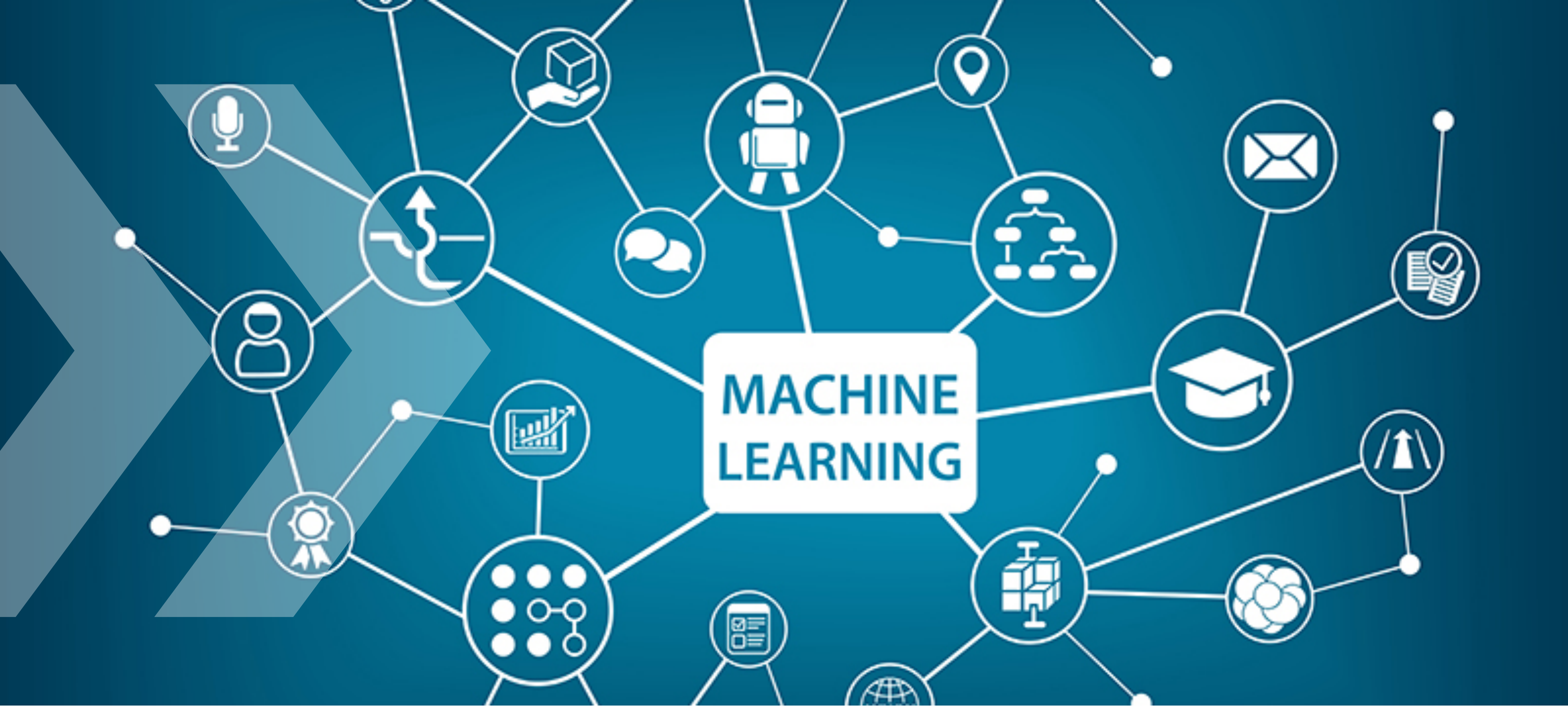

CS489/698: Intro to ML

Lecture 08: Kernels

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