

# An Introduction to Optimization with Application to Machine Learning

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#### Motivation: Machine Learning

Linear Regression

minimize 
$$\sum_{i=1}^{n} ||w^{t}x_{i} + b - y_{i}||^{2}$$

SVM

$$\begin{aligned} & \underset{w,b}{\text{minimize}} & & \|w\|^2 + C \sum_{i=1}^n \varepsilon_i \\ & subject \ to & \ y_i(w^T x_i + b) \geq 1 - \varepsilon_i \ i = 1, \dots n \\ & \ \varepsilon_i \geq 0 \ i = 1, \dots, n \end{aligned}$$

PGDM metric learning

minimize 
$$\sum_{(x_i, x_j) \in S} ||x_i - x_j||_P$$
  
subject to  $\sum_{(x_i, x_j) \in D} ||x_i - x_j||_P \ge 1$   
 $P \ge 0$ 

#### Optimization Problem

```
minimize f_0(x)

subject to f_i(x) \le 0 i = 1, ..., m

h_i(x) = 0 i = 1, ..., p
```

- $x \in \mathbb{R}^n$  is the variable to find
- $f_0: \mathbb{R}^n \to \mathbb{R}$  is called the objective (cost or utility) function
- $f_i: \mathbb{R}^n \to \mathbb{R}, i = 1, ... m$  are the inequality constraints (defines a set)
- $h_i: \mathbb{R}^n \to \mathbb{R}, i = 1, ... p$  are the equality constraints (defines a set)
- Solution:  $p^* = \inf\{f_0(x)|f_i(x) \le 0 \ i = 1, ... m, h_i(x) = 0 \ i = 1, ..., p\}$
- Constrained vs. unconstrained problems: whether you have the constrains or not.
- A feasible point x is optimal if  $f_0(x) = p^*$ ;  $X_{OPT}$  is the set of optimal points.

#### Feasibility

- An optimization problem is feasible
  - if  $x \in dom f_0$  (implicit constraints) and it satisfies all the (explicit) constraints  $f_i(x) \le 0$  i = 1, ..., m &  $h_i(x) = 0$  i = 1, ..., p.
- For infeasible problems, we say  $p^* = +\infty$
- Feasibility problem

find 
$$x$$
  
subject to  $f_i(x) \le 0$   $i = 1, ..., m$   
 $h_i(x) = 0$   $i = 1, ..., p$ 

Equivalent to the following optimization problem

minimize 0  
subject to 
$$f_i(x) \le 0$$
  $i = 1, ..., m$   
 $h_i(x) = 0$   $i = 1, ..., p$ 

## Locally Optimal Points

For the following problem

minimize 
$$f_0(x)$$
  
 $s.t.$   $f_i(x) \le 0$   $i = 1, ..., m$   
 $h_i(x) = 0$   $i = 1, ..., p$ 

x is locally optimum if there is an R > 0 such that x is optimal for the following problem

minimize 
$$f_0(z)$$
  
 $s.t. \ f_i(z) \le 0 \ i = 1, ... m$   
 $h_i(z) = 0 \ i = 1, ..., p$   
 $\|z - x\|_2 \le R$ 

#### Regularization

- A form of limiting the feasible search space of an optimization problem
- Can be considered as the prior information that the solution is located in the neighborhood of point x

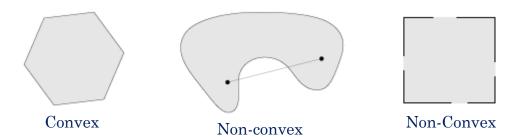
- $\blacktriangleright$  Leads to sparse solution for x =0 and small p
- I will get back to this.

#### Convexity

- ▶ An optimization problem is convex if
  - $f_0: \mathbb{R}^n \to \mathbb{R}$  is a convex function
  - Constrains  $f_i(x) \le 0$   $i = 1, ..., m \& h_i(x) = 0$  i = 1, ..., p are convex sets.
  - $f_0: \mathbb{R}^n \to \mathbb{R}, f_i: \mathbb{R}^n \to \mathbb{R}, i = 1, ..., m, h_i: \mathbb{R}^n \to \mathbb{R}, i = 1, ..., p \text{ can be linear or nonlinear}$
- Importance
  - Any local optimum is a global optimum
  - Local optimality can be verified. No general tractable global optimum test
  - So, for convex problems, it is easy to check if a point is a global optimum.
- Feasible set of a convex optimization problem is convex.
- Convex set and convex function??

