Learning From Data Locally and Globally

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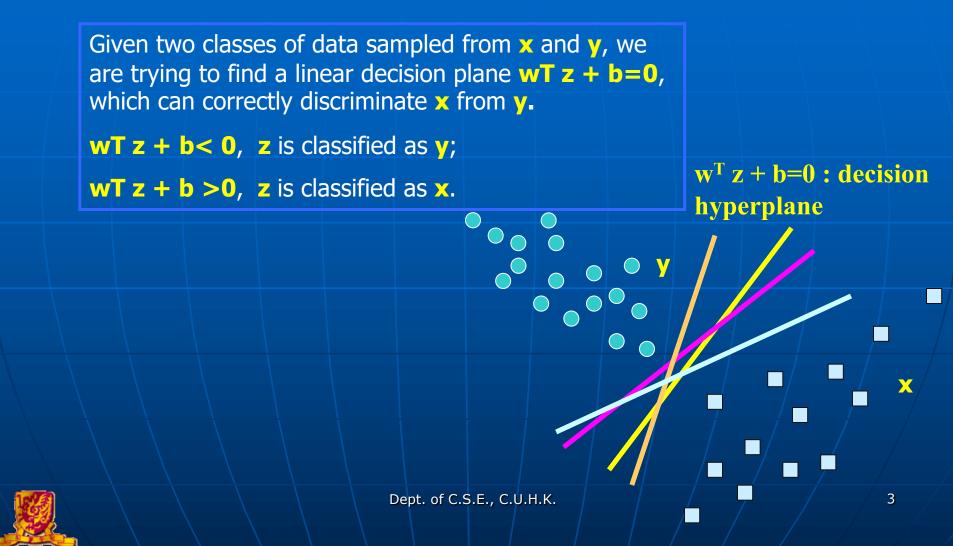
Outline

Background

- Linear Binary classifier
- Global Learning
 - Bayes optimal Classifier
- Local Learning
 - Support Vector Machine
- Contributions
- Minimum Error Minimax Probability Machine (MEMPM)
 - Biased Minimax Probability Machine (BMPM)
- Maxi-Min Margin Machine (M⁴)
 - Local Support Vector Regression (LSVR)
- Future work
- Conclusion



Background - Linear Binary Classifier



Background - Global Learning (I)

- Global learning
 - Basic idea: Focusing on summarizing data usually by estimating a distribution
 - Example
 - 1) Assume Gaussinity for the data
 - 2) Learn the parameters via MLE or other criteria
 - 3) Exploit Bayes theory to find the optimal thresholding for classification



Traditional Bayes Optimal Classifier

Background - Global Learning (II)

Problems

Usually have to assume specific models on data, which may NOT always coincide with data

"all models are wrong but some are useful..."—by George Box

Estimating distributions may be wasteful and imprecise

Finding the ideal generator of the data, i.e., the distribution, is only an intermediate goal in many settings, e.g., in classification or regression. **Optimizing an intermediate objective may be inefficient or wasteful**.



Background-Local Learning (I)

Local learning

- Basic idea: Focus on exploiting part of information, which is <u>directly related to the</u> objective, e.g., the classification accuracy instead of describing data in a holistic way
- Example

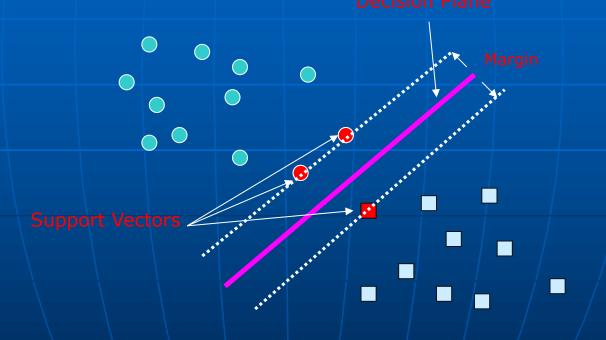
In classification, we need to accurately model the data around the (possible) separating plane, while inaccurate modeling of other parts is certainly acceptable (as is done in SVM).



Background - Local Learning (II)

Support Vector Machine (SVM)

---The current state-of-the-art classifier





Background - Local Learning (III)

Problems

The fact that the objective is exclusively determined by local information may lose the overall view of data



Background-Local Learning (IV)

An illustrative example

Along the dashed axis, the y data is obviously more likely to scatter than the x data. Therefore, a more reasonable hyerplane may lie closer to the x data rather than locating itself in the middle of two classes as in SVM.

A more reasonable hyperplane

SVM

Learning Locally and Globally

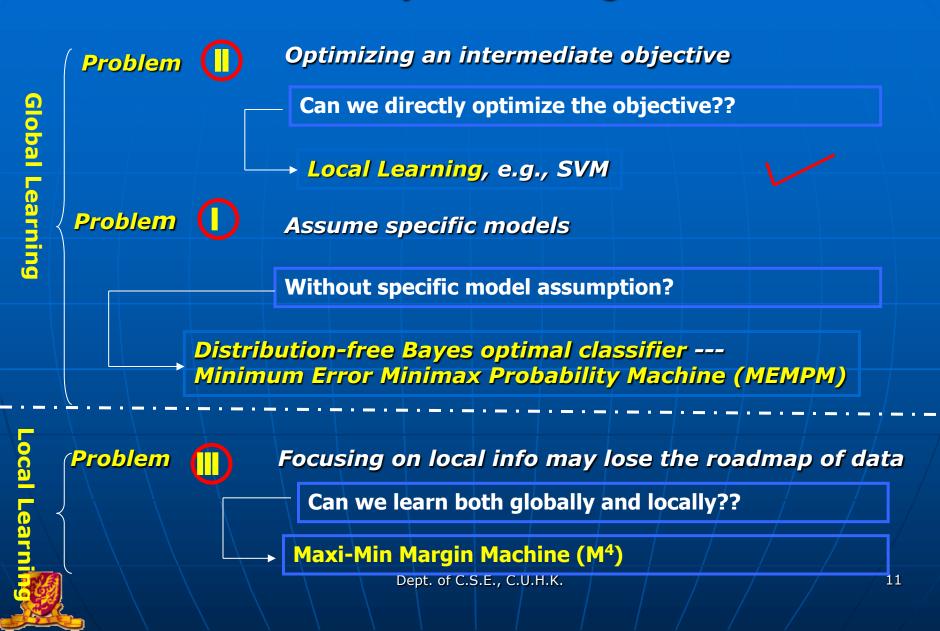


Learning Locally and Globally

- Basic idea: Focus on using both local information and certain robust global information
 - Do not try to estimate the distribution as in global learning, which may be inaccurate and indirect
 - Consider robust global information for providing a roadmap for local learning



Summary of Background



Contributions

 Mininum Error Minimax Probability Machine (Accepted by JMLR 04)

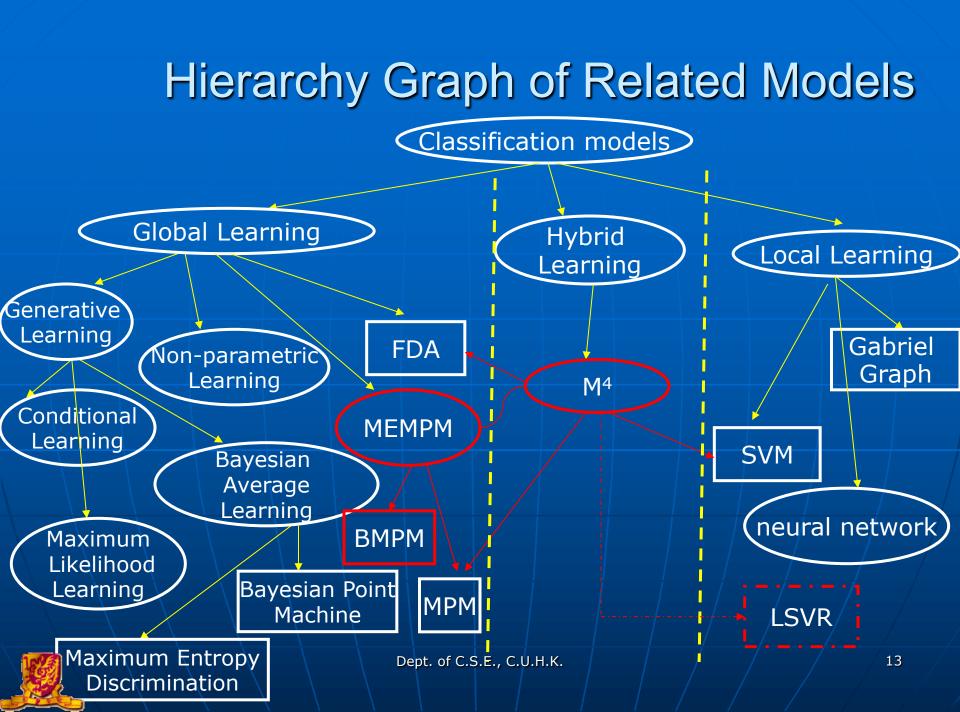
• A worst-case distribution-free Bayes Optimal Classifier

 Containing Minimax Probability Machine (MPM) and Biased Minimax Probability Machine (BMPM)(AMAI04,CVPR04) as special cases

Maxi-Min Margin Machine (M⁴) (ICML 04+Submitted)