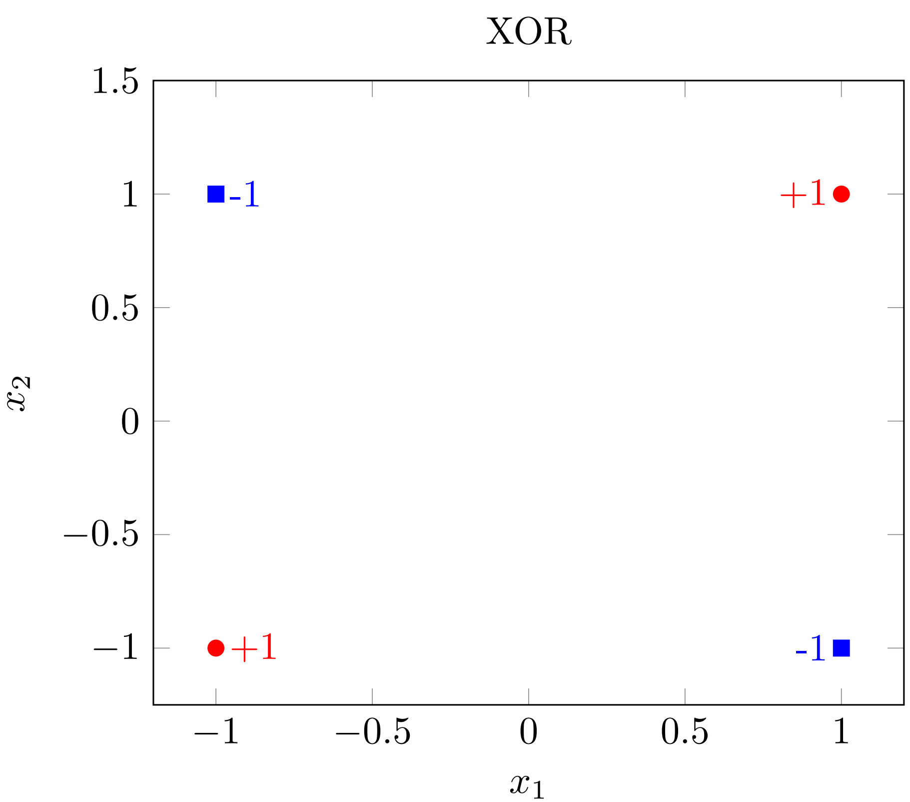
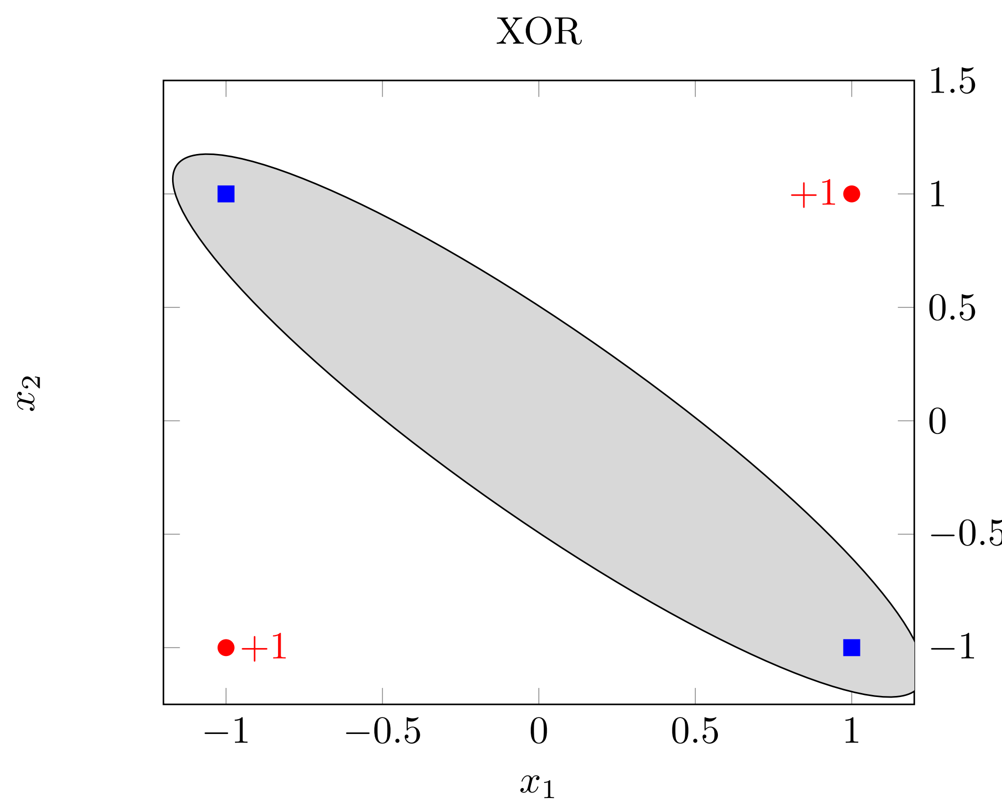
Outline

