Machine learning: lecture 8

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Topics

- Support vector machines
  - training, prediction
  - other kernel methods
- Kernels
  - examples, properties, construction
  - feature vectors and sparsity

SVM summary

- **Training:** We can find the optimal setting of the Lagrange multipliers α_i by maximizing

$$\sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} y_i y_j \alpha_i \alpha_j K(\mathbf{x}_i, \mathbf{x}_j)$$

subject to $0 \leq \alpha_i \leq C$ and $\sum_i \alpha_i y_i = 0$.

  - larger C means larger penalty for errors
  - $\hat{\alpha}_i = 0$ except for "support vectors"
  - all misclassified examples will be support vectors
  - $\hat{w}_0$ can be found based on examples for which $\hat{\alpha}_i$ is between 0 and C (when classification constraints are satisfied with equality)

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- **Prediction:** We make predictions according to the sign of the discriminant function

$$\hat{y} = \text{sign}\big(\hat{w}_0 + \sum_{i \in SV} \hat{\alpha}_i y_i K(\mathbf{x}, \mathbf{x}_i)\big)$$

Other kernel methods: linear regression

- A linear regression model with feature vectors:

$$f(\mathbf{x}; \mathbf{w}) = \phi(\mathbf{x})^T \mathbf{w}_1 + w_0,$$

where $\phi(\mathbf{x}) = [\phi_1(\mathbf{x}), \ldots, \phi_m(\mathbf{x})]^T$.

We can train these models via regularized least squares

$$\min \quad \frac{1}{2} \sum_{i=1} (y_i - f(\mathbf{x}; \mathbf{w}))^2 + \frac{\lambda}{2} \|\mathbf{w}_1\|^2$$

- We'd like to turn these models into kernel methods where the examples (feature vectors) appear only in inner products $K(\mathbf{x}, \mathbf{x}') = \phi^T(\mathbf{x}) \phi(\mathbf{x}')$.

Other kernel methods: linear regression

- **Training**: maximize

$$\sum_{i=1}^{n} \left(\alpha_i y_i - \lambda \alpha_i^2 / 2\right) - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j K(\mathbf{x}_i, \mathbf{x}_j)$$

subject to $\alpha_i \in \mathcal{R}$ and $\sum_i \alpha_i = 0$.

The offset parameter $\hat{w}_0$ can be obtained directly from the solution:

$$\hat{w}_0 = \frac{1}{n} \sum_{i=1}^{n} \big(y_i - \sum_{j=1}^{n} \hat{\alpha}_j K(\mathbf{x}_i, \mathbf{x}_j)\big)$$

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- **Prediction**: the predicted output for a new point $\mathbf{x}$ is

$$f(\mathbf{x}; \hat{\alpha}, \hat{w}_0) = \hat{w}_0 + \sum_{i=1}^{n} \hat{\alpha}_i K(\mathbf{x}, \mathbf{x}_i)$$

Other kernel methods: logistic regression

- A logistic regression model with feature vectors

$$P(y = 1|\mathbf{x}, \mathbf{w}) = g\left(\, \phi(\mathbf{x})^T \mathbf{w}_1 + w_0 \,\right)$$

where $\phi(\mathbf{x}) = [\phi_1(\mathbf{x}), \ldots, \phi_m(\mathbf{x})]^T$

As before we can train these models by minimizing the following regularized empirical loss (maximizing penalized log-likelihood):

$$\min \quad \sum_{i=1}^{n} -\log P(y_i|\mathbf{x}_i, \mathbf{w}) + \frac{\lambda}{2} \|\mathbf{w}_1\|^2$$

Other kernel methods: logistic regression

- **Training**: maximize

$$\sum_{i=1}^{n} H(\lambda \alpha_i)/\lambda - \frac{1}{2} \sum_{i,j=1}^{n} y_i y_j \alpha_i \alpha_j K(\mathbf{x}_i, \mathbf{x}_j)$$

subject to $0 \leq \alpha_i \leq 1/\lambda$ and $\sum_i \alpha_i y_i = 0$.