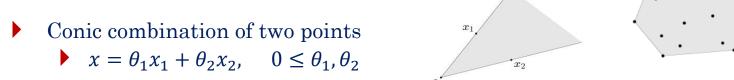
#### Affine and Convex Sets

- Affine sets: the line through any two disjoint points
  - $x = \theta x_1 + (1 \theta) x_2, \quad \theta \in \mathbb{R}$
  - Or equivalently, solution set of linear equation  $\{x | Ax = b\}$
- Line segment: line segment between two points
  - $x = \theta x_1 + (1 \theta) x_2, \quad 0 \le \theta \le 1$
- Convex Sets: a set that contains the line segment of any two points of the set
  - $x_1, x_2 \in S, 0 \le \theta \le 1 \implies \theta x_1 + (1 \theta)x_2 \in S$

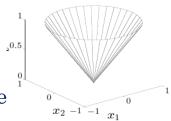


## Convex Sets (examples)

- Convex hull of set  $S = \{x_1, x_2, ..., x_k\}$ : Set of all convex combinations of points in S



- Convex cone of set S: a set that contains all conic combinations of points in S
- $\qquad \qquad \text{Hyperplanes } (a^T x + b = 0, \text{ linear equality})$
- ► Halfspaces  $(a^T x + b \le 0$ , linear inequality)
- Euclidean balls and Ellipsoids:  $\{x | (x x_c)^T P^{-1} (x x_c) \le 1\}$  ( $P \in S^n_{++}$ , i.e. P is positive-definite P)
- Norm ball:  $\{x | ||x x_c|| \le r\}$
- Norm cone:  $C = \{(x, t) | ||x|| \le t\} \in \mathbb{R}^{n+1}$ 
  - Euclidean norm cone ( $||x||_2$ ) is called second order cone

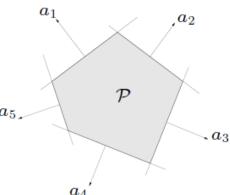


#### Operations that preserve convexity

- Intersection of convex sets
- ▶ The image of a convex set under affine (linear) function
  - $F: \mathbb{R}^n \to \mathbb{R}^m: F(x)=Ax+b$
  - scaling (aS), translation(S+a), projection
- Perspective function
  - $F: \mathbb{R}^{n+1} \to \mathbb{R}^n: F(x,t)=x/t, \quad \text{dom}(F)=\{(x,t) \mid t>0\}$
  - Image and inverse image of convex sets under perspective are convex
- ▶ Linear-fractional functions:
  - $F: \mathbb{R}^n \to \mathbb{R}^m: F(\mathbf{x}, \mathbf{t}) = \frac{Ax + b}{c^T x + d}, \quad \text{dom}(F) = \{\mathbf{x} \mid c^T x + d > 0\}$
  - ▶ Image and inverse image of convex sets under linearfractional functions are convex

#### Convexity preserving operations (cont.)

- Intersection of convex sets is convex.
- Polyhedra is convex
  - Intersection of finite number of halfspaces and hyperplanes



- Positive semidefinite (PSD) cone: Set of all PSD matrices is convex
  - Intersection of infinite number of halfspaces and hyperspaces passing through origin  $(\bigcap_{z\neq 0} \{X \in S^n \mid z^T X z \geq 0\})$
  - We denote it by  $S^n_+$

#### Generalized Inequalities

- Definition: A cone  $K \subseteq \mathbb{R}^n$  is a proper cone if
  - K is convex
  - K is closed
  - K is solid: it has nonempty interior
  - K is pointed: it contains no line
- Generalized inequalities: defined by a proper cone K, is a partial ordering

$$x \leq_K y \iff y - x \in K$$
  
 $x <_K y \iff y - x \in int \ K \ (interior \ of \ K)$ 

- Examples
  - Componentwise inequality:

$$x \prec_{R_+} n y \iff y_i \ge x_i$$

Matrix inequality

$$X \prec_{S_+}^n Y \iff Y - X \text{ is PSD}$$

#### **Dual Cones**

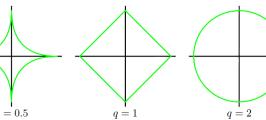
- Dual cone of a cone K:  $K^* = \{y \mid y^T x \ge 0 \text{ for all } x \in K\}$   $x \le_K y \iff y - x \in K$  $x <_K y \iff y - x \in int K \text{ (interior of } K\text{)}$
- Examples
  - $K = R_{+}^{n}$ :  $K^* = R_{+}^{n}$
  - $K = S_{+}^{n}$ :  $K^* = S_{+}^{n}$ ,  $(tr(XY) \ge 0)$
  - $K = \{(x,t) \mid ||x||_2 \le t\}: K^* = \{(x,t) \mid ||x||_2 \le t\}$
  - $K = \{(x,t) \mid ||x||_1 \le t\} : K^* = \{(x,t) \mid ||x||_\infty \le t\}$

