ECE597ML-697ML: Kernel Trick

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Big Picture: So Far

- Cost function paradigm for supervised machine learning
  - Input $\mathbf{x}$
  - Output $\mathbf{y}$
  - Find $h_{\boldsymbol{\theta}}(\mathbf{x})$ such that $h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) \approx y^{(i)}$
  - Cost function $J(\boldsymbol{\theta})$
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  - Regularization to avoid overfitting
- Everything so far has been based on **linear models**
  $h_{\boldsymbol{\theta}}(\mathbf{x}) = g(\boldsymbol{\theta}^T \mathbf{x})$

Kernel-Trick Motivation

- But what we really want are flexible non-linear classifers!
  - How can we get this with linear methods?
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  - Kernel trick!
- Wait... feature expansions already allow non-linear learning...

$$(x_1, x_2) \mapsto (1, x_1, x_2, x_1^2, x_2^2, x_1 x_2)$$

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- **Kernel trick**: non-linear feature expansions in implicit way way
  - Computationally efficient
  - Don't actually do expansion

Kernel Trick Starting Point

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- $\boldsymbol{\theta}$ in span of feature vectors
- We'll discuss later how to find $\alpha_1, \ldots, \alpha_m$

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- How to find $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_m)$? Minimize $J(\boldsymbol{\alpha})$. (More later)
- Note: (*) only needs to hold for $\boldsymbol{\theta}$ that minimizes $J(\boldsymbol{\theta})$

Takeaway

$$\boxed{\begin{aligned} h_{\boldsymbol{\theta}}(\mathbf{x}) &= \sum_{i=1}^{m} \alpha_i K(\mathbf{x}^{(i)}, \mathbf{x}) \\ J(\boldsymbol{\theta}) &= \frac{1}{2} \sum_{k=1}^{m} \left(\sum_{i=1}^{m} \alpha_i K(\mathbf{x}^{(i)}, \mathbf{x}^{(k)}) - y^{(k)} \right)^2 \end{aligned}}$$

Thought experiment: I hold feature vectors in a box. You can ask me only for dot products. Can you still train model? Make predictions?

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Concrete Example: “Kernelized” Linear Regression

- **Observation:** can rewrite linear regression as a *different* linear regression model:

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- Map $\mathbf{x}$ to new "feature vector" $k(\mathbf{x})$ (= kernel evaluation between $\mathbf{x}$ and each training feature vector.

- What happens to original data matrix X under this mapping? (Recall: ith row of X is ith feature vector $\mathbf{x}^{(i)}$.)

- We get a new "data matrix" K, whose ith row is holds dot products between $\mathbf{x}^{(i)}$ and each *other* training point:

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- Note: this equivalance is only exact without regularization. In practice: use a different optimization method to find $\boldsymbol{\alpha}$ to minimize $J(\boldsymbol{\alpha})$

Linear Models

Same reasoning applies more generally to any linear model of this form:

$$\boxed{\begin{aligned} h_{\boldsymbol{\theta}}(\mathbf{x}) &= g(\boldsymbol{\theta}^T\mathbf{x}) \\ J(\boldsymbol{\theta}) &= \sum_{k=1}^{m} \mathsf{cost}(\boldsymbol{\theta}^T\mathbf{x}^{(k)}, y^{(k)}) \end{aligned}}$$

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- Can fit model by substituting kernel matrix for data matrix.

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Example: Polynomial Kernel

Important trick: we can often compute kernel without actually doing the expansion

$$K(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^T \mathbf{z})^2$$

Claim: this is the kernel corresponding to $\phi(\mathbf{x}) = \begin{bmatrix} x_1 x_1 \\ x_1 x_2 \\ x_2 x_1 \\ x_2 x_2 \end{bmatrix}$

Exercise: verify this on board

More Polynomial Kernels

Claim: these two are equivalent

$$\phi(\mathbf{x}) = \begin{bmatrix} 1 \\ \sqrt{2}x_1 \\ \sqrt{2}x_2 \\ x_1x_1 \\ x_1x_2 \\ x_2x_1 \\ x_2x_2 \end{bmatrix} \qquad K(\mathbf{x},\mathbf{z}) = (\mathbf{x}^T\mathbf{z}+1)^2$$

- Complexity of computing $\phi(\mathbf{x})^T\phi(\mathbf{z})$?
- Complexity of computing $\mathbf{x}^T\mathbf{z}$?
- Complexity of computing $(\mathbf{x}^T\mathbf{z}+1)^2$?

Polynomial Kernel: Significance

- Compute $\phi(\mathbf{x})^T\phi(\mathbf{z})$: $O(n^2)$
- Compute $\mathbf{x}^T\mathbf{z}$: $O(n)$
- Compute $(\mathbf{x}^T\mathbf{z}+1)^2$: $O(n)$

Polynomial Kernel: Significance

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- Compute $\mathbf{x}^T\mathbf{z}$: $O(n)$
- Compute $(\mathbf{x}^T\mathbf{z}+1)^2$: $O(n)$

If using *kernel trick*, can implement a non-linear feature expansion at no additional cost

Even More Polynomial Kernels

$$K(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^T \mathbf{z} + 1)^d$$

Corresponds to ϕ that takes all products of up to d original features

$O(n)$ time to compute kernel instead of $O(n^d)$

Gaussian Kernel

$$K(\mathbf{x}, \mathbf{z}) = \exp(-\gamma ||\mathbf{x} - \mathbf{z}||^2)$$

- Highly flexible, non-linear kernel
- Corresponds to infinite dimensional ϕ (cannot implement feature mapping, but can still use kernel)
- Demos
  - Gaussian kernel intuition: similarity function
  - Linear regression

A Word on Regularization

- Suppose we want to combine feature expansion with regularization

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(derivation next slide)

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- This is *not* the same as penalizing $\|\boldsymbol{\alpha}\|^2$
  - Tip: use regularization with kernelized linear models
  - Tip: Use a custom optimizer for to minimize $J(\boldsymbol{\alpha})$

A Word on Regularization

Derivation of regularization term:

$$\boldsymbol{\theta}^T\boldsymbol{\theta} = \left(\sum_{i=1}^{m}\alpha_i\phi(\mathbf{x}^{(i)})\right)^T\left(\sum_{j=1}^{m}\alpha_i\phi(\mathbf{x}^{(j)})\right)$$

$$=$$

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&= \boldsymbol{\alpha}^T K\boldsymbol{\alpha}
\end{aligned}$$

Practical Tips

- Use support vector machines (SVMs) for kernelized classification
  - Like logistic regression, with *slightly* different loss function. (Derivation based on geometric principles, but end point the same.)
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- Use Gaussian kernels

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Demos

- Kernel logistic regression
- SVM loss
- SVM classification