COMP5211: Machine Learning

Lecture 5

Adagrad

$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{\varepsilon I + diag(G_t)}} \cdot g_t, \tag{1}$$

$$g_t = \frac{1}{n} \sum_{i=1}^n \nabla_{\theta} \mathcal{L}(x^{(i)}, y^{(i)}, \theta_t), \tag{2}$$

$$G_t = \sum_{\tau=1}^t g_\tau g_\tau^\top. \tag{3}$$

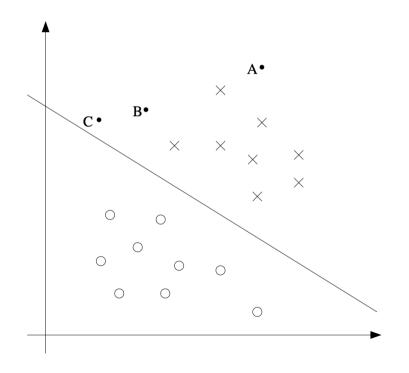
$$\begin{bmatrix} \theta_{t+1}^{(1)} \\ \theta_{t+1}^{(2)} \\ \vdots \\ \theta_{t+1}^{(m)} \end{bmatrix} = \begin{bmatrix} \theta_{t}^{(1)} \\ \theta_{t}^{(2)} \\ \vdots \\ \theta_{t}^{(m)} \end{bmatrix} - \begin{bmatrix} \frac{\eta}{\sqrt{\varepsilon + G_{t}^{(1,1)}}} & 0 & \cdots & 0 \\ 0 & \frac{\eta}{\sqrt{\varepsilon + G_{t}^{(2,2)}}} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{\eta}{\sqrt{\varepsilon + G_{t}^{(m,m)}}} \end{bmatrix} \cdot \begin{bmatrix} g_{t}^{(1)} \\ g_{t}^{(2)} \\ \vdots \\ g_{t}^{(m)} \end{bmatrix}$$
(5)

Support Vector Machine Margin

- Intuition
 - Confidence of A,B,C
- Let our decision function as

$$\bullet \ h_{w,b} = g(w^T x + b)$$

- g(z) = 1 if $z \ge 0$, g(z) = -1 otherwise
- Function margins: $\hat{\gamma}^{(i)} = y^{(i)}(w^Tx + b)$
- However, it will double just replace w with 2w, b with 2b



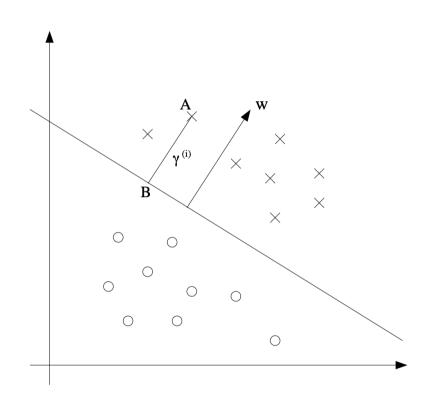
Margin

• Find point B:

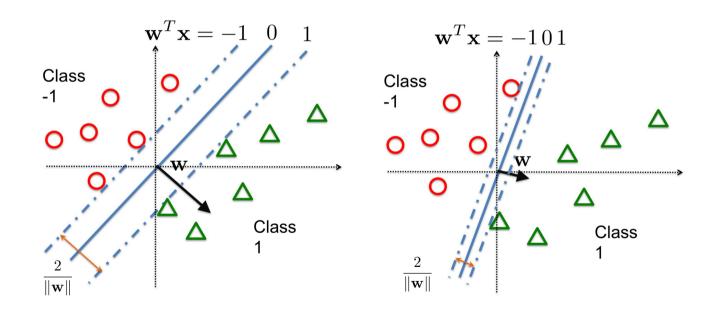
•
$$w^{T}(x^{(i)} - \gamma^{(i)} \frac{w}{\|w\|}) + b = 0$$