Here $H(p) = -p \log(p) - (1-p)\log(1-p)$ is the binary entropy function. $\hat{w}_0$ has to be solved iteratively after obtaining $\hat{\alpha}$.

Other kernel methods: logistic regression

- **Training**: maximize

$$\sum_{i=1}^{n} H(\lambda \alpha_i)/\lambda - \frac{1}{2} \sum_{i,j=1}^{n} y_i y_j \alpha_i \alpha_j K(\mathbf{x}_i, \mathbf{x}_j)$$

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Here $H(p) = -p \log(p) - (1-p)\log(1-p)$ is the binary entropy function. $\hat{w}_0$ has to be solved iteratively after obtaining $\hat{\alpha}$.

- **Prediction:** the predicted probabilities over possible labels for a new point $\mathbf{x}$ are given by

$$P(y = 1|\mathbf{x}, \hat{\alpha}, \hat{w}_0) = g\left(\, \hat{w}_0 + \sum_{i=1}^{n} \hat{\alpha}_i y_i K(\mathbf{x}, \mathbf{x}_i) \,\right)$$

Example kernels

- **Linear kernel**

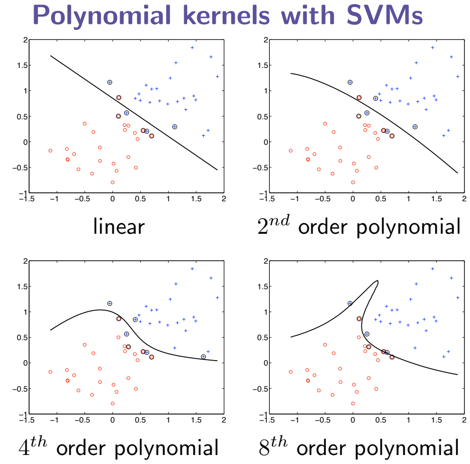
$$K(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^T \mathbf{x}')$$

- **Polynomial kernel**

$$K(\mathbf{x}, \mathbf{x}') = \left(1 + (\mathbf{x}^T \mathbf{x}')\right)^p$$

where $p = 2, 3, \ldots$. To get the feature vectors we concatenate all up to p^{th} order polynomial terms of the components of $\mathbf{x}$ (weighted appropriately)

Polynomial kernels with SVMs

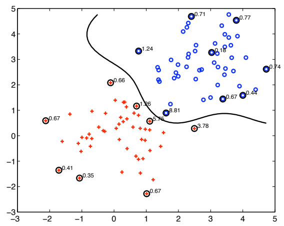


Example kernels

- **Radial basis kernel**

$$K(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{1}{2}\|\mathbf{x} - \mathbf{x}'\|^2\right)$$

In this case the feature space is infinite dimensional function space (use of the kernel results in a *non-parametric* classifier).



– support vectors need not appear close to the boundary in the input space, only in the feature space

Definition of kernels

- We can think of kernels in terms of explicit or implicit feature mappings
  – Definition 1: $K(\mathbf{x}, \mathbf{x}')$ is a kernel if it can be written as an inner product $\phi(\mathbf{x})^T\phi(\mathbf{x}')$ for some feature mapping ϕ.
  – Definition 2: $K(\mathbf{x}, \mathbf{x}')$ is a kernel if for any finite set of training examples, $\mathbf{x}_1, \ldots, \mathbf{x}_n$, the $n \times n$ matrix $K_{ij} = K(\mathbf{x}_i, \mathbf{x}_j)$ is positive semi-definite.

Kernels and construction

- We can build kernels from simpler ones. For example:
  – If $K_1(\mathbf{x}, \mathbf{x}')$ and $K_2(\mathbf{x}, \mathbf{x}')$ are valid kernels then

$$\begin{aligned} f(\mathbf{x})K_1(\mathbf{x}, \mathbf{x}')f(\mathbf{x}') &\quad \text{(scaling)} \\ K_1(\mathbf{x}, \mathbf{x}') + K_2(\mathbf{x}, \mathbf{x}') &\quad \text{(sum)} \\ K_1(\mathbf{x}, \mathbf{x}')K_2(\mathbf{x}, \mathbf{x}') &\quad \text{(product)} \end{aligned}$$

  are valid kernels.