#### **Convex Functions**

Definition: function f(x):  $\mathbb{R}^n \to \mathbb{R}$  is convex if the graph of the function lies between the line segment joining any two points of the graph.



- Formally: f(x):  $\mathbb{R}^n \to \mathbb{R}$  is convex if dom(f) is convex and  $f(\theta x + (1 \theta)y) \le \theta f(x) + (1 \theta)f(y)$
- $\blacktriangleright$  Examples in  $\mathbb{R}$ :
  - affine, exponential, powers  $(x^{\alpha}, \alpha \leq 0 \text{ or } \alpha \geq 1)$ , power of absolute value  $(|x|^{\alpha}, \alpha \geq 1)$
- Example on  $\mathbb{R}^n$ 
  - Norm $||x||_{\alpha} = (\sum_{i=1}^{n} |x_i|^{\alpha})^{1/\alpha}, \alpha \ge 1$
- Example on  $\mathbb{R}^{n \times m}$ 
  - Affine function  $\operatorname{tr}(A^TX) + b = \sum_{i=1}^m \sum_{j=1}^n A_{ij} X_{ij} + b$



## Convex Functions (verification tricks)

*f*(*x*):  $R^n$  → R is convex if and only if the following function of one variable is convex in t for any  $x \in dom(f) \& v \in \mathbb{R}^n$ :

$$g(t): R \to R: g(t) = f(x + tv), \operatorname{dom}(g) = \{t \mid x + tv \in \operatorname{dom}(f)\}\$$

First order condition: Differentiable f with convex domain is convex if and only if

$$f(y) \ge f(x) + \nabla f(x)^T (y - x)$$

 $f(x) + \nabla f(x)^{T} (y - x)$ 

Second order condition: twice differentiable function f with convex domain is convex if and only if

$$\nabla^2 f(x) \ge 0$$
 for all  $x \in dom(f)$ 

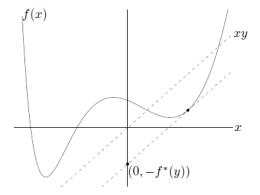
Example: quadratic function  $1/2x^TPx + q^Tx + r$  is convex if P is PSD

#### Operations that preserve convexity:

- Nonnegative weighted sum
  - $\sum_{i=1}^{n} \alpha_i f_i(x)$  is convex if  $f_i(x)$ , i = 1,2,...n are convex Jensen's inequality:  $f(\mathbb{E}(x)) \leq \mathbb{E}f(x)$
- Composition with affine function
  - f(Ax + b) is convex if f(x) is convex
  - Examples:  $f(x) = -\sum_{i=1}^{n} \log(b_i a_i^T x)$
- **Minimization** 
  - $g(x) = \min_{y \in C} f(x, y)$  is convex if f(x, y) is convex in (x, y) and C is a convex set
  - Examples:  $dist(x, S) = \min_{y \in S} ||x y||$  is convex if S is convex
- Perspective  $g(x,t) = tf\left(\frac{x}{t}\right), t > 0$ 
  - Example:  $g(x,t) = \frac{x^T x}{t}, t > 0$
- Pointwise maximum and suprimum

  - Piecewise linear function:  $f(x) = \max_{i=1,\dots,n} a_i^T x + b_i$   $g(x) = \sup_{x \in A} f(x,y)$  is convex if f(x,y) is convex in x for each  $y \in A$
  - Example: max eigenvalue of a symmetric function  $\lambda_{max}(X) = \sup_{\|y\|=1} y^T X y$