- A unified framework that learns locally and globally
 - Support Vector Machine (SVM)
 - Minimax Probability Machine (MPM)
 - Fisher Discriminant Analysis (FDA)
 - Can be linked with MEMPM
- Can be extended into regression: Local Support Vector Regression (LSVR) (submitted)

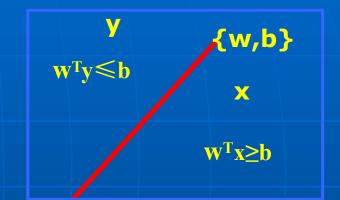




Minimum Error Minimax Probability Machine (MEMPM)

Model Definition:

max α,β, ₩ ≠0,b	$\theta \alpha + (1-\theta)\beta$, s.t
$\inf_{\mathbf{x}\sim(\bar{\mathbf{x}},\Sigma_{\mathbf{x}})}$	$\Pr\{\mathbf{W}^T\mathbf{x}\geq b\}\geq\alpha,$
$\inf_{\mathbf{y} \sim (\overline{\mathbf{y}}, \Sigma_{\mathbf{y}})}$	$\Pr\{\mathbf{W}^T\mathbf{y}\leq b\}\geq \boldsymbol{\beta}.$



• θ : prior probability of class **x**; $a(\beta)$: represents the worstcase accuracy for class x (y)

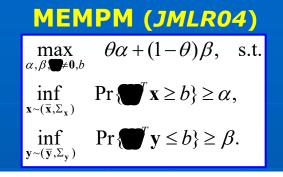
 $\mathbf{x} \sim (\overline{\mathbf{x}}, \Sigma_{\mathbf{x}})$: The class of distributions that have prescribed

mean $\overline{\mathbf{x}}$ and covariance $\Sigma_{\mathbf{x}}$

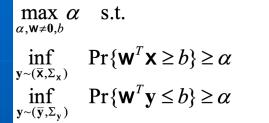
likewise

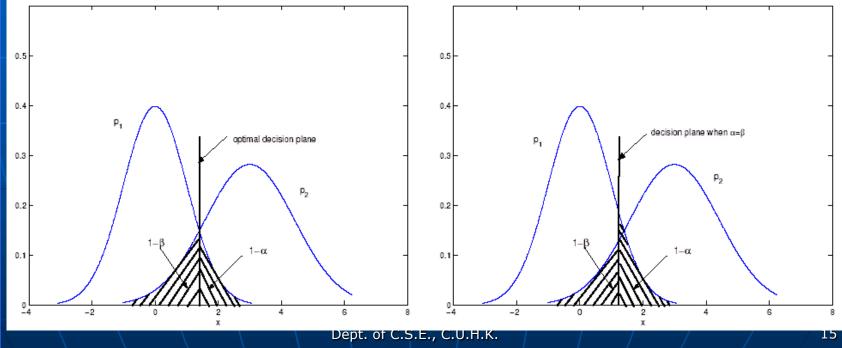


MEMPM: Model Comparison



MPM (Lanckriet et al. JMLR 2002)





MEMPM: Advantages

- A distribution-free Bayes optimal Classifier in the worst-case scenario
- Containing an explicit accuracy bound, namely, $\theta \alpha + (1-\theta)\beta$

 Subsuming a special case Biased Minimax Probability Machine for biased classification

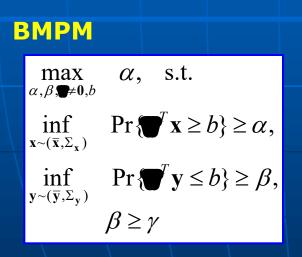


MEMPM: Biased MPM

Biased Classification:

Diagnosis of epidemical disease: Classifying a patient who is infected with a disease into an opposite class results in more serious consequence than the other way around. The classification accuracy should **be biased towards the class with**

disease.



An ideal model for biased classification.

A typical setting: We should maximize the accuracy for the important class as long as the accuracy for the less important class is acceptable (greater than an acceptable level γ).



MEMPM: Biased MPM (I)

Objective

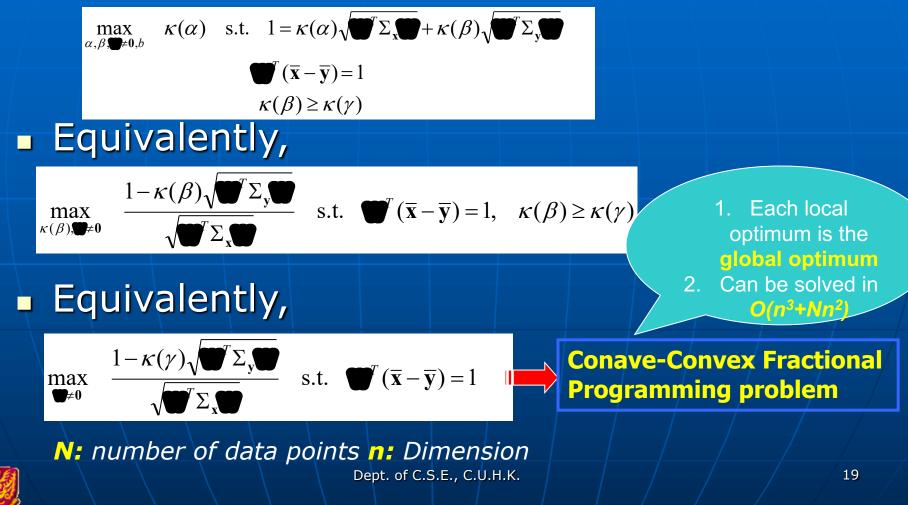
$$\max_{\alpha,\beta,\mathbf{a}\neq\mathbf{0},b} \alpha \quad \text{s.t.} \quad \inf_{\mathbf{x}\sim(\bar{\mathbf{x}},\Sigma_{\mathbf{x}})} \Pr\{\mathbf{\nabla}^T \mathbf{x} \ge b\} \ge \alpha$$
$$\inf_{\mathbf{y}\sim(\bar{\mathbf{y}},\Sigma_{\mathbf{y}})} \Pr\{\mathbf{\nabla}^T \mathbf{y} \le b\} \ge \beta$$
$$\beta \ge \gamma$$

Equivalently

$$\max_{\alpha,\beta,\mathbf{p}\neq\mathbf{0},b} \quad \kappa(\alpha) \quad \text{s.t.} \quad 1 = \kappa(\alpha)\sqrt{\mathbf{p}^{T}}\Sigma_{\mathbf{x}}\mathbf{p} + \kappa(\beta)\sqrt{\mathbf{p}^{T}}\Sigma_{\mathbf{y}}\mathbf{p}$$
$$\mathbf{p}^{T}(\mathbf{\bar{x}}-\mathbf{\bar{y}}) = 1$$
$$\kappa(\beta) \ge \kappa(\gamma)$$
$$\kappa(\alpha) = \sqrt{\frac{\alpha}{1-\alpha}}, \quad \kappa(\beta) = \sqrt{\frac{\beta}{1-\beta}}$$

MEMPM: Biased MPM (II)

Objective



MEMPM: Optimization (I)

Objective

$$\max_{\alpha,\beta,\mathbf{y}\neq\mathbf{0}} \quad \theta\alpha + (1-\theta)\beta, \quad \text{s.t.}$$
$$1 = \kappa(\alpha)\sqrt{\mathbf{w}^T \Sigma_{\mathbf{x}}} + \kappa(\beta)\sqrt{\mathbf{w}^T \Sigma_{\mathbf{y}}}$$
$$\mathbf{w}^T(\mathbf{\overline{x}} - \mathbf{\overline{y}}) = 1$$

$$\min_{\kappa(\alpha),\kappa(\beta),\Psi\neq 0} \frac{\theta}{\kappa(\alpha)^2 + 1} + \frac{1 - \theta}{\kappa(\beta)^2 + 1}, \quad \text{s.t.}$$
$$1 = \kappa(\alpha) \sqrt{\Psi^T \Sigma_x \Psi} + \kappa(\beta) \sqrt{\Psi^T \Sigma_y \Psi}$$
$$\Psi^T(\bar{\mathbf{x}} - \bar{\mathbf{y}}) = 1$$



MEMPM: Optimization (II)

Objective

$$\max_{\alpha,\beta,\Psi\neq 0} \frac{\theta\kappa(\alpha)^2}{\kappa(\alpha)^2 + 1} + (1 - \theta)\beta, \quad \text{s.t.}$$

$$\mathbf{\Psi}^T(\mathbf{\bar{x}} - \mathbf{\bar{y}}) = 1,$$
where $\kappa(\alpha) = \frac{1 - \kappa(\beta)\sqrt{\mathbf{\Psi}^T \Sigma_y \mathbf{\Psi}}}{\sqrt{\mathbf{\Psi}^T \Sigma_y \mathbf{\Psi}}}$

Line search + BMPM method



MEMPM: Problems

As a global learning approach, the decision plane is exclusively dependent on global information, i.e., up to second-order moments.

These moments may NOT be accurately estimated! –We may need local information to neutralize the negative effect caused.