- Feature map
- Kernels
- The Kernel Trick
- Advanced

XOR revisited





Quadratic classifier

Weights
(to be learned)

$$\mathbf{x}^\top \boxed{Q}\mathbf{x} + \sqrt{2}\mathbf{x}^\top \boxed{\mathbf{p}} + \boxed{\gamma} \geq 0$$

$$\Updownarrow$$

$$\hat{y} = f(\mathbf{x}) = 1$$

The power of lifting

$$\mathbf{x}^\top Q\mathbf{x} + \sqrt{2}\mathbf{x}^\top \mathbf{p} + \gamma \geq 0$$

$$\Vert$$

$$\mathbf{w}^\top \phi(\mathbf{x}) \geq 0$$

$R^d \rightarrow R^{d*d+d+1}$

Feature map

$$\phi(\mathbf{x}) = \begin{bmatrix} \overrightarrow{\mathbf{x}\mathbf{x}^\top} \\ \sqrt{2}\mathbf{x} \\ 1 \end{bmatrix} \qquad \mathbf{w} = \begin{bmatrix} \overrightarrow{Q} \\ \mathbf{p} \\ \gamma \end{bmatrix}$$

Example

$$\phi(\mathbf{x}) = [x_1^2, \sqrt{2}x_1x_2, x_2^2, \sqrt{2}x_1, \sqrt{2}x_2, 1]$$

$$\phi(\mathbf{x}) = [x_1^2, x_1x_2, x_1x_2, x_2^2, \sqrt{2}x_1, \sqrt{2}x_2, 1]$$

Curse of dimensionality?

$$\phi : \mathbf{R}^d \to \mathbf{R}^{\boxed{d^2+d+1}}$$

computation in this space now

$$\phi(\mathbf{x}) = \begin{bmatrix} \overrightarrow{\mathbf{x}\mathbf{x}^\top} \\ \sqrt{2}\mathbf{x} \\ 1 \end{bmatrix}$$

But, all we need is the dot product !!!

$$\begin{aligned} \phi(\mathbf{x})^\top \phi(\mathbf{x}') &= (\mathbf{x}^\top \mathbf{x}')^2 + 2\mathbf{x}^\top \mathbf{x}' + 1 \\ &= (\mathbf{x}^\top \mathbf{x}' + 1)^2 \end{aligned}$$

- This is still computable in O(d)!

Feature transform

$$\phi : \mathbf{R}^d \to \mathbf{R}^h$$

- NN: learn φ simultaneously with **w**

- Here: choose a nonlinear φ so that for some *f* : R→R

$$\phi(\mathbf{x})^\top \phi(\mathbf{x}') = \boxed{f(\mathbf{x}^\top \mathbf{x}')}$$

save computation

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Reverse engineering

- Start with some function $k : \mathbf{R}^d \times \mathbf{R}^d \to \mathbf{R}$, s.t. exists feature transform φ with

$$\phi(\mathbf{x})^\top \phi(\mathbf{x}') = k(\mathbf{x}, \mathbf{x}')$$

- As long as *k* is efficiently computable, don't care the dim of φ (could be infinite!)

- Such *k* is called a (reproducing) kernel.

Examples

- Polynomial kernel

$$k(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^\top \mathbf{x}')^p$$

$$k(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^\top \mathbf{x}' + 1)^p$$

- Gaussian Kernel

$$k(\mathbf{x}, \mathbf{x}') = \exp(-\|\mathbf{x} - \mathbf{x}'\|_2^2 / \sigma)$$

- Laplace Kernel

$$k(\mathbf{x}, \mathbf{x}') = \exp(-\|\mathbf{x} - \mathbf{x}'\|_2 / \sigma)$$

- Matérn Kernel

$$\frac{1}{2^{\nu-1}\Gamma(\nu)} \Big(\frac{2\sqrt{\nu}\|\mathbf{x} - \mathbf{x}'\|_2}{\theta}\Big)^\nu H_\nu \Big(\frac{2\sqrt{\nu}\|\mathbf{x} - \mathbf{x}'\|_2}{\theta}\Big)$$

Verifying a kernel

For any n, for any x_1, x_2, …, x_n, the kernel matrix K with

$$K_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$$

is symmetric and positive semidefinite ($K \in \mathbb{S}_+^d$)