. Geometric margin: $\gamma^{(i)} = \frac{w^T x^{(i)} + b}{||w||}$

$$\gamma = \min_{i=1,\dots,N} \gamma^{(i)}$$

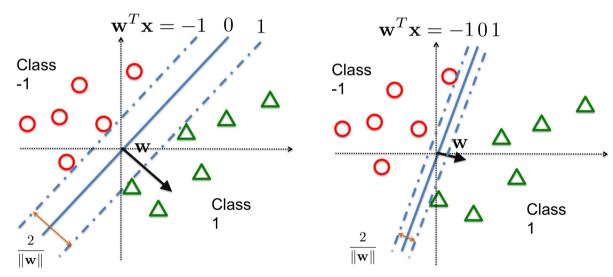


Max margin



Linear SVM

• Goal: Find a hyperplane to separate these two classes of data: if $y_i = 1, w^T x_i \ge 1$; if $y_i = -1, w^T x_i \ge -1$



Prefer a hyperplane with maximum margin

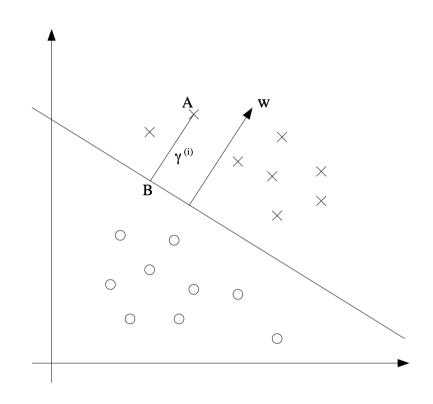
Margin

$$\gamma^{(i)} = \frac{w^T x^{(i)} + b}{\|w\|}$$

$$\gamma = \min_{i=1}^{m} \gamma^{(i)}$$

$$\max_{\gamma,w,b} \frac{\gamma}{\|w\|}$$

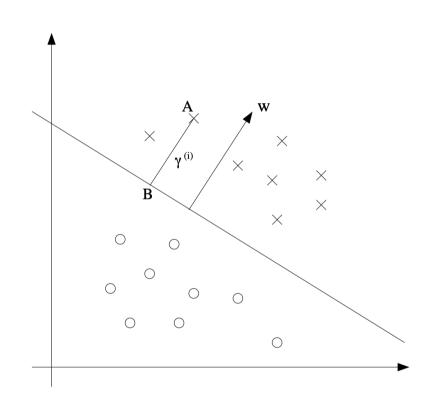
 $\max_{\gamma,w,b} \frac{\gamma}{\|w\|}$ s.t. $y_i(w^Tx_i + b) \ge \gamma, i = 1,...,n$



Margin

$$\max_{\gamma,w,b} \frac{\gamma}{\|w\|}$$

- s.t. $y_i(w^T x_i + b) \ge \gamma, i = 1,...,n$
- γ will increase linearly with w, b
- Just set $\gamma = 1$



Support Vector Machine Margin

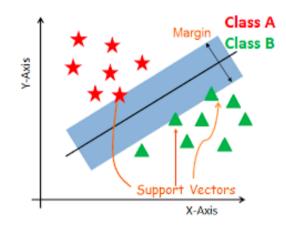
Margin

$$\max_{\gamma,w,b} \frac{\gamma}{\|w\|}$$

- s.t. $y_i(w^T x_i + b) \ge \gamma, i = 1,...,n$
- γ will increase linearly with w, b
- Just set $\gamma = 1$

$$\max_{w,b} \frac{1}{\|w\|}$$

• s.t. $y_i(w^T x_i + b) \ge 1, i = 1, ..., n$



Linear SVM (hard constraint)

• SVM primal problem (with hard constraints):

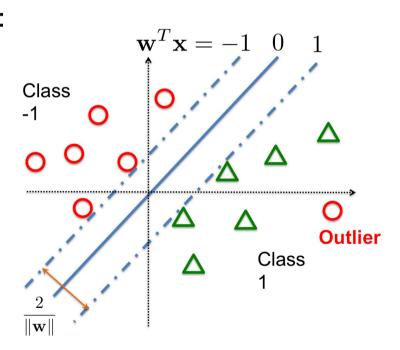
$$\min_{w} \frac{1}{2} w^{T} w$$
s.t. $y_{i}(w^{T} x_{i}) \ge 1, i = 1,...,n$

Linear SVM (hard constraint)

SVM primal problem (with hard constraints):

$$\min_{w} \frac{1}{2} w^T w$$

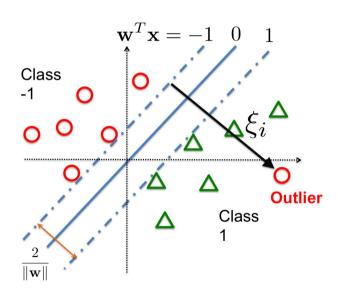
- s.t. $y_i(w^T x_i) \ge 1, i = 1, ..., n$
- What if there are outliers?