Learning Locally and Globally: Maxi-Min Margin Machine (M⁴)

A more reasonable hyperplane

SVM

Model Definition

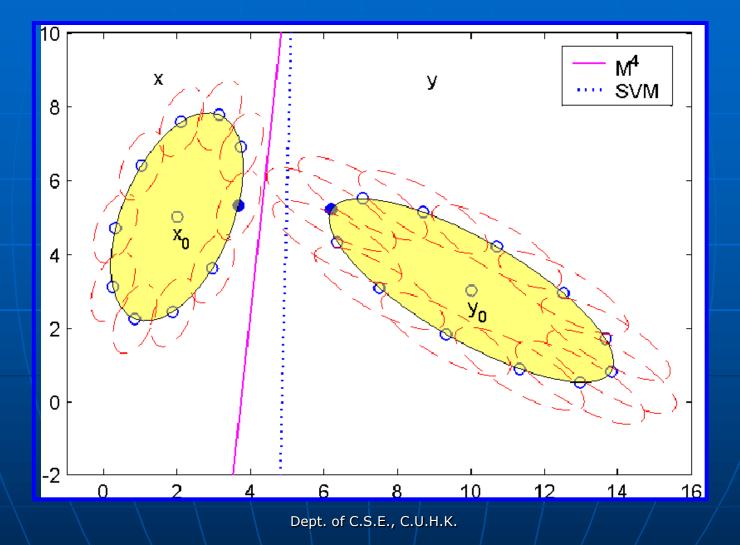
The formulation for M^4 can be written as:

$$\frac{\max_{\rho, \mathbf{w} \neq \mathbf{0}, b} \quad \rho \quad s.t.}{\sqrt{\mathbf{w}^T \mathbf{x}_i + b}} \geq \rho, \quad i = 1, 2, \dots, N_{\mathbf{x}},$$
$$\frac{-(\mathbf{w}^T \mathbf{y}_j + b)}{\sqrt{\mathbf{w}^T \Sigma_{\mathbf{y}} \mathbf{w}}} \geq \rho, \quad j = 1, 2, \dots, N_{\mathbf{y}},$$

where $\Sigma_{\mathbf{x}}$ and $\Sigma_{\mathbf{y}}$ refer to the covariance matrices of the \mathbf{x} and the \mathbf{y} data, respectively.



M⁴: Geometric Interpretation





M⁴: Solving Method (I)

Divide and Conquer:

If we fix ρ to a specific ρ_n , the problem changes to check whether this ρ_n satisfies the following constraints:

$$(\mathbf{w}^T \mathbf{x}_i + b) \ge \rho_n \sqrt{\mathbf{w}^T \Sigma_{\mathbf{x}} \mathbf{w}}, \ i = 1, \dots, N_{\mathbf{x}},$$

$$-(\mathbf{w}^T \mathbf{y}_j + b) \ge \rho_n \sqrt{\mathbf{w}^T \Sigma_{\mathbf{y}} \mathbf{w}}, \ j = 1, \dots, N_{\mathbf{y}}$$

If yes, we increase ρ_n ; otherwise, we decrease it.

Second Order Cone Programming Problem!!!



M⁴: Solving Method (II)

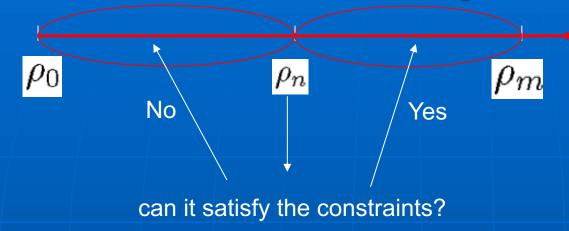
Iterate the following two Divide and Conquer steps:

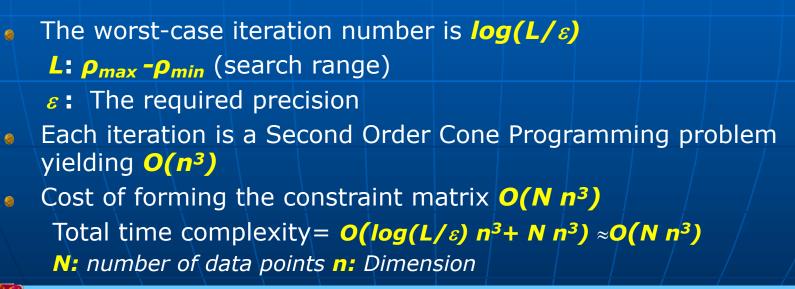
- 1. **Divide:** Set $\rho_n = (\rho_0 + \rho_m)/2$, where ρ_0 is a feasible ρ , ρ_m is an infeasible ρ , and $\rho_0 \leq \rho_m$.
- Conquer: Call the Modified Second Order Cone Programming (MSOCP) procedure elaborated in the following to check whether ρ_n is a feasible ρ. If yes, set ρ₀ = ρ_n; otherwise, set ρ_m = ρ_n;

Sequential Second Order Cone Programming Problem!!!

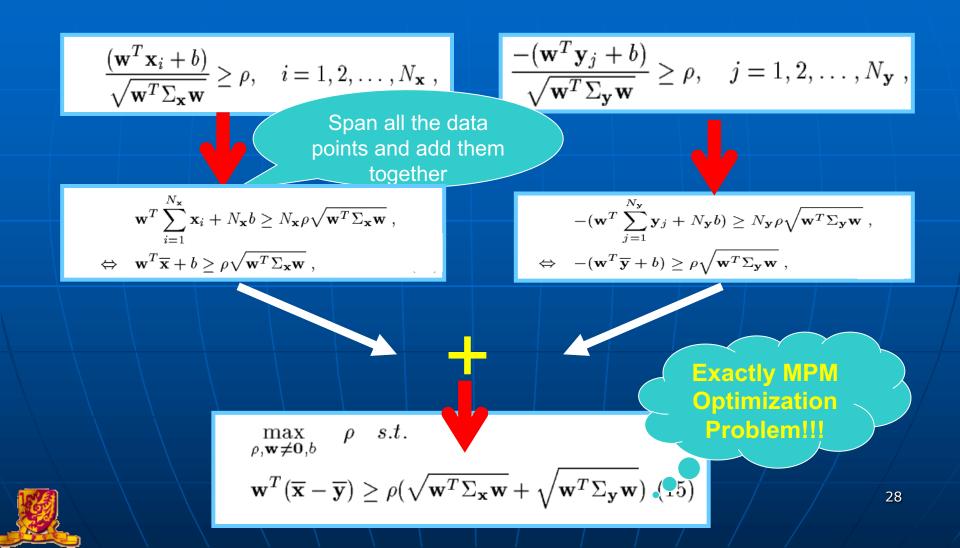


M⁴: Solving Method (III)





M⁴: Links with MPM (I)



M⁴: Links with MPM (II)

Remarks:

- The procedure is not reversible: MPM is a special case of M4
 - MPM focuses on building decision boundary GLOBALLY, i.e., it exclusively depends on the means and covariances.
- However, means and covariances may not be accurately estimated.

The formulation for M^4 can be written as:

$$\max_{\substack{\rho, \mathbf{w} \neq \mathbf{0}, b}} \rho \quad s.t. \\
\frac{(\mathbf{w}^T \mathbf{x}_i + b)}{\sqrt{\mathbf{w}^T \Sigma_{\mathbf{x}} \mathbf{w}}} \ge \rho, \quad i = 1, 2, \dots, N_{\mathbf{x}} , \\
\frac{-(\mathbf{w}^T \mathbf{y}_j + b)}{\sqrt{\mathbf{w}^T \Sigma_{\mathbf{y}} \mathbf{w}}} \ge \rho, \quad j = 1, 2, \dots, N_{\mathbf{y}} ,$$

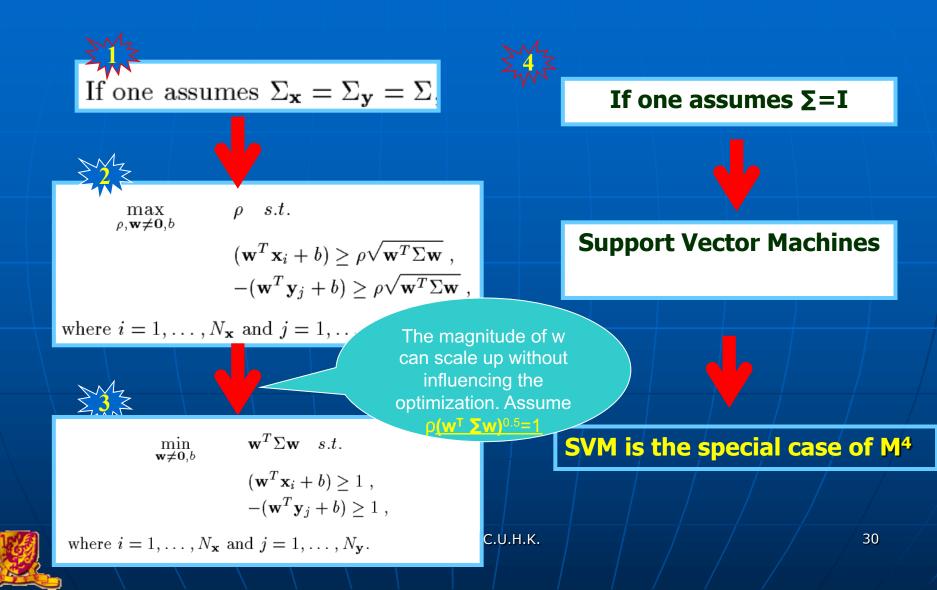
where $\Sigma_{\mathbf{x}}$ and $\Sigma_{\mathbf{y}}$ refer to the covariance matrices of the \mathbf{x} and the \mathbf{y} data, respectively.

