# Topic 7: KERNEL METHODS

CMSC 35400/STAT 37710 Machine Learning
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# General form of kernel methods

$k\colon \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a PSD kernel and $\mathcal{H}_k$ is the associated RKHS. Kernel methods (aka. Hilbert space learning algorithms) solve the RRM problem

$$\widehat{f} = \operatorname*{argmin}_{f \in \mathcal{H}_k} \Bigg[ \underbrace{\frac{1}{m} \sum_{i=1}^{m} \ell(f(x_i), y_i)}_{\text{training error}} + \underbrace{\Omega(\|f\|_{\mathcal{H}_k})}_{\text{regularizer}} \Bigg].$$

- $\Omega$ can be any increasing function $\mathbb{R}^+ \to \mathbb{R}^+$ .
- The final hypothesis is $\widehat{h}(x) = \sigma(\widehat{f}(x))$ . For example, in the SVM, simply $\widehat{h}(x) = \operatorname{sgn}(\widehat{f}(x))$ .
- $\ell$ is the **surrogate loss**. For example, in classification, the hinge loss is a surrogate for the zero-one loss.

Instead of actually having to search over a function space, all such problems reduce to $m$ dimensional optimization thanks to the reproducing property $f(x) = \langle f, k_x \rangle$ and the Representer Theorem.

# The modularity of kernel methods

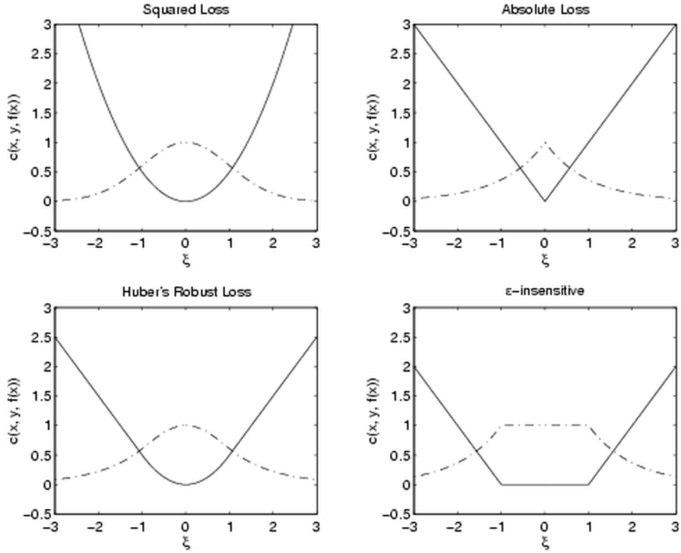
Regularized risk minimization in RKHSs is a powerful paradigm because it has distinct moving parts:

- **The loss**
  - Reflects the nature of the problem (classification/regression/ranking/...).
  - Determines exactly what type of optimization problem we end up with.
- **The kernel**
  - Regulates overfitting by determining the regularization term.
  - Reflects our prior knowledge about the problem.

Can dream up virtually any kernel machine and solve it efficiently as long as

1. The loss only involves function evaluations $f(x) = \langle f, k_x \rangle$ at data points;
2. The regularizer is an increasing function of $\| f \|_{\mathcal{F}}$ .

# Loss functions for regression



# 1. The kernel perceptron

# The vanilla perceptron

```
$\mathbf{w} \leftarrow 0$ ;
$t \leftarrow 1$ ;
while(true){
  if $\mathbf{w} \cdot \mathbf{x}_t \geq 0$ predict $\hat{y}_t = 1$ ; else predict $\hat{y}_t = -1$ ;
  if $((\hat{y}_t = -1)$ and $(y_t = 1))$ let $\mathbf{w} \leftarrow \mathbf{w} + \mathbf{x}_t$ ;
  if $((\hat{y}_t = 1)$ and $(y_t = -1))$ let $\mathbf{w} \leftarrow \mathbf{w} - \mathbf{x}_t$ ;
  $t \leftarrow t + 1$ ;
}
```

At any $t$, the weight vector is of the form

$$\mathbf{w} = \sum_{i=1}^{t-1} c_i \, \mathbf{x}_i \qquad \text{where} \qquad c_i \in \{-1, 0, +1\}\,.$$

# The kernel perceptron

```
$t \leftarrow 1$ ;
while(1){
  if $\sum_{i=1}^{t-1} c_i k(\mathbf{x}_i, \mathbf{x}_t) \geq 0$ predict $\hat{y}_t = 1$ ; else $\hat{y}_t = -1$ ;
  $c_t \leftarrow 0$ ;
  if $((\hat{y}_t = -1)$ and $(y_t = 1))$ let $c_t = 1$ ;
  if $((\hat{y}_t = 1)$ and $(y_t = -1))$ let $c_t = -1$ ;
  $t \leftarrow t + 1$ ;
}
```

# 2. Kernel PCA

# PCA in feature space

Recall that in $\mathbb{R}^D$ (after centering), the first principal component is given by

$$\boldsymbol{v}_1 = \arg \max_{\|\boldsymbol{v}\|=1} \frac{1}{m} \sum_{i=1}^{m} (\mathbf{x}_i \cdot \boldsymbol{v})^2.$$

Clearly, $\boldsymbol{v}_1$ lies in the span, i.e., $\boldsymbol{v}_1 = \sum_{i=1}^m \alpha_i \, \mathbf{x}_i$ .

Kernel analog:

$$f_1 = \underset{f \in \mathcal{F} \quad \|f\|=1}{\operatorname{argmax}} \sum_{i=1}^{m} \langle f, \phi(x_i) \rangle^2 .$$

Once again, $f = \sum_{i=1}^m \alpha_i \, \phi(x_i)$ for some $\alpha_1, \ldots, \alpha_m \in \mathbb{R}$ .

# Kernel PCA

As in $\mathbb{R}^D$ , $f$ will be the highest e-value e-vector of the sample covariance operator

$$\Sigma(f) = \frac{1}{m} \sum_{i=1}^{m} \phi(x_i) \langle f, \phi(x_i) \rangle \, .$$