- Symmetric: $K_{ij} = K_{ji}$
- Positive semidefinite (PSD): for all $\boldsymbol{\alpha} \in \mathbf{R}^n$

$$\boldsymbol{\alpha}^\top K \boldsymbol{\alpha} = \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j K_{ij} \geq 0$$

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Kernel calculus

- If k is a kernel, so is λk for any $\lambda \geq 0$
- If k_1 and k_2 are kernels, so is k_1+k_2
- If k_1 and k_2 are kernels, so is $k_1 k_2$

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Kernel SVM (dual)

$$\min_{C \geq \alpha \geq 0} \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \boxed{K_{ij}} - \sum_{i=1}^{n} \alpha_i$$

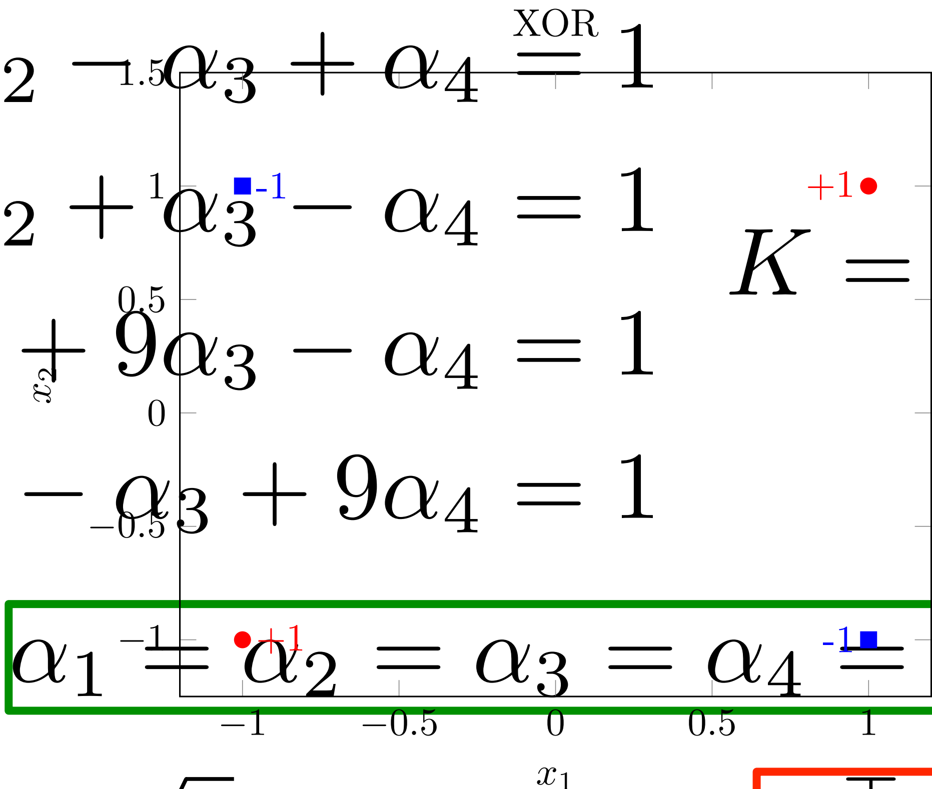
$$\text{s.t.} \sum_{i} \alpha_i y_i = 0$$

With **α**, $\mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \phi(\mathbf{x}_i)$ but φ is implicit…

Does it work?

$$9\alpha_1 - \alpha_2 - \alpha_3 + \alpha_4 = 1$$
$$-\alpha_1 + 9\alpha_2 + \alpha_3 - \alpha_4 = 1$$
$$-\alpha_1 + \alpha_2 + 9\alpha_3 - \alpha_4 = 1$$
$$\alpha_1 - \alpha_2 - \alpha_3 + 9\alpha_4 = 1$$

$$K = \begin{bmatrix} 9 & 1 & 1 & 1 \\ 1 & 9 & 1 & 1 \\ 1 & 1 & 9 & 1 \\ 1 & 1 & 1 & 9 \end{bmatrix}$$



$$\boxed{\alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = 1/8}$$

$$\mathbf{w} = [0, -1/\sqrt{2}, 0, 0, 0, 0] \qquad \boxed{\mathbf{w}^\top \phi(\mathbf{x}) = -x_1 x_2}$$

$$\phi(\mathbf{x}) = [x_1^2, \sqrt{2}x_1x_2, x_2^2, \sqrt{2}x_1, \sqrt{2}x_2, 1]$$

Testing

- Given test sample **x**', how to perform testing?