$$\max_{\substack{\rho, \mathbf{w} \neq \mathbf{0}, b}} \rho \quad s.$$

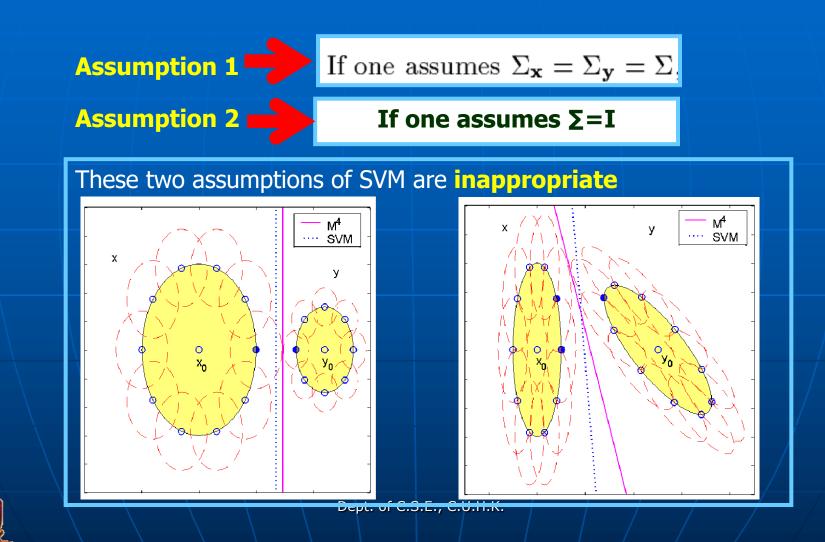
$$\mathbf{w}^{T}(\overline{\mathbf{x}} - \overline{\mathbf{y}}) \geq \rho(\sqrt{\mathbf{w}^{T} \Sigma_{\mathbf{x}} \mathbf{w}} + \sqrt{\mathbf{w}^{T} \Sigma_{\mathbf{y}} \mathbf{w}})$$



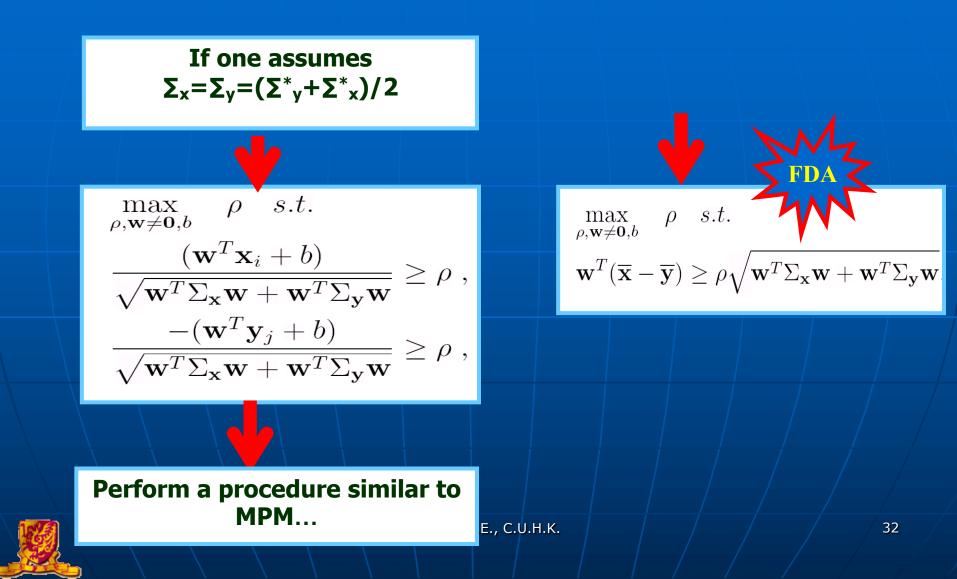
M⁴: Links with SVM (I)



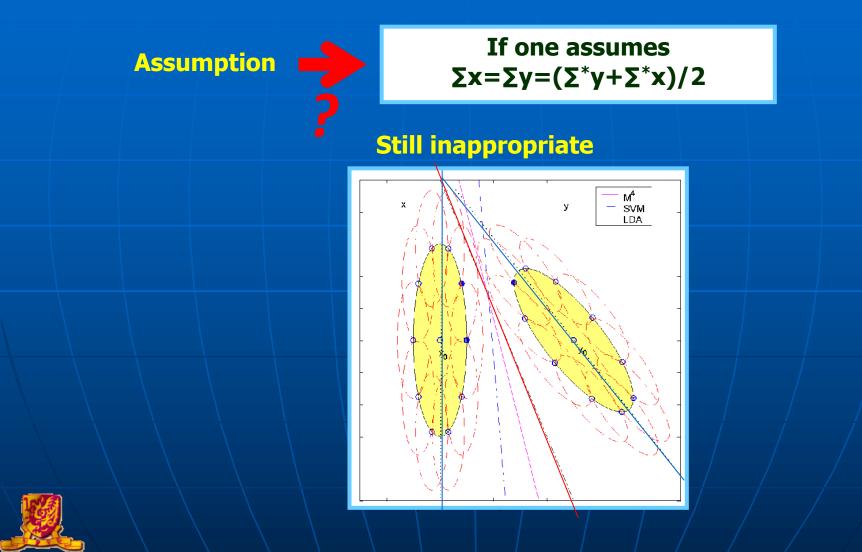
M⁴: Links with SVM (II)



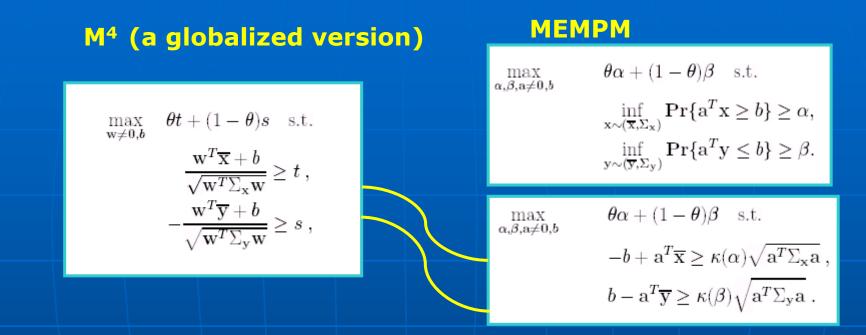
M⁴: Links with FDA (I)



M⁴: Links with FDA (II)



M⁴: Links with MEMPM



T and s \iff K(a) and K(β):

The margin from the mean to the decision plane

The globalized M⁴ maximizes the weighted margin, while MEMPM Maximizes the weighted worst-case accuracy.



M⁴ :Nonseparable Case

Introducing slack variables

$$\max_{\substack{\rho, \mathbf{w} \neq \mathbf{0}, b, \boldsymbol{\xi}}} \rho - C \sum_{k=1}^{N_{\mathbf{x}}+N_{\mathbf{y}}} \boldsymbol{\xi}_{k} \quad s.t.$$

$$(\mathbf{w}^{T}\mathbf{x}_{i} + b) \geq \rho \sqrt{\mathbf{w}^{T}\Sigma_{\mathbf{x}}\mathbf{w}} - \boldsymbol{\xi}_{i} ,$$

$$- (\mathbf{w}^{T}\mathbf{y}_{j} + b) \geq \rho \sqrt{\mathbf{w}^{T}\Sigma_{\mathbf{y}}\mathbf{w}} - \boldsymbol{\xi}_{j+N_{\mathbf{x}}} ,$$

$$\boldsymbol{\xi}_{k} \geq 0 ,$$

How to solve?? Line Search+Second Order Cone Programming

Step 1. Generate a new ρ_n from three previous ρ_1, ρ_2, ρ_3 by using the Quadratic Interpolation method.

Step 2. Fix $\rho = \rho_n$, perform the optimization based on SOCP algorithms. Update ρ_1, ρ_2, ρ_3 . M⁴ : Extended into Regression----Local Support Vector Regression (LSVR) Regression: Find a function $f(x) = w^T x + b$, $w, x \in \mathbb{R}^d, b \in \mathbb{R}$. to approximate the data $\{(x_i, y_i) \mid x_i \in \mathbb{R}^d, y_i \in \mathbb{R}, i = 1, ..., N\}$

LSVR Model Definition

SVR Model Definition

$$\min_{\mathbf{w},b,\xi_{i},\xi_{i}^{*}} \quad \frac{1}{N} \sum_{i=1}^{N} \sqrt{\mathbf{w}^{T} \Sigma_{i} \mathbf{w}} + C \sum_{i=1}^{N} (\xi_{i} + \xi_{i}^{*}), \\
\text{s.t.} \quad y_{i} - (\mathbf{w}^{T} \mathbf{x}_{i} + b) \leq \epsilon \sqrt{\mathbf{w}^{T} \Sigma_{i} \mathbf{w}} + \xi_{i}, \\
(\mathbf{w}^{T} \mathbf{x}_{i} + b) - y_{i} \leq \epsilon \sqrt{\mathbf{w}^{T} \Sigma_{i} \mathbf{w}} + \xi_{i}^{*}, \\
\xi_{i} \geq 0, \quad \xi_{i}^{*} \geq 0, \quad i = 1, \dots, N,
\end{cases} \qquad \min_{\mathbf{w},b,\xi_{i},\xi_{i}^{*}} \quad \|\mathbf{w}\| + C \sum_{i=1}^{N} (\xi_{i} + \xi_{i}^{*}), \\
\text{s.t.} \quad y_{i} - (\mathbf{w} \mathbf{x}_{i} + b) \leq \epsilon + \xi_{i}, \\
(\mathbf{w} \mathbf{x}_{i} + b) - y_{i} \leq \epsilon + \xi_{i}^{*}, \\
\xi_{i} \geq 0, \quad \xi_{i}^{*} \geq 0, \quad i = 1, \dots, N,
\end{cases}$$

$$\therefore y_{i} = w^{T} x_{i} + b, \quad \overline{y}_{i} = w^{T} \overline{x}_{i} + b$$