- Given training examples $(x_1, y_1), ..., (x_n, y_n)$
 - Consider binary classification: $y_i \in \{+1, -1\}$
- Linear Support Vector Machine (SVM):

$$\min_{w} \quad \frac{1}{2} w^T w + C \sum_{i=1}^{n} \xi_i$$

. s.t. $y_i(w^Tx_i) \geq 1 - \xi_i, i = 1, \dots, n$ $\xi_i \geq 0$



• SVM primal problem:

$$\min_{w} \frac{1}{2} w^{T} w + C \sum_{i=1}^{n} \xi_{i}$$
• s.t. $y_{i}(w^{T} x_{i}) \ge 1 - \xi_{i}, i = 1, ..., n$

- s.t. $y_i(w^T x_i) \ge 1 \xi_i, i = 1, ..., r$ $\xi_i \ge 0$
- · Equivalent to

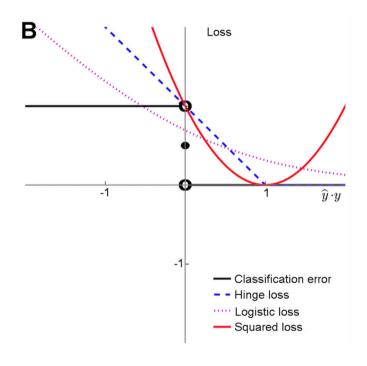
$$\underset{w}{\operatorname{arg\,min}} C \sum_{i=1}^{n} \max(1 - y_{i}w^{T}x_{i}, 0) + \underbrace{\frac{1}{2}w^{T}w}_{\text{hinge loss}}$$
 L2 regularization

• None-differentiable when $y_i w^T x_i = 1$ for some i

- Given training examples $(x_1, y_1), ..., (x_n, y_n)$
 - Consider binary classification: $y_i \in \{+1, -1\}$
- Linear Support Vector Machine (SVM):

•
$$\arg\min_{w} C \sum_{i=1}^{n} \max(1 - y_i w^T x_i, 0) + \frac{1}{2} w^T w$$

(Hinge loss with I2 regularization)



Stochastic subgradient method for SVM

• A sub gradient of $\ell_i(w) = \max(0, 1 - y_i w^T x_i)$:

$$\nabla_{w} \mathcal{E}_{i}(w) = \begin{cases} -y_{i} x_{i}, & \text{if } 1 - y_{i} w^{T} x_{i} > 0 \\ 0, & \text{if } 1 - y_{i} w^{t} x_{i} < 0 \\ 0, & \text{if } 1 - y_{i} w^{T} x_{i} = 0 \end{cases}$$

Stochastic subgradient descent for SVM:

For
$$t=1,2,\ldots$$
 Randomly pick an index i If $y_i \boldsymbol{w}^T \boldsymbol{x}_i < 1$, then $\boldsymbol{w} \leftarrow (1-\eta_t) \boldsymbol{w} + \eta_t n C y_i \boldsymbol{x}_i$ Else (if $y_i \boldsymbol{w}^T \boldsymbol{x}_i \geq 1$): $\boldsymbol{w} \leftarrow (1-\eta_t) \boldsymbol{w}$

• SVM primal problem:

$$\min_{w} \quad \frac{1}{2} w^{T} w + C \sum_{i=1}^{n} \xi_{i}$$
• s.t. $y_{i}(w^{T} x_{i}) \geq 1 - \xi_{i}, i = 1, ..., n$
 $\xi_{i} \geq 0$