## Conjugate function:



The conjugate function of f is defined as

$$f^*(y) = \sup_{x \in dom(f)} (y^T x - f(x))$$

- The conjugate function of  $f^*$  is the max cap between the linear function  $y^Tx$  and f(x). For differentiable functions, this occurs at a point x where  $y = \nabla f(x)$
- $f^*$  is convex even if f is not. Because it is a pointwise suprimum of a family of affine functions
- Also known as Lengendre-Fenchel Transformation or Fenchel Transformation
- Examples
  - $f(x) = -\log(x) \to f^*(y) = -1 \log(-y), y < 0$
  - $f(x) = \exp(x) \to f^*(y) = y\log(y) y, y > 0$
  - $f(x) = x\log(x) \to f^*(y) = \exp(y-1), y \neq 0$
  - $f(x) = 1/x \rightarrow f^*(y) = -2(-y)^{1/2}, y \le 0$

#### Slack variables

Converting inequality constraints to equality constrains

minimize 
$$f_0(x)$$
  $\rightarrow$  minimize  $f_0(x)$   
 $s.t.$   $f_i(x) \le 0$   $i = 1, ... m$   $s.t.$   $f_i(x) + b_i = 0$   $i = 1, ... m$   
 $b_i \ge 0$   $i = 1, ... m$ 

Introducing equality constraints

minimize 
$$f_0(A_0x + b_0)$$
  $\rightarrow$  minimize  $f_0(y_0)$   
 $s.t.$   $f_i(A_ix + b_i) \le 0$   $i = 1, ... m$   $s.t.$   $f_i(y_i) \le 0$   $i = 1, ... m$   
 $A_ix + b_i = y_i$   $i = 0, ... m$ 

Converting an infeasible problem to feasible by relaxing the constraints

minimize 
$$f_0(x)$$
  $\rightarrow$  minimize  $f_0(x) + C \sum_{i=1}^m b_i$   
 $s.t.$   $f_i(x) \le 0$   $i = 1, ... m$   $s.t.$   $f_i(x) - b_i \le 0$   $i = 1, ... m$   
 $b_i \ge 0$   $i = 1, ... m$ 

## Duality

The following optimization problem

minimize 
$$f_0(x)$$
  
subject to  $f_i(x) \le 0$   $i = 1, ..., m$   
 $h_i(x) = 0$   $i = 1, ..., p$ 

Can be written in the Lagrangian form

$$L(x, \lambda, \nu) = f_0(x) + \sum_{i=1}^{m} \lambda_i f_i(x) + \sum_{i=1}^{p} \nu_i h_i(x)$$

- $\lambda_i$ , i=1,...,m are called the Lagrange multipliers associated with the inequalities and  $\nu_i$ , i=1,...,m are called the Lagrange multipliers associated with the equalities. They are also called the dual variables.
- ▶ The Lagrange dual function is defined as

$$g(\lambda, \nu) = \inf_{x} L(x, \lambda, \nu) = \inf_{x} f_0(x) + \sum_{i=1}^{m} \lambda_i f_i(x) + \sum_{i=1}^{p} \nu_i h_i(x)$$

- $\mathbf{g}(\lambda, \nu)$  is the lower bound for the optimal value of original problem
  - $g(\lambda, \nu) \leq P^*$

#### The dual problem

The following optimization problem is called the dual problem (original problem is called primal)

maximize 
$$g(\lambda, \nu)$$
  
subject to  $\lambda \ge 0$ 

- Finds the best lower bound on  $p^*$ 
  - A convex optimization problem with optimal value denoted by  $d^*$
  - L( $\lambda$ ,  $\nu$ ) is concave since it is pointwise infimum of a family of affine functions

$$g(\lambda, \nu) = \inf_{x} L(x, \lambda, \nu) = \inf_{x} f_0(x) + \sum_{i=1}^{m} \lambda_i f_i(x) + \sum_{i=1}^{p} \nu_i h_i(x)$$

▶ This automatically gives a procedure to optimize the non-convex problems.

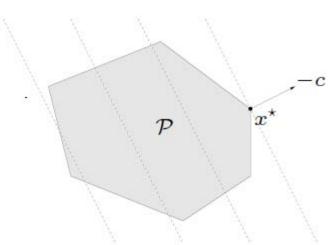
#### Solving dual problems

- Solve the dual problem which is convex
- Question: how good it is?
  - ▶ The duality gap  $p^* d^*$  is a measure of how good it is
  - Not usually easy to show that the gap is small
- Strong duality  $p^* d^* = 0$ 
  - Usually (but not always) holds for convex problems
  - Non-convex problem can have strong duality as well so you can get lucky if you use the dual
- If the strong duality holds and x,  $\lambda$ ,  $\nu$  are optimal, then they must satisfy the following conditions, called KKT conditions
  - Primal constraints:  $f_i(x) \le 0$ , i = 1, ... m
  - Dual constraints:  $\lambda_i > 0$ , i = 1, ... m
  - Complementary slackness:  $\lambda_i f_i(x) = 0$ , i = 1, ... m
  - Gradient of Lagrangian vanishes:  $\nabla f_0(x) + \sum_{i=1}^m \lambda_i \nabla f_i(x) + \sum_{i=1}^p \nu_i \nabla h_i(x)$