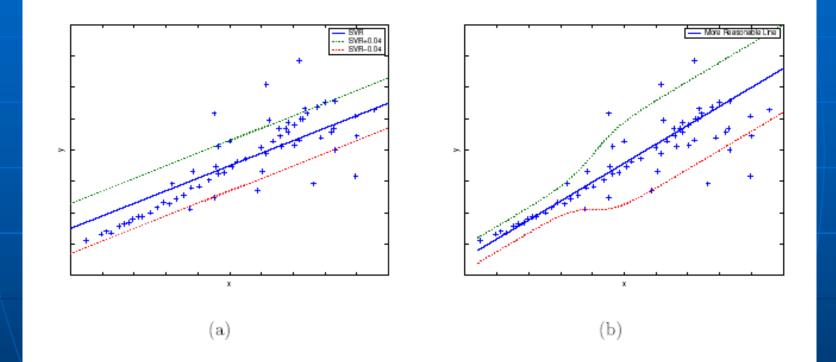
$$\therefore \Delta_{i} = \frac{1}{2k+1} \sum_{j=-k}^{k} (y_{i+j} - \overline{y}_{i})^{2} = \frac{1}{2k+1} \sum_{j=-k}^{k} [w^{T} (x_{i+j} - \overline{x}_{i})]^{2} = w^{T} \Sigma_{i} w$$

Local Support Vector Regression (LSVR)

When supposing Σ_i=I for each observation, LSVR is equivalent with l₁-SVR under a mild assumption.

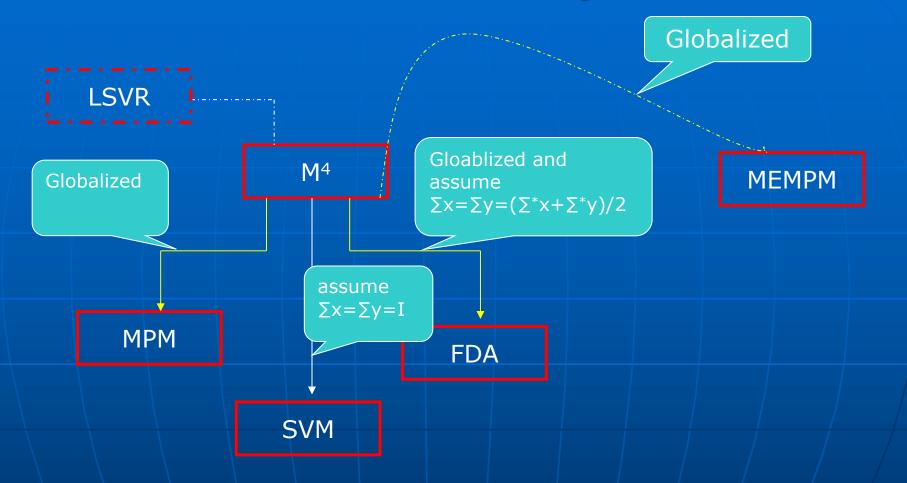
The LSVR model with setting $\Sigma_i = \mathbf{I}$ is equivalent to the ℓ_1 -norm Lemma SVR in the sense that: (1) Assuming a unique ϵ_1^* exists for making ℓ_1 -norm SVR optimal (i.e. setting ϵ to ϵ_1^* will make the objective function minimal), if for ϵ_1^* the ℓ_1 -norm SVR achieves a solution $\{\mathbf{w}^*, b^*\} = \text{SVR}(\epsilon_1^*)$, then the LSVR can produce the same solution by setting the parameter $\epsilon = \frac{\epsilon_1^*}{\|\mathbf{w}_1^*\|}$, i.e., $\text{LSVR}(\frac{\boldsymbol{\epsilon}_1^*}{\|\mathbf{w}_1^*\|}) = \text{SVR}(\boldsymbol{\epsilon}_1^*);$ (2) Assuming a unique $\boldsymbol{\epsilon}_2^*$ exists for making the special case of LSVR optimal (i.e. setting ϵ to ϵ_2^* will make the objective function minimal), if for ϵ_2^* the special case of LSVR achieves a solution $\{\mathbf{w}_2^*, b_2^*\} =$ $LSVR(\epsilon_2^*)$, then the ℓ_1 -norm SVR can produce the same solution by setting the parameter $\boldsymbol{\epsilon} = \boldsymbol{\epsilon}_2^* \| \mathbf{w}_2^* \|$, i.e., $\text{SVR}(\boldsymbol{\epsilon}_2^* \| \mathbf{w}_2^* \|) = \text{LSVR}(\boldsymbol{\epsilon}_1^*)$.

SVR vs. LSVR





Short Summary





Non-linear Classifier : Kernelization (I)

 Previous discussions of MEMPM, BMPM, M⁴, and LSVR are conducted in the scope of linear classification.

How about non-linear classification problems?

Using Kernelization techniques



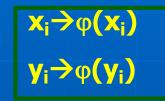
Non-linear Classifier : Kernelization (II)

 In the next slides, we mainly discuss the kernelization on M^{4,} while the proposed kernelization method is also applicable for MEMPM, BMPM, and LSVR.



Nonlinear Classifier: Kernelization (III)

Map data to higher dimensional feature space R^f



• Construct the linear decision plane $f(y,b)=y^T z + b$ in the feature space R^f , with $y \in R^f$, $b \in R$

•In R^f, we need to solve

$$\max_{\substack{\boldsymbol{\rho}, \boldsymbol{\gamma} \neq \mathbf{0}, b}} \rho \quad s.t. \\
\frac{(\boldsymbol{\gamma}^T \varphi(\mathbf{x}_i) + b)}{\sqrt{\boldsymbol{\gamma}^T \Sigma_{\varphi(\mathbf{x})} \boldsymbol{\gamma}}} \ge \rho, \quad i = 1, 2, \dots, N_{\mathbf{x}}, \\
\frac{-(\boldsymbol{\gamma}^T \varphi(\mathbf{y}_j) + b)}{\sqrt{\boldsymbol{\gamma}^T \Sigma_{\varphi(\mathbf{y})} \boldsymbol{\gamma}}} \ge \rho, \quad j = 1, 2, \dots, N_{\mathbf{y}}$$

• However, we do not want to solve this in an explicit form of φ . Instead, we want to solve it in a kernelization form

$$K(z_{1},z_{2}) = \phi(z_{1})^{T}\phi(z_{2})$$



Nonlinear Classifier: Kernelization (IV)

Corollary If the estimates of means and covariance matrices are given in M^4 as the following plug-in estimates:

$$\begin{split} \overline{\varphi(\mathbf{x})} &= \frac{1}{N_{\mathbf{x}}} \sum_{i=1}^{N_{\mathbf{x}}} \varphi(\mathbf{x}_{i}), \qquad \overline{\varphi(\mathbf{y})} = \frac{1}{N_{\mathbf{x}}} \sum_{j=1}^{N_{\mathbf{x}}} \varphi(\mathbf{y}_{j}) ,\\ \Sigma_{\varphi(\mathbf{x})} &= \frac{1}{N_{\mathbf{y}}} \sum_{i=1}^{N_{\mathbf{x}}} (\varphi(\mathbf{x}_{i}) - \overline{\varphi(\mathbf{x})}) (\varphi(\mathbf{x}_{i}) - \overline{\varphi(\mathbf{x})})^{T} ,\\ \Sigma_{\varphi(\mathbf{y})} &= \frac{1}{N_{\mathbf{y}}} \sum_{j=1}^{N_{\mathbf{y}}} (\varphi(\mathbf{y}_{j}) - \overline{\varphi(\mathbf{y})}) (\varphi(\mathbf{y}_{j}) - \overline{\varphi(\mathbf{y})})^{T} , \end{split}$$

then the optimal γ in (4.37-4.39) lies in the space spanned by the training

points.

$$oldsymbol{\gamma} = \sum_{i=1}^{N_{\mathbf{x}}} \mu_i arphi(\mathbf{x}_i) + \sum_{j=1}^{N_{\mathbf{y}}} v_j arphi(\mathbf{y}_j) \;,$$



Nonlinear Classifier: Kernelization (V)