Equivalent to

$$\operatorname{arg\,min}_{w} C \sum_{i=1}^{n} \max(1 - y_{i}w^{T}x_{i}, 0) + \underbrace{\frac{1}{2}w^{T}w}_{\text{hinge loss}}$$
L2 regularization

- None-differentiable when $y_i w^T x_i = 1$ for some i
- Alternatively, we show how to derive the dual form of SVM

Linear SVM dual

• SVM primal problem:

$$\min_{w} \quad \frac{1}{2}w^T w + C \sum_{i=1}^{n} \xi_i$$

- s.t. $y_i(w^Tx_i) \ge 1 \xi_i, i = 1,...,n$ $\xi_i \ge 0$
- Equivalent to: (using Lagrange multiplier):

$$\min_{w,\xi} \max_{\alpha \ge 0, \beta \ge 0} \frac{1}{2} ||w||^2 + C \sum_{i} \xi_i - \sum_{i} \alpha_i (y_i w^T x_i - 1 + \xi_i) - \sum_{i} \beta_i \xi_i$$

Linear SVM dual form

• SVM primal problem:

$$\min_{w} \quad \frac{1}{2} w^T w + C \sum_{i=1}^{n} \xi_i$$

- s.t. $y_i(w^T x_i) \ge 1 \xi_i, i = 1,...,n$ $\xi_i \ge 0$
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• Under certain condition (e.g., Slater's condition), exchanging min, max will not change the optimal solution:

$$\max_{\alpha \ge 0, \beta \ge 0} \min_{w, \xi} \frac{1}{2} ||w||^2 + C \sum_{i} \xi_i - \sum_{i} \alpha_i (y_i w^T x_i - 1 + \xi_i) - \sum_{i} \beta_i \xi_i$$

Linear SVM dual form

• Reorganize the equation:

$$\max_{\alpha \ge 0, \beta \ge 0} \min_{w, \xi} \frac{1}{2} ||w||^2 - \sum_{i} \alpha_i y_i w^T x_i + \sum_{i} \xi_i (C - \alpha_i - \beta_i) + \sum_{i} \alpha_i$$

• Now, for any given α, β , the minimizer of w will satisfy

$$\frac{\partial L}{\partial w} = w - \sum_{i} \alpha_{i} y_{i} x_{i} = 0 \Rightarrow w^{*} = \sum_{i} y_{i} \alpha_{i} x_{i}$$

- Also, we have $C = \alpha_i + \beta_i$, otherwise ξ_i can make the objective function $-\infty$
- Subsititue these two equations back we get

$$\max_{\alpha \ge 0, \beta \ge 0, C = \alpha + \beta} - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j x_i^T x_j + \sum_i \alpha_i$$

Linear SVM dual

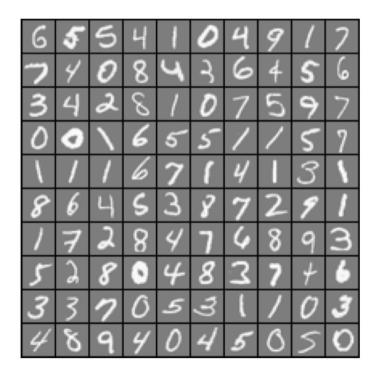
- Therefore, we get the following dual problem
 - $\max_{C>\alpha>0} \left\{ -\frac{1}{2} \alpha^T Q \alpha + e^T \alpha \right\} := D(\alpha),$
 - Where Q is an $n \times n$ matrix with $Q_{ij} = y_i y_j x_i^T x_j$
- Based on the derivations, we know
 - Primal minimum = dual maximum (under Slater's condition)
 - Let α^* be the dual solution and w^* be the primal solution, we have

$$w^* = \sum_i y_i \alpha_i^* x_i$$

We can solve the dual problem instead of primal problem

Multi-class

- n data points, L labels, d features
- Input: training data $\{x_i, y_i\}_{i=1}^n$:
 - Each x_i is a d dimensional feature vector
 - Each $y_i \in \{1,...,L\}$ is the corresponding label
 - Each training data belongs to one category
- Goal: find a function to predict the correct label
 - $f(x) \approx y$



Reduction to binary classification

- Many algorithms for binary classification
- Idea: transform multi-class or multi-label problems to multiple binary classification problems
- Two approaches:
 - One versus All (OVA)
 - One versus One (OVO)