  – If $\mathbf{x} = [x_1, \ldots, x_d]^T \in \mathcal{R}^d$ and $K_i(x_i, x_i')$ are valid 1-dimensional kernels, then

$$K(\mathbf{x}, \mathbf{x}') = \prod_{i=1}^{d} K_i(x_i, x_i')$$

  is a valid kernel in $\mathcal{R}^d$.

Kernels and sequences

- We can also derive kernels for variable length sequences. For example:

$\mathbf{x} = $ `... my first day this term was ...`
$\mathbf{x}' = $ `... Last year the midterm had ...`

Gap-weighted subsequence kernel:

$$K(\mathbf{x}, \mathbf{x}') = \sum_{u \in \Sigma^d} \sum_{\vec{i}: u = \mathbf{x}[\vec{i}]} \sum_{\vec{j}: u = \mathbf{x}[\vec{j}]} \lambda^{(i_d - i_1)} \lambda^{(j_d - j_1)}$$

where $\lambda \in (0, 1)$ and Σ^d is the set of all sequences of length d. The kernel reflects the degree to which the sequences have common subsequences penalizing non-contiguous subsequences.

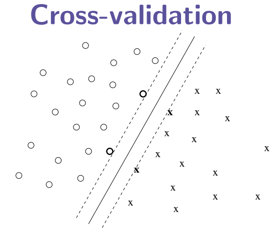
Dimensionality and complexity

- Many of these kernels correspond to very high dimensional feature spaces
  – polynomial kernel for large p or $dim(\mathbf{x})$
  – radial basis kernel (infinite)
  – subsequence kernel (combinatorial)
  etc.
- The dimensionality of the feature space determines the number of parameters in the primal formulation

$$\min \;\; \|\mathbf{w}_1\|^2 \;\; \text{subject to} \;\; y_i[w_0 + \phi(\mathbf{x}_i)^T\mathbf{w}_1] - 1 \geq 0, \;\; \forall i$$

Can these methods generalize?

Cross-validation



- For SVMs the leave-one-out cross-validation error does not depend on the dimensionality of the feature space but only on the # of support vectors

$$\text{Leave-one-out CV error} \leq \frac{\#\ \text{support vectors}}{\#\ \text{of training examples}}$$

(similar results exist for kernel logistic regression)

Kernels, examples, sparsity

- High dimensional feature vectors (many basis functions) can still permit a sparse solution in terms of the number of training examples

$$\underbrace{\begin{array}{c}\phi(\mathbf{x}_1)\\ \begin{bmatrix}\phi_1(\mathbf{x}_1)\\ \phi_2(\mathbf{x}_1)\\ \phi_3(\mathbf{x}_1)\\ \ldots\\ \phi_d(\mathbf{x}_1)\end{bmatrix}\end{array} \quad \begin{array}{c}\phi(\mathbf{x}_2)\\ \begin{bmatrix}\phi_1(\mathbf{x}_2)\\ \phi_2(\mathbf{x}_2)\\ \phi_3(\mathbf{x}_2)\\ \ldots\\ \phi_d(\mathbf{x}_2)\end{bmatrix}\end{array}}_{\text{a few examples)}} \quad \ldots \quad \begin{array}{c}\phi(\mathbf{x}_n)\\ \begin{bmatrix}\phi_1(\mathbf{x}_n)\\ \phi_2(\mathbf{x}_n)\\ \phi_3(\mathbf{x}_n)\\ \ldots\\ \phi_d(\mathbf{x}_n)\end{bmatrix}\end{array} \left.\begin{array}{l} \\ \\ \end{array}\right\} \text{a few components}$$

- Alternatively, we could try to find a few basis functions (components) that solve the classification/regression task