Kernelization Theorem of M⁴ The optimal decision hyperplane for M⁴ involves solving the following optimization problem:

$$\begin{split} & \underset{\boldsymbol{\rho}, \boldsymbol{\eta} \neq \boldsymbol{0}, \boldsymbol{b}}{\underset{\boldsymbol{\eta}, \boldsymbol{\eta} \neq \boldsymbol{0}, \boldsymbol{b}}{\underset{\boldsymbol{\eta}, \boldsymbol{\eta} \neq \boldsymbol{0}, \boldsymbol{b}}{\underbrace{(\boldsymbol{\eta}^{T} \mathbf{K}_{i} + \boldsymbol{b})}}} \geq \boldsymbol{\rho}, \quad i = 1, 2, \dots, N_{\mathbf{X}}, \\ & \frac{(\boldsymbol{\eta}^{T} \mathbf{K}_{i} + \boldsymbol{b})}{\sqrt{\frac{1}{N_{\mathbf{x}}} \boldsymbol{\eta}^{T} \tilde{\mathbf{K}}_{\mathbf{x}}^{T} \tilde{\mathbf{K}}_{\mathbf{x}} \boldsymbol{\eta}}} \geq \boldsymbol{\rho}, \quad j = 1, 2, \dots, N_{\mathbf{y}}, \\ & \frac{-(\boldsymbol{\eta}^{T} \mathbf{K}_{j+N_{\mathbf{x}}} + \boldsymbol{b})}{\sqrt{\frac{1}{N_{\mathbf{y}}} \boldsymbol{\eta}^{T} \tilde{\mathbf{K}}_{\mathbf{y}}^{T} \tilde{\mathbf{K}}_{\mathbf{y}} \boldsymbol{\eta}}} \geq \boldsymbol{\rho}, \quad j = 1, 2, \dots, N_{\mathbf{y}} \,. \end{split}$$
Notation
$$\boldsymbol{\eta} := [\mu_{1}, \dots, \mu_{N_{\mathbf{x}}}, \upsilon_{1}, \dots, \upsilon_{N_{\mathbf{y}}}]^{T} \\ \tilde{\mathbf{K}}_{\mathbf{x}}, \tilde{\mathbf{k}}_{\mathbf{y}} \in \mathbb{R}^{N_{\mathbf{x}} + N_{\mathbf{y}}} \quad [\tilde{\mathbf{k}}_{\mathbf{x}}]_{i} := \frac{1}{N_{\mathbf{x}}} \sum_{j=1}^{N_{\mathbf{x}}} \mathbf{K}(\mathbf{x}_{j}, \mathbf{z}_{i}) \,. \\ & [\tilde{\mathbf{k}}_{\mathbf{y}}]_{i} := \frac{1}{N_{\mathbf{y}}} \sum_{j=1}^{N_{\mathbf{y}}} \mathbf{K}(\mathbf{y}_{j}, \mathbf{z}_{i}) \,. \\ \mathbf{1}_{N_{\mathbf{x}}} \in \mathbb{R}^{N_{\mathbf{x}}} \quad \mathbf{1}_{i} := 1 \quad i = 1, 2, \dots, N_{\mathbf{x}} \,. \\ \mathbf{1}_{N_{\mathbf{y}}} \in \mathbb{R}^{N_{\mathbf{y}}} \quad \mathbf{1}_{i} := 1 \quad i = 1, 2, \dots, N_{\mathbf{y}} \,. \\ & \tilde{\mathbf{K}} := \left(\begin{array}{c} \tilde{\mathbf{K}}_{\mathbf{x}} \\ \mathbf{K}_{\mathbf{y}} \end{array}\right) := \left(\begin{array}{c} \mathbf{K}_{\mathbf{x}} - \mathbf{1}_{N_{\mathbf{x}}} \tilde{\mathbf{k}}_{\mathbf{x}}^{T} \\ \mathbf{K}_{\mathbf{y}} - \mathbf{1}_{N_{\mathbf{y}}} \tilde{\mathbf{k}}_{\mathbf{y}}^{T} \end{array}\right) \,. \end{split}$$



Experimental Results ---MEMPM (I)

Six benchmark data sets From UCI Repository

	Dataset	Attributes #	Instances#
1	Twonorm	20	7400
2	Breast	9	699
3	Ionosphere	34	351
4	Pima	8	768
5	Heart-disease	13	270
6	Vote	16	435



45

Platform: Windows 2000 Developing tool: Matlab 6.5

Evaluate both the linear and the Gaussian kernel with the wide parameter for Gaussian chosen by cross validations.

Experimental Results ---MEMPM(II)

Dataset	MEMPM			MPM		
	α	β	heta lpha + (1 - heta) eta	Accuracy	α	Accuracy
Twonorm(%)	$80.3\pm0.2\%$	$79.9\pm0.1\%$	$80.1\pm0.1\%$	$97.9\pm0.1\%$	$80.1\pm0.1\%$	$97.9\pm0.1\%$
Breast(%)	$77.8\pm0.8\%$	$91.4\pm0.5\%$	$86.7\pm0.5\%$	$96.9\pm0.3\%$	$84.4\pm0.5\%$	$97.0\pm0.2\%$
Ionosphere(%)	$95.9\pm1.2\%$	$36.5\pm2.6\%$	$74.5\pm0.8\%$	$88.5 \pm 1.0\%$	$63.4 \pm 1.1\%$	$84.8\pm0.8\%$
Pima(%)	$0.9\pm0.0\%$	$62.9\pm1.1\%$	$41.3\pm0.8\%$	$76.8\pm0.6\%$	$32.0 \pm 0.8\%$	$76.1\pm0.6\%$
Heart-disease(%)	$43.6\pm2.5\%$	$66.5\pm1.5\%$	$56.3\pm1.4\%$	$84.2\pm0.7\%$	$54.9 \pm 1.4\%$	$83.2\pm0.8\%$
Vote(%)	$82.6\pm1.3\%$	$84.6\pm0.7\%$	$83.9\pm0.9\%$	$94.9\pm0.4\%$	$83.8\pm0.9\%$	$94.8\pm0.4\%$

Table 2: Lower bound α , β , and test accuracy compared to MPM in the linear setting.

Dataset	MEMPM				MPM	
	α	β	$\theta \alpha + (1 - \theta)\beta$	Accuracy	α	Accuracy
Twonorm(%)	$91.7\pm0.2\%$	$91.7\pm0.2\%$	$91.7\pm0.2\%$	$97.9\pm0.1\%$	$91.7\pm0.2\%$	$97.9\pm0.1\%$
Breast(%)	$88.4\pm0.6\%$	$90.7 \pm 0.4\%$	$89.9 \pm 0.4\%$	$96.9\pm0.2\%$	$89.9 \pm 0.4\%$	$96.9\pm0.3\%$
Ionosphere(%)	$94.2\pm0.8\%$	$80.9\pm3.0\%$	$89.4\pm0.8\%$	$93.8\pm0.4\%$	$89.0 \pm 0.8\%$	$92.2\pm0.4\%$
Pima(%)	$2.6\pm0.1\%$	$62.3\pm1.6\%$	$41.4\pm1.1\%$	$77.0\pm0.7\%$	$32.1 \pm 1.0\%$	$76.2\pm0.6\%$
Heart-disease(%)	$47.1 \pm 2.2\%$	$66.6\pm1.4\%$	$58.0\pm1.5\%$	$83.9\pm0.9\%$	$57.4 \pm 1.6\%$	$83.1\pm1.0\%$
Vote(%)	$85.1\pm1.3\%$	$84.3\pm0.7\%$	$84.7\pm0.8\%$	$94.7\pm0.5\%$	$84.4\pm0.8\%$	$94.6\pm0.4\%$

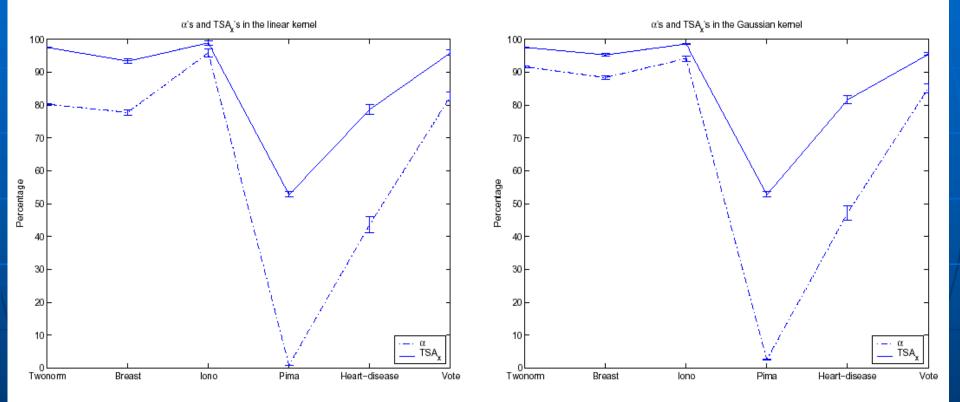
Table 3: Lower bound α , β , and test accuracy compared to MPM with the Gaussian kernel.

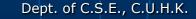
Dept. of C.S.E., C.U.H.K.