Multi problems One Versus All (OVA)

- Multi-class/multi-label problems with *L* categories
- Build *L* different binary classifiers
- For the *t*-th classifier:
 - Positive samples: all the points in class t ($\{x_i : t \in y_i\}$)
 - Negative samples: all the points not in class t ($\{x_i : t \notin y_i\}$)
 - $f_t(x)$: the decision value for the *t*-th classifier
 - (Larger $f_t \Rightarrow$ higher probability that x in class t)
- · Prediction:
 - $f(x) = \arg\max_{t} f_t(x)$
- Example: using SVM to train each binary classifier

Multi problems One Versus One (OVO)

- Multi-class/multi-label problems with L categories
- Build L(L-1) different binary classifiers
- For the (s, t)-th classifier:
 - Positive samples: all the points in class s ($\{x_i : s \in y_i\}$)
 - Negative samples: all the points in class t $(\{x_i : t \notin y_i\})$
 - $f_{s,t}(x)$: the decision value for the *t*-th classifier
 - (Larger $f_{s,t}(x) \Rightarrow$ label s has higher probability than label t)
 - $f_{t,s}(x) = -f_{s,t}(x)$
- Prediction:

$$f(x) = \arg\max_{s} (\sum_{t} f_{s,t}(x))$$

• Example: using SVM to train each binary classifier

Another approach for multi-class classification

- OVA and OVO: decompose the problem by labels
 - But good binary classifiers may not imply good multi-class prediction
- Design a multi-class loss function and solve a single optimization problem

Another approach for multi-class classification

- OVA and OVO: decompose the problem by labels
 - But good binary classifiers may not imply good multi-class prediction
- Design a multi-class loss function and solve a single optimization problem
- Minimize the regularized training error:

•
$$\min_{w_1,...,w_L} \sum_{i=1}^n loss(x_i, y_i) + \lambda \sum_{j=1,...,L} w_j^T w_j$$

Main idea

- For simplicity, we assume a linear model
- Model parameters: $w_1, ..., w_L$
- For each data point *x*, compute the decision value for each label:
 - $w_1^T x, w_2^T x, ..., w_L^T x$
- Prediction:
 - $y = \arg\max_{t} w_{t}^{T} x$
- For training data x_i , y_i is the true label, so we want
 - $y_i \approx \arg\max_t w_t^T x_i$, $\forall i$

Softmax

- The predicted score for each class:
 - $w_1^T x_i, w_2^T x_i, ...$
- Loss for the i-th data is defined by
 - $-\log(\frac{e^{w_{y_i}^T x_i}}{\sum_{j} e^{w_j^T x_i}}) \text{ (probability of choosing the correct label)}$
- Solve a single optimization problem

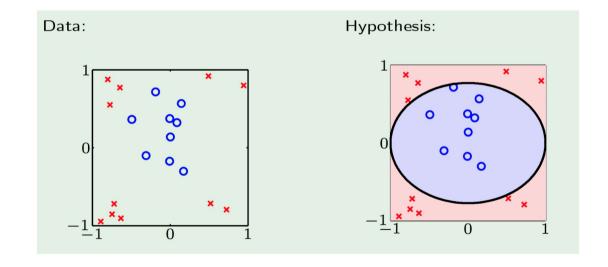
$$\min_{w_1, ..., w_L} \sum_{i=1}^n -\log(\frac{e^{w_{y_i}^T x_i}}{\sum_j e^{w_j^T x_i}}) + \lambda \sum_j w_j^T w_j$$

Loss functions for multi-class classification

- Ranking based approaches: directly minimizes the ranking loss:
 - For multi-class classification, the score of y_i should be larger than other labels
- Soft-max loss:
 - Measure the probability of predicting correct class

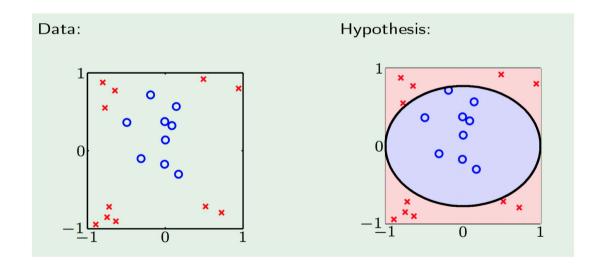
Linear hypotheses

- Up to now: linear hypotheses
 - Perception, Linear regression, Logistic regression, ...
- Many problems are not linearly separable