$$\mathbf{w}^\top \phi(\mathbf{x}') = \sum_{i=1}^{n} \alpha_i y_i \phi(\mathbf{x}_i)^\top \phi(\mathbf{x}')$$

$$= \sum_{i=1}^{n} \alpha_i y_i k(\mathbf{x}_i, \mathbf{x}')$$

No explicit access to φ, again!

dual variables

training set

kernel

Tradeoff

- Previously: training O(nd), test O(d)
- Kernel: training $O(n^2)$, test O(n)
- Nice to avoid explicit dependence on h (could be inf)
- But if n is also large… ~~(maybe later)~~

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Learning the kernel (Lanckriet et al.'04)

$$\min_{C \geq \alpha \geq 0} \max_{\zeta \geq 0} \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \left[\sum_{s=1}^{t} \zeta_s K_{ij}^{(s)} \right] - \sum_{i=1}^{n} \alpha_i$$

$$\text{s.t.} \quad \sum_{i} \alpha_i y_i = 0$$

- Nonnegative combination of *t* pre-selected kernels, with coefficients ζ simultaneously learned

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Logistic regression revisited

$$\min_{\mathbf{w}\in\mathbf{R}^d} \sum_i \log(1 + e^{-y_i \mathbf{w}^\top \mathbf{x}_i}) + \lambda\|\mathbf{w}\|_2^2$$

kernelize

$$\min_{\mathbf{w}\in\mathbf{R}^h} \sum_i \log(1 + e^{-y_i \mathbf{w}^\top \phi(\mathbf{x}_i)}) + \boxed{\lambda\|\mathbf{w}\|_2^2}$$

Representer Theorem (Wabha, Schölkopf, Herbrich, Smol Dinuzzo, …).

The optimal w has the following form:

$$\mathbf{w} = \sum_i \alpha_i \phi(\mathbf{x}_i)$$

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Kernel Logistic Regression (primal)

$$\boxed{\min_{\boldsymbol{\alpha} \in \mathbf{R}^n} \ \sum_i \log(1 + e^{-y_i \boldsymbol{\alpha}^\top K_{:i}}) + \lambda \boldsymbol{\alpha}^\top K \boldsymbol{\alpha}}$$

$$\min_{\mathbf{w} \in \mathbf{R}^d} \ \sum_i \log(1 + e^{-y_i \mathbf{w}^\top \mathbf{x}_i}) + \lambda \mathbf{w}^\top \mathbf{w}$$

$$\boldsymbol{\alpha}_{t+1} \leftarrow \boldsymbol{\alpha}_t - \eta_t [\nabla^2 f(\boldsymbol{\alpha}_t)]^{-1} \cdot \nabla f(\boldsymbol{\alpha}_t)$$

$$\nabla^2 f(\boldsymbol{\alpha}_t) = \sum_i p_i (1 - p_i) K_{:i} K_{:i}^\top + 2\lambda K$$

$$\nabla f(\boldsymbol{\alpha}_t) = K^\top (\mathbf{p} - \mathbf{y}) + \lambda K \boldsymbol{\alpha}_t$$

$$p_i = \frac{1}{1 + e^{-\boldsymbol{\alpha}_t^\top K_{:i}}}$$

uncertain predictions get bigger weight

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Universal approximation (Micchelli, Xu, Zhang'06)

Universal kernel. For any compact set Z, for any continuous function $f : Z \to \mathbf{R}$, for any $\varepsilon > 0$, there exist $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$ in Z and $\alpha_1, \alpha_2, \ldots, \alpha_n$ in $\mathbf{R}$ such that

$$\max_{\mathbf{x} \in Z} \left| f(\mathbf{x}) - \sum_{i=1}^{n} \alpha_i k(\mathbf{x}, \mathbf{x}_i) \right| \leq \epsilon$$

decision boundary

kernel methods

Example. The Gaussian kernel. $\exp(-\|\mathbf{x} - \mathbf{x}'\|_2^2 / \sigma)$

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Kernel mean embedding (Smola, Song, Gretton, Schölkopf, …)

$$\mathbf{P} \mapsto \mu_{\mathbf{P}} := \mathbf{E}(\phi(X)), \quad \text{where } X \sim \mathbf{P}$$

feature map of some kernel

- Characteristic kernel: the above mapping is 1-1
- Completely preserve the information in the distribution P
- Lots of applications

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Questions?