At the Significance level 0.05

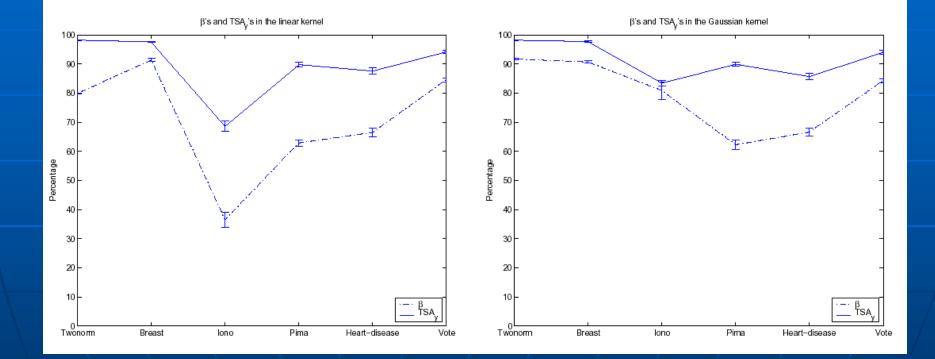
Experimental Results ---MEMPM (III)

 α vs. The test-set accuracy for x (TSAx)



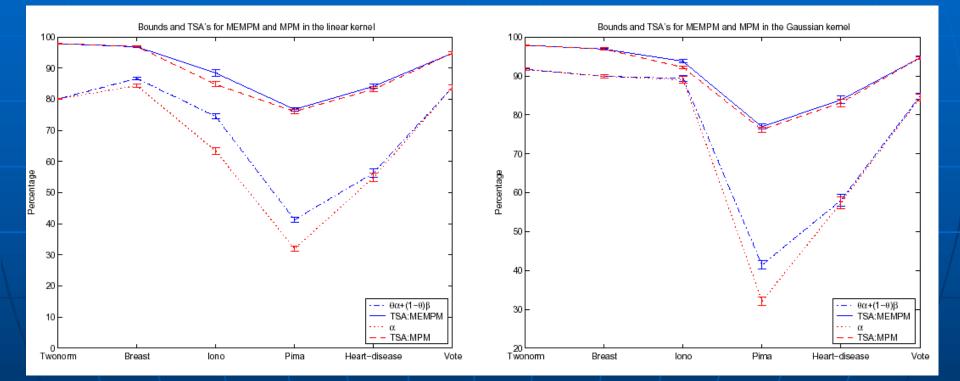


Experimental Results ---MEMPM (IV) *S vs. The test-set accuracy for y (TSAy)*





Experimental Results ---MEMPM (V) $\theta \alpha + (1-\theta)\beta$ vs. The overall test-set accuracy (TSA)

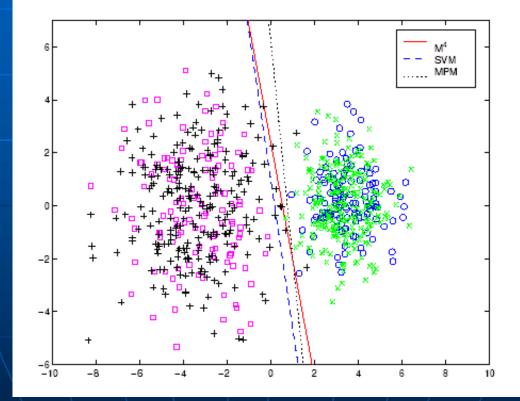




Experimental Results ----M⁴ (I)

Synthetic Toy Data (1)

Two types of data with the same data orientation but different data magnitude

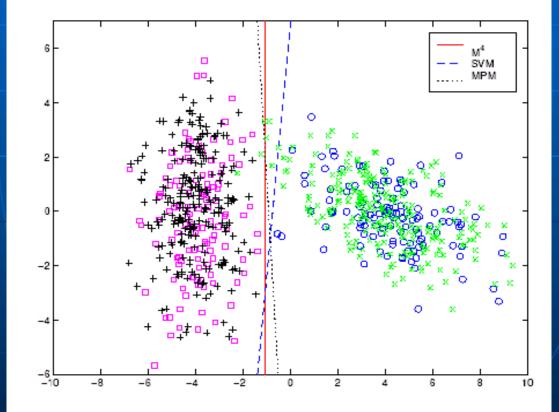




Experimental Results ----M⁴ (II)

Synthetic Toy Data (2)

Two types of data with the same data magnitude but different data orientation

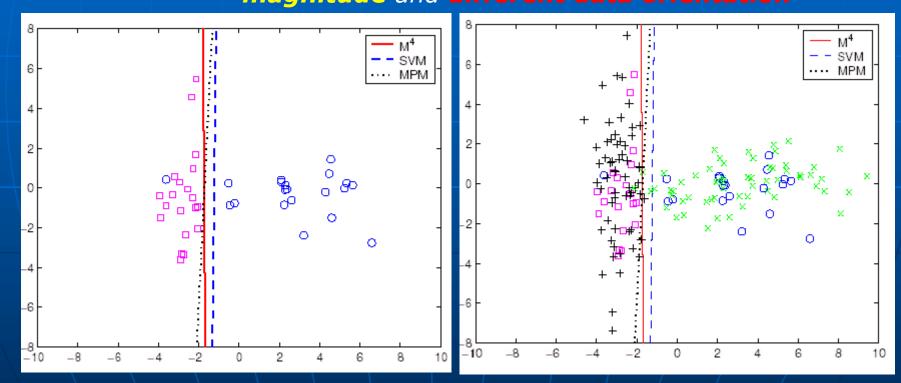




Experimental Results ----M⁴ (III)

Synthetic Toy Data (3)

Two types of data with the different data magnitude and different data orientation



Experimental Results ----M⁴ (IV)

Benchmark Data from UCI

Data set	Linear kernel				Gaussian kerne	el
	M^4	SVM	MPM	M^4	SVM	MPM
Twonorm(%)	96.5 ± 0.6	95.1 ± 0.7	97.6 ± 0.5	96.5 ± 0.7	96.1 ± 0.4	97.6 ± 0.5
Breast(%)	97.5 ± 0.7	96.6 ± 0.5	96.9 ± 0.8	97.5 ± 0.6	96.7 ± 0.4	96.9 ± 0.8
Ionosphere(%)	87.7 ± 0.8	86.9 ± 0.6	84.8 ± 0.8	94.5 ± 0.4	94.2 ± 0.3	92.3 ± 0.6
Pima(%)	77.7 ± 0.9	77.9 ± 0.7	76.1 ± 1.2	77.6 ± 0.8	78.0 ± 0.5	76.2 ± 1.2
$\operatorname{Sonar}(\%)$	77.6 ± 1.2	76.2 ± 1.1	75.5 ± 1.1	84.9 ± 1.2	86.5 ± 1.1	87.3 ± 0.8
Vote(%)	96.1 ± 0.5	95.1 ± 0.4	94.8 ± 0.4	96.2 ± 0.5	95.9 ± 0.6	94.6 ± 0.4
Heart-disease(%)	86.6 ± 0.8	84.1 ± 0.7	83.2 ± 0.8	86.2 ± 0.8	83.8 ± 0.5	83.1 ± 1.0

Table 2: Comparisons of classification accuracies among M⁴, SVM, and MPM.



Future Work

Speeding up M⁴ and MEMPM

- Contain support vectors—can we employ its sparsity as has been done in SVM?
- Can we reduce redundant points??

 How to impose constrains on the kernelization for keeping the topology of data?

Generalization error bound?

SVM and MPM have both error bounds.

How to extend to multi-category classifications?

- One vs. One or One vs. All?
- Or seeking a principled way to construct multi-way boundary in a step??



Conclusion

- We propose a general global learning model MEMPM
 - A Worst-case distribution-free Bayes Optimal classifier
 - Containing an explicit error bound for future data
 - Subsuming BMPM which is idea for biased classification
- We propose a hybrid framework M⁴ by learning from data locally and globally
 - This model subsumes three important models as special cases
 - SVM
 - MPM
 - FDA
 - Extended into regression tasks



Discussion (I)

■ In linear cases, M⁴ outperforms SVM and MPM

In Gaussian cases, M⁴ is slightly better or comparable than SVM

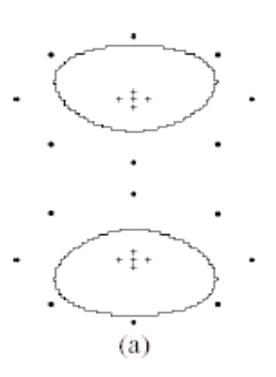
•(1) Sparsity in the feature space results in inaccurate estimation of covariance matrices

• (2) Kernelization may not keep data topology of the original data.— Maximizing Margin in the feature space does not necessarily maximize margin in the original space



Discussion (II)

An example to illustrate that maximizing the margin in the feature space does not necessarily maximize the margin in the original space



(a) SVM using degree 4 polynomial kernel. From Simon Tong et al. *Restricted Bayesian Optimal classifiers*, AAAI, 2000.



Setup

Three concerns:

Binary classification data sets

For easy comparison. MPM (Lanckriet et al. JMLR 02 or nips02) also uses these data sets.