## Linear Program (LP)

Convex problem with affine objective and constraints functions

minimize 
$$c^T x + d$$
  
 $s.t. Gx \le h$   
 $Ax = b$ 



- Feasible set is a polyhedron
- linprog command in MATLAB

## Quadratic Program (QP)

Convex problem with quadratic convex objective and affine constraints functions (P is PSD)

minimize 
$$1/2x^TPx + q^Tx + r$$
  
 $s.t. Gx \le h$   
 $Ax = b$ 

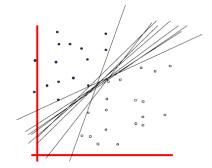


Quadprog command in matlab

#### SVM: a QP Example

- Many linear classifiers separating two separable set of examples
- Pick the one with maximum margin

$$\label{eq:subject_to_problem} \begin{split} & \underset{w,b}{\text{minimize}} & \|w\|^2 \\ & subject \ to \ \ y_i(w^Tx_i+b) \geq 1, \ i=1, \dots n \end{split}$$



- If the examples are not separable, the feasible set of this problem is empty (infeasible problem)
- Utilizing slack variables to relax the constraints and make a feasible problem

$$\begin{aligned} & \underset{w,b}{\text{minimize}} & & \|w\|^2 + C \sum_{i=1}^n \varepsilon_i \\ & subject \ to & \ y_i(w^T x_i + b) \geq 1 - \varepsilon_i \ i = 1, \dots n \\ & \ \varepsilon_i \geq 0 \ i = 1, \dots, n \end{aligned}$$

#### SVM: dual formulation

Define the Lagrangian:

$$L(\mathbf{w}, \mathbf{b}, \lambda, \nu) = \|\mathbf{w}\|^2 + C \sum_{i=1}^n \varepsilon_i - \sum_{i=1}^m \alpha_i (y_i(\mathbf{w}^T x_i + b) - 1 + \varepsilon_i) - \sum_{i=1}^n \mu_i \varepsilon_i$$

Finding  $L(\lambda, \nu) = \inf_{w,b} L(w, b, \lambda, \nu)$ 

$$\frac{\partial L(w, b, \lambda, \nu)}{\partial w} = 0 \to w = \sum_{i=1}^{n} \alpha_i y_i x_i$$
$$\frac{\partial L(w, b, \lambda, \nu)}{\partial b} = 0 \to \sum_{i=1}^{n} \alpha_i y_i = 0$$
$$\frac{\partial L(w, b, \lambda, \nu)}{\partial \varepsilon_i} = 0 \to \alpha_i = C - \mu_i$$

KKT conditions: 1) 
$$\alpha_i \ge 0$$
,  $\Sigma_{i=1}^m \alpha_i (y_i(w^T x_i + b) - 1 + \varepsilon_i) = 0$ , 6)  $\mu_i \varepsilon_i = 0$ 

KKT conditions: 1) 
$$\alpha_i \ge 0$$
, 2)  $y_i(w^T x_i + b) - 1 + \varepsilon_i \ge 0$ , 3)  $\sum_{i=1}^m \alpha_i (y_i(w^T x_i + b) - 1 + \varepsilon_i) = 0$ , 4)  $\mu_i \ge 0$ , 5)  $\varepsilon_i \ge 0$ ,

#### SVM: dual formulation

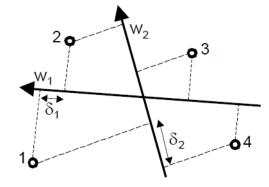
Using these results, we obtain the dual problem

maximize 
$$\sum_{i=1}^{n} \alpha_{i} - 1/2 \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{i} x_{j}$$
subject to  $0 \le \alpha_{i} \le C$ 

Useful form for using the kernel trick

maximize 
$$\sum_{i=1}^{n} \alpha_i - 1/2 \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j K(x_i, x_j)$$
subject to  $0 \le \alpha_i \le C$ 

