vec{x})$

Can derive a **simple algorithm** (the projected Gradient Descent):

Initialize $\vec{x}^0$

for t = 1,2,…do

$\vec{x}'^t := \vec{x}^{t-1} - \eta \nabla_x f(\vec{x}^{t-1})$ *(step in the gradient direction)*

$\vec{x}^t := \Pi_{g_i}(\vec{x}'^t)$ *(project back onto the constraints)*

terminate when no progress can be made, ie, $|f(\vec{x}^t) - f(\vec{x}^{t-1})| \leq \epsilon$

Back to Constrained Opt.: Duality Theorems

Theorem (weak Lagrangian duality):

$$d^* \leq p^*$$

Theorem (strong Lagrangian duality):

If *f* is convex and for a feasible point *x**

$g_i(\vec{x}^*) < 0$, or

$g_i(\vec{x}^*) \leq 0$ when *g* is affine

Then $d^* = p^*$

Optimization problem:

Minimize: $f(\vec{x})$

Such that: $g_i(\vec{x}) \leq 0$

(for all i)

Lagrange function:

$$L(\vec{x}, \vec{\lambda}) := f(\vec{x}) + \sum_{i=1}^{n} \lambda_i g_i(\vec{x})$$

Primal:

$$p^* = \min_{\vec{x}} \max_{\lambda_i \geq 0} L(\vec{x}, \vec{\lambda})$$

Dual:

$$d^* := \max_{\lambda_i \geq 0} \min_{\vec{x}} L(\vec{x}, \vec{\lambda})$$

Ok, Back to SVMs

Observations:

- object function is convex
- the constraints are affine, inducing a polytope constraint set.

So, SVM is a convex optimization problem (in fact a **quadratic program**)

Moreover, **strong duality holds**.

Let's examine the dual… the Lagrangian is:

$$L(\vec{w}, b, \vec{\alpha}) = \frac{1}{2}\|\vec{w}\|^2 + \sum_{i=1}^{n} \alpha_i \big(1 - y_i(\vec{w} \cdot \vec{x}_i - b)\big)$$

SVM standard (primal) form:

Minimize: $\frac{1}{2}\|\vec{w}\|^2$
(w,b)

Such that: $y_i(\vec{w} \cdot \vec{x}_i - b) \geq 1$
(for all i)

SVM Dual

Lagrangian:

$$L(\vec{w}, b, \vec{\alpha}) = \frac{1}{2}\|\vec{w}\|^2 + \sum_{i=1}^{n} \alpha_i \left(1 - y_i(\vec{w}\cdot\vec{x}_i - b)\right)$$

Primal: $p^* = \min_{\vec{w},b} \max_{\alpha_i \geq 0} L(\vec{w}, b, \vec{\alpha})$

Dual: $d^* = \max_{\alpha_i \geq 0} \min_{\vec{w},b} L(\vec{w}, b, \vec{\alpha})$

Unconstrained, let's calculate

SVM standard (primal) form:

Minimize: *(w,b)*	$\frac{1}{2}\|\vec{w}\|^2$
Such that: *(for all i)*	$y_i(\vec{w}\cdot\vec{x}_i - b) \geq 1$

$$\frac{\partial}{\partial \vec{w}} L(\vec{w}, b, \vec{\alpha}) = \vec{w} - \sum_{i=1}^{n} \alpha_i y_i \vec{x}_i \qquad \Longrightarrow \qquad \vec{w} = \sum_{i=1}^{n} \alpha_i y_i \vec{x}_i$$

- *when $\alpha_i > 0$, the corresponding x_i is the support vector*
- *w is only a function of the support vectors!*

$$\frac{\partial}{\partial b} L(\vec{w}, b, \vec{\alpha}) = \sum_{i=1}^{n} \alpha_i y_i \qquad \Longrightarrow \qquad \sum_{i=1}^{n} \alpha_i y_i = 0$$

SVM Dual (contd.)

Lagrangian:

$$L(\vec{w}, b, \vec{\alpha}) = \frac{1}{2}\|\vec{w}\|^2 + \sum_{i=1}^{n} \alpha_i \left(1 - y_i(\vec{w} \cdot \vec{x}_i - b)\right)$$

Primal: $p^* = \min_{\vec{w}, b} \max_{\alpha_i \geq 0} L(\vec{w}, b, \vec{\alpha})$

Dual: $d^* = \max_{\alpha_i \geq 0} \min_{\vec{w}, b} L(\vec{w}, b, \vec{\alpha})$

Unconstrained, let's calculate

$$\min_{\vec{w}, b} L(\vec{w}, b, \vec{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j (x_i \cdot x_j)$$

So:

$$d^* = \max_{\alpha_i \geq 0} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j (x_i \cdot x_j)$$

subject to $\sum_{i=1}^{n} \alpha_i y_i = 0$

SVM standard (primal) form:

Minimize: $\frac{1}{2}\|\vec{w}\|^2$
(w,b)

Such that: $y_i(\vec{w} \cdot \vec{x}_i - b) \geq 1$
(for all i)

SVM Optimization Interpretation

SVM standard (primal) form:

Minimize: $\frac{1}{2}\|\vec{w}\|^2$
(w,b)

Such that: $y_i(\vec{w} \cdot \vec{x}_i - b) \geq 1$
(for all i)

Maximize γ = 2/||w||

SVM standard (dual) form:

Maximize: $\sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j (x_i \cdot x_j)$
(α_i)

Such that: $\sum_{i=1}^{n} \alpha_i y_i = 0 \qquad \alpha_i \geq 0$
(for all i)

Kernelized version

Only a function of "support vectors"

What We Learned…

- Support Vector Machines
- Maximum Margin formulation
- Constrained Optimization
- Lagrange Duality Theory
- Convex Optimization
- SVM dual and Interpretation
- How get the optimal solution

Questions?

Next time…

Parametric and non-parametric Regression