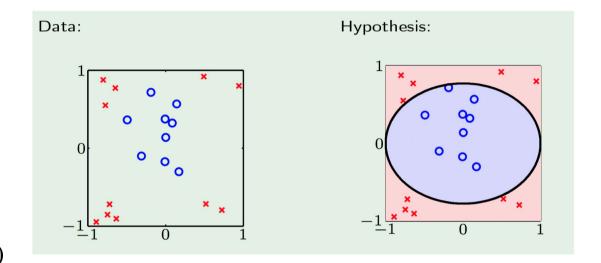
Circular Separable

 Data is not linear separable



Circular Separable

- Data is not linear separable
- But circular separable by a circle of radius $\sqrt{0.6}$ centered at origin:
 - $h_{SEP}(x) = sign(-x_1^2 x_2^2 + 0.6)$



Circular Separable and Linear Separable

•
$$h(x) = sign(0.6 \cdot 1 + (-1) \cdot x_1^2 + (-1) \cdot x_2^2)$$

Circular Separable and Linear Separable

$$h(x) = \operatorname{sign}(\underbrace{0.6} \cdot \underbrace{1} + \underbrace{(-1)} \cdot \underbrace{x_1^2} + \underbrace{(-1)} \cdot \underbrace{x_2^2})$$

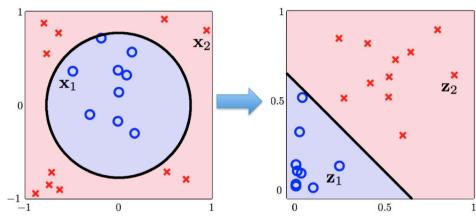
$$\overset{\tilde{w}_0}{\tilde{v}_0} \overset{\tilde{z}_0}{\tilde{z}_0} \overset{\tilde{w}_1}{\tilde{w}_1} \overset{\tilde{z}_1}{\tilde{z}_1} \overset{\tilde{w}_2}{\tilde{w}_2} \overset{\tilde{z}_2}{\tilde{z}_2}$$

$$= \operatorname{sign}(\tilde{w}^T z)$$

Circular Separable and Linear Separable

$$\begin{split} h(x) &= \mathrm{sign}(\underbrace{0.6}_{\tilde{w_0}} \cdot \underbrace{1}_{\tilde{z_0}} + \underbrace{(-1)}_{\tilde{w_1}} \cdot \underbrace{x_1^2}_{\tilde{z_1}} + \underbrace{(-1)}_{\tilde{w_2}} \cdot \underbrace{x_2^2}_{\tilde{z_2}}) \\ &= \mathrm{sign}(\tilde{w}^T z) \end{split}$$

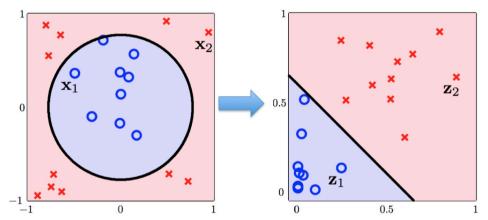
• $\{(x_n, y_n)\}$ circular separable \Rightarrow $\{(z_n, y_n)\}$ linear separable



Circular Separable and Linear Separable

$$h(x) = \operatorname{sign}(\underbrace{0.6}_{\tilde{w_0}} \cdot \underbrace{1}_{\tilde{z_0}} + \underbrace{(-1)}_{\tilde{w_1}} \cdot \underbrace{x_1^2}_{\tilde{z_1}} + \underbrace{(-1)}_{\tilde{w_2}} \cdot \underbrace{x_2^2}_{\tilde{z_2}})$$
$$= \operatorname{sign}(\tilde{w}^T z)$$

- $\{(x_n, y_n)\}$ circular separable \Rightarrow $\{(z_n, y_n)\}$ linear separable
- $x \in \mathcal{X} \to x \in \mathcal{Z}$ (using a nonlinear transformation ϕ)