Medium or smaller size Data sets

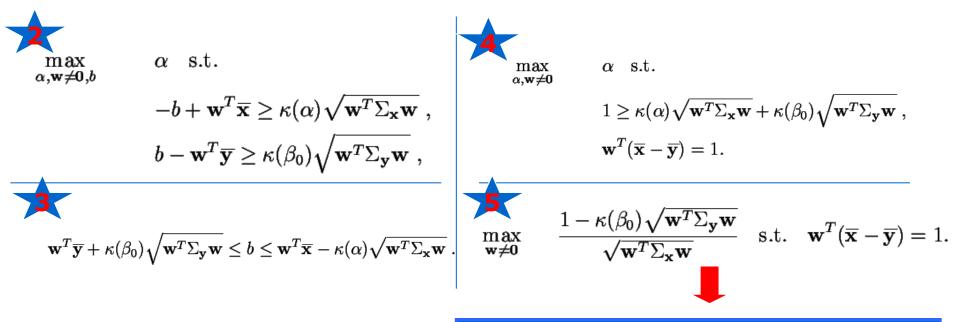
Appendix A: MEMPM- BMPM (I)

ima Given $\mathbf{w} \neq \mathbf{0}$ and b, such that $\mathbf{w}^T \mathbf{y} \leq b$ and $\beta \in [0, 1)$, the

condition

$$\inf_{\mathbf{y} \sim (\bar{\mathbf{y}}, \Sigma_{\mathbf{y}})} \mathbf{Pr} \{ \mathbf{w}^T \mathbf{y} \le b \} \ge \beta,$$

holds if and only if $b - \mathbf{w}^T \overline{\mathbf{y}} \ge \kappa(\beta) \sqrt{\mathbf{w}^T \Sigma_{\mathbf{y}} \mathbf{w}}$ with $\kappa(\beta) = \sqrt{\frac{\beta}{1-\beta}}$.





Fractional Programming

Appendix A: MEMPM- BMPM (II)

Solving Fractional Programming problem

$$\max_{\mathbf{a}\neq\mathbf{0}} 1 - \kappa(\gamma) \sqrt{\mathbf{\mathbf{f}}^T \Sigma_{\mathbf{y}} \mathbf{\mathbf{f}}} - \lambda \sqrt{\mathbf{\mathbf{f}}^T \Sigma_{\mathbf{x}} \mathbf{\mathbf{f}}} \quad \text{s.t.} \quad \mathbf{\mathbf{f}}^T (\mathbf{\overline{x}} - \mathbf{\overline{y}}) = 1$$

Update

$$\lambda \leftarrow \frac{1 - \kappa(\gamma) \sqrt{\nabla^{T} \Sigma}}{\sqrt{\nabla^{T} \Sigma}}$$

Equivalently

$$\min_{\mathbf{w}\neq\mathbf{0}} \kappa(\gamma) \sqrt{\mathbf{w}^T \Sigma_{\mathbf{y}} \mathbf{w}} + \lambda \sqrt{\mathbf{w}^T \Sigma_{\mathbf{x}} \mathbf{w}} \quad \text{s.t.} \quad \mathbf{w}^T (\overline{\mathbf{x}} - \overline{\mathbf{y}}) = 1$$



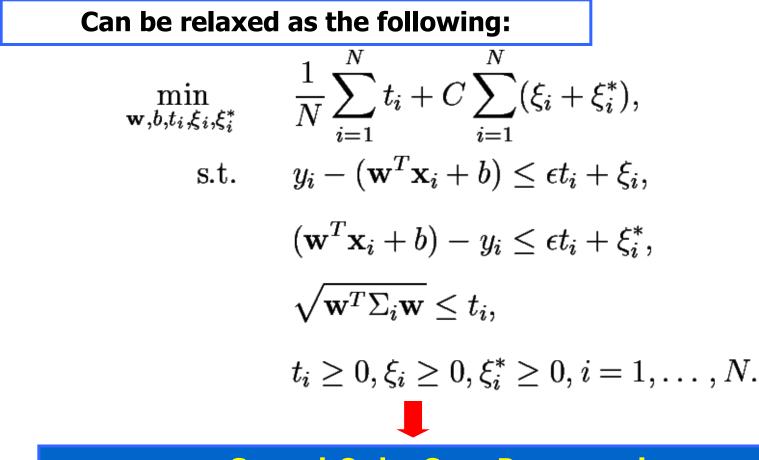
Least-squares approach

Appendix B: Optimization of LSVR(I)

$$\min_{\mathbf{w},b,t_i,\xi_i,\xi_i^*} \quad \frac{1}{N} \sum_{i=1}^N t_i + C \sum_{i=1}^N (\xi_i + \xi_i^*),$$
s.t. $y_i - (\mathbf{w}^T \mathbf{x}_i + b) \le \epsilon \sqrt{\mathbf{w}^T \Sigma_i \mathbf{w}} + \xi_i,$
 $(\mathbf{w}^T \mathbf{x}_i + b) - y_i \le \epsilon \sqrt{\mathbf{w}^T \Sigma_i \mathbf{w}} + \xi_i^*,$
 $\sqrt{\mathbf{w}^T \Sigma_i \mathbf{w}} \le t_i,$
Hard to be solved...



Appendix B: Optimization of LSVR(II)



Second-Order Cone Programming



Appendix C: Convex Optimization

Linear Program:

$$\min_{x} c^{T} x \quad \text{s.t.} \quad Ax \preceq b$$
$$Fx = g$$

Quadratic Program:

$$\min_{x} x^{T} P x + 2q^{T} x + r \quad \text{s.t.} \quad Ax \leq b$$
$$Fx = g$$

Quadratic Constrained Quadratic Program:

$$\min_{x} x^T P_0 x + 2q_0^T x + r_0 \quad \text{s.t.} \quad x^T P_i x + 2q_i^T x + r_i \le 0$$
$$i = 1, \dots, L \quad (\text{convex if } P_i \succeq 0)$$

LP SVM (Mangasarian, Bennett)

SVM

(Vapnik)

Kernel Fisher Discriminant (Mika et al.)

Second Order Cone Program:

$$\min_{x} c^{T} x \quad \text{s.t.} \quad ||A_{i}x + b_{i}||_{2} \le e_{i}^{T} x + d_{i}$$
$$i = 1, \dots, L$$

Semi-Definite Program:

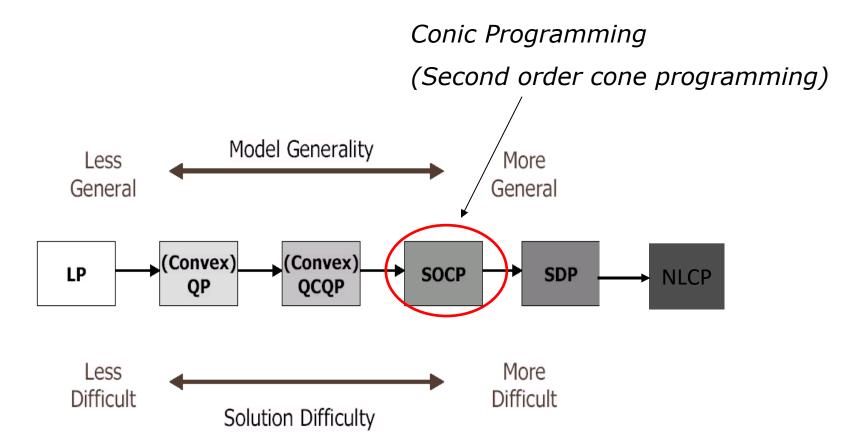
$$\min_{x} c^{T} x \quad \text{s.t.} \quad A(x) = A_0 + \sum_{i=1}^{n} x_i A_i \succeq 0 \quad (A_i = A_i^T \in \mathbb{R}^{p \times p})$$
$$Fx = g$$

Minimax Probability Machine (Lanckriet et al.)

Kernel matrix learning (Lanckriet, Cristianini et al.)



Appendix C: Convex Optimization





Appendix C: Convex Optimization -SOCP

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min
$$f^T x$$

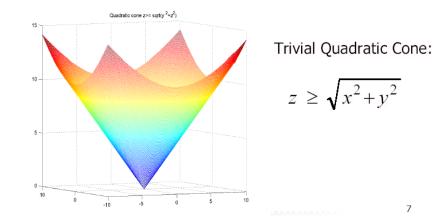
s.t. $\|C_i x + d_i\| \le a_i^T x + b_i, \quad i = 1, ..., N$

$$x \in \mathfrak{R}^{n}$$
 $f, a_i \in \mathfrak{R}^{n}$ $C_i \in \mathfrak{R}^{(k_i-1) \times n}$ $d_i \in \mathfrak{R}^{k_i-1}$ $b_i \in \mathfrak{R}$

Equivalent to conic program

- Linear constraints: cone dimension k=1
- Cone constraints: change of variables (vector) $y = C_i x + d_i$, $z = a_i^T x + b_i$

Quadractic cone C sometimes also called Lorentz cone (or ice cream cone)



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Appendix C: SOCP-Solver

Sedumi (MATLAB) Loqo (C, MATLAB) MOSEK (C, MATLAB) SDPT3 (MATLAB+C or FORTRAN)

The worst-case cost is $O(n^3)$



Time Complexity

Models	Time
	Complexity
MEMPM	O(Ln ³ +Nn ²)
BMPM	O(n ³ +Nn ²)
M ⁴	O(Nn³)
LS-SVM	O(n ³ +Nn ²)
LSVR	O(Nn³)
LS-SVR	O(n ³ +Nn ²)



Time Complexity

Thus we believe that for practical purposes the cost of solving an SOCP is roughly equal to the cost of solving a modest number (5–50) of systems of the form (40). If no special structure in the problem data is exploited, the cost of solving the system is $O(n^3)$, and the cost of forming the system matrix is $O(n^2 \sum_{i=1}^{N} n_i)$. In practice, special problem structure (*e.g.*, sparsity) often allows forming the equations faster, or solving the systems (39) or (40) more efficiently.

> ----"Applications of Second Order Cone Programming", Lobo, Boyd et al. in Linear Algebra and Applications.