## SVM^Rank: a QP Example



- Ranking problem:
  - n queries  $q_i$ , i = 1, ..., n
  - for query  $q_i$ , a list of items  $d_j^i$ ,  $j = 1, ..., m_i$  (feature vector) with their respect relevancy  $r_i^i$ ,  $j = 1, ..., m_i$  to the query.
  - Assume also that  $r_j^i$  are discrete [1..k]
- Objective: obtain a linear classifier that respects ordering information
  - Suppose W is such a classifier
  - Construct a set on pair of examples  $S = \{(x, z) | x = d_i^i, z = d_k^i, r_k^i r_j^i = 1\}$
  - Find W that maximizes the margin between each two items

minimize 
$$||w||^2 + C \sum_{r_i - r_j = 1} \varepsilon_{ij}$$
  
subject to  $w^T(x_j - x_i) \ge 1 - \varepsilon_{ij}$ ,  $(x_i, x_j) \in S$   
 $\varepsilon_{ij} \ge 0$   $i = 1, ..., n$ 

#### Multi-Task Learning

- Problem setup
  - T classification problems, each with different set of training examples.
  - ► Task t has  $n_t$  training examples  $(x_i^t, y_i^t)$ ,  $i = 1, ..., n_t$
  - Feature vector of all task are in the same space
  - Tasks are related (digits recognition, medical domains, etc)
- Objective: to learn linear classifiers  $w^t$ , t = 1, ..., T for tasks by considering that the tasks are similar
- $\blacktriangleright$  Solution: assume all tasks are similar to a central unknown task  $\mu$

▶ How to write the dual of this problem? (Next lecture)

## Quadratically Constrained QP (QCQP)

Convex problem with quadratic convex objective and constraints functions ( $P_i$  are SDP)

minimize 
$$1/2x^{T}P_{0}x + q_{0}^{T}x + r_{0}$$
s. t. 
$$1/2x^{T}P_{i}x + q_{i}^{T}x + r_{i} \le 0$$

$$Ax = b$$

- Objective and constrains are convex quadratic
- Can be solved with standard toolbox

#### Semidefinite Programming

Convex problem with quadratic convex objective and constraints functions

minimize 
$$c^Tx + d$$
  
 $s.t.$   $x_1P_1 + \cdots + x_nP_n + Q \le 0$  (Linear Matrix Inequality)  
 $Gx \le b$  (General inequalities)  
 $Ax = b$ 

Or

minimize 
$$tr(CX)$$
  
 $s.t.$   $tr(A_iX) = b_i$   
 $X \ge 0$ 

- If  $P_1, ..., P_n$  and Q are all diagonal, the SDP programming reduces to linear programming
- ▶ SeDuMi is a good tool to model this type of problems

## Local and Global Consistency SSL

Local and global Consistency, minimize

$$Q(F) = \underbrace{\frac{1}{2} \sum_{i,j=1}^{N} W_{ij} \left\| \frac{F_i}{\sqrt{D_{ii}}} - \frac{F_j}{\sqrt{D_{jj}}} \right\|^2}_{Smoothness} + \underbrace{\mu \sum_{i=1}^{N} \left\| F_i - Y_i \right\|^2}_{Fitting}$$

▶ Question: convex or non-convex?

$$Q(F) = F D^{-\frac{1}{2}} L D^{-\frac{1}{2}} F + \underbrace{\mu \sum_{i=1}^{N} \|F_i - Y_i\|^2}_{Fitting}$$

▶ How to solve such problems? (Next lecture)

## PGDM metric learning

PGDM metric learning

minimize 
$$\sum_{(x_i, x_j) \in S} ||x_i - x_j||_P$$
  
subject to  $\sum_{(x_i, x_j) \in D} ||x_i - x_j||_P \ge 1$   
 $P \ge 0$ 

- Question: convex or non-convex?
- ▶ How should we solve such problems? (next lecture)

#### LMNN metric learning

▶ LMNN metric learning

minimize 
$$\sum_{(x_i, x_j) \in S} ||x_i - x_j||_P$$
  
 $s.t ||x_i - x_k||_P - ||x_i - x_j||_P \ge 1, (x_i, x_j, x_k) \in R$   
 $P \ge 0$ 

- in  $(x_i, x_j, x_k) \in R$ ,  $(x_i, x_j)$  are of the same class and neighbor according to Euclidean distance.  $(x_i, x_k)$  are from two different classes.
- Question: convex or non-convex?
- ▶ How should we solve such problems? (next lecture)