Definition

- Define nonlinear transformation
 - $\phi(\mathbf{x}) = (1, x_1^2, x_2^2) = (z_0, z_1, z_2) = \mathbf{z}$

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 - $\phi(\mathbf{x}) = (1, x_1^2, x_2^2) = (z_0, z_1, z_2) = \mathbf{z}$
- Linear hypotheses in ${\mathcal Z}$ space:
 - $\operatorname{sign}(\tilde{h}(\mathbf{z})) = \operatorname{sign}(\tilde{h}(\phi(\mathbf{x}))) = \operatorname{sign}(w^T \phi(\mathbf{x}))$

Definition

- Define nonlinear transformation
 - $\phi(\mathbf{x}) = (1, x_1^2, x_2^2) = (z_0, z_1, z_2) = \mathbf{z}$
- Linear hypotheses in \mathscr{Z} -space:
 - $\operatorname{sign}(\tilde{h}(\mathbf{z})) = \operatorname{sign}(\tilde{h}(\phi(\mathbf{x}))) = \operatorname{sign}(w^T \phi(\mathbf{x}))$
- Line in \mathcal{Z} -space \Leftrightarrow some quadratic curves in \mathcal{X} -space

- A "bigger " ${\mathcal Z}$ space:
 - $\phi_2(\mathbf{x}) = (1, x_1, x_2, x_1^2, x_1 x_2, x_2^2)$

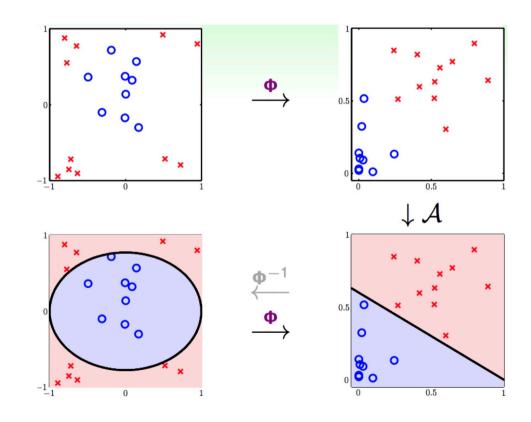
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 - $\phi_2(\mathbf{x}) = (1, x_1, x_2, x_1^2, x_1 x_2, x_2^2)$
- Linear in \mathscr{Z} -space \Leftrightarrow quadratic hypotheses in \mathscr{X} -space
- The hypotheses space:
 - $\mathcal{H}_{\phi_2} = \{h(x) : h(x) = \tilde{w}^T \phi_2(x) \text{ for some } \tilde{w}\}$ (quadratic hypotheses)

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 - $\phi_2(\mathbf{x}) = (1, x_1, x_2, x_1^2, x_1 x_2, x_2^2)$
- Linear in \mathcal{Z} -space \Leftrightarrow quadratic hypotheses in \mathcal{X} -space
- The hypotheses space:
 - $\mathcal{H}_{\phi_2} = \{h(x) : h(x) = \tilde{w}^T \phi_2(x) \text{ for some } \tilde{w}\}$ (quadratic hypotheses)
- Also include linear model as a degenerate case

Learning a good quadratic function

- Transform original data $\{x_n, y_n\}$ to $\{z_n = \phi(x_n), y_n\}$
- Solve a linear problem on $\{z_n, y_n\}$ using your favorite algorithm $\mathscr A$ to get a good model $\tilde w$
- Return the model $h(x) = \text{sign}(\tilde{w}^T \phi(x))$



Polynomial mappings

• Can now freely do quadratic classification, quadratic regression

Polynomial mappings

- Can now freely do quadratic classification, quadratic regression
- Can easily extend to any degree of polynomial mappings
 - E.g., $\phi(x) = (x_1, x_2, x_3, x_1x_2, x_1x_3, x_2x_3, x_1x_2^2, x_1x_3^2, x_1x_2^2, x_2^2x_3, x_2^2x_3, x_1^3, x_2^3, x_3^3)$

SVM with nonlinear mapping

• SVM with nonlinear mapping $\varphi(\cdot)$:

$$\min_{w} \quad \frac{1}{2} w^T w + C \sum_{i=1}^{n} \xi_i$$

- s.t. $y_i(w^T \varphi(x_i)) \ge 1 \xi_i, i = 1,...,n$ $\xi_i \ge 0$
- Hard to solve if $\varphi(\,\cdot\,)$ maps to very high or infinite dimensional space

SVM with nonlinear mapping

- · Similarly, we could derive
 - $\max_{C \ge \alpha \ge 0} \left\{ -\frac{1}{2} \alpha^T Q \alpha + e^T \alpha \right\} := D(\alpha),$
 - Where Q is an $n \times n$ matrix with $Q_{ij} = y_i y_j \varphi(x_i)^T \varphi(x_j)$
- · Based on the derivations, we know
 - Primal minimum = dual maximum (under Slater's condition)
 - Let α^* be the dual solution and w^* be the primal solution, we have

$$w^* = \sum_i y_i \alpha_i^* \varphi(x_i)$$

The price we pay: computational complexity

• *Q*-th oder polynomial transform:

$$\phi(x) = (1, x_1, x_2, ..., x_d, x_1^2, x_1 x_2, ..., x_d^2, ..., x_d^2, ..., x_d^2, ..., x_d^2, ..., x_1^Q, x_1^Q, x_1^{Q-1} x_2, ..., x_d^Q)$$

• $O(d^Q)$ dimensional vector \Rightarrow High computational cost

Kernel trick

- Do not directly define $\varphi(\,\cdot\,)$
- Instead, define "kernel"
 - $K(x_i, x_j) = \varphi(x_i)^T \varphi(x_j)$

Kernel trick

- Do not directly define $\varphi(\,\cdot\,)$
- Instead, define "kernel"
 - $K(x_i, x_j) = \varphi(x_i)^T \varphi(x_j)$
- Examples:
 - Gaussian kernel: $K(x_i, x_j) = e^{-\gamma ||x_i x_j||^2}$
 - Polynomial kernel: $K(x_i, x_j) = (\gamma x_i^T x_j + c)^d$
 - Other kernels for specific problems:
 - Graph kernels (Vishwanathan et al., "Graph Kernels", JMLR, 2010)
 - Pyramid kernel for image matching (Grauman and Darrell, "The Pyramid Match Kernel: Discriminative Classification with Sets of Image Features". In ICCV, 2005)
 - String kernel (Lodhi et al., "Text classification using string kernels". JMLR, 2002)

SVM with kernel

• Training: compute $\alpha = [\alpha_1, ..., \alpha_n]$ by solving the quadratic optimization problem:

$$\min_{0 \le \alpha \le C} \frac{1}{2} \alpha^T Q \alpha - e^T \alpha$$

• Where $Q_{ij} = y_i y_j K(x_i, x_j)$

SVM with kernel

- Training: compute $\alpha = [\alpha_1, ..., \alpha_n]$ by solving the quadratic optimization problem:
 - $\min_{0 < \alpha < C} \frac{1}{2} \alpha^T Q \alpha e^T \alpha$
 - Where $Q_{ij} = y_i y_j K(x_i, x_j)$
- Prediction: for a test data x,

$$w^T \varphi(x) = \sum_{i=1}^n y_i \alpha_i \varphi(x_i)^T \varphi(x) = \sum_{i=1}^n y_i \alpha_i K(x_i, x)$$

Kernel trick

Kernel Ridge Regression

- Actually, this "kernel method" works for many different losses
- Example: ridge regression

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$$\min_{w} \frac{1}{2} ||w||^2 + \frac{1}{2} \sum_{i=1}^{n} (w^T \varphi(x_i) - y_i)^2$$

- Dual problem:
 - $\min_{\alpha} \alpha^T Q \alpha + \|\alpha\|^2 2\alpha^T y$

Kernel trick Scalability

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 - Space: $O(n^2)$ for storing the $n \times n$ kernel matrix (can be reduced in some cases);
 - Time: $O(n^3)$ for computing the exact solution

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- Good packages available:
 - LIBSVM (can be called in scikit-learn)
 - LIBLINEAR (for linear SVM, can be called in scikit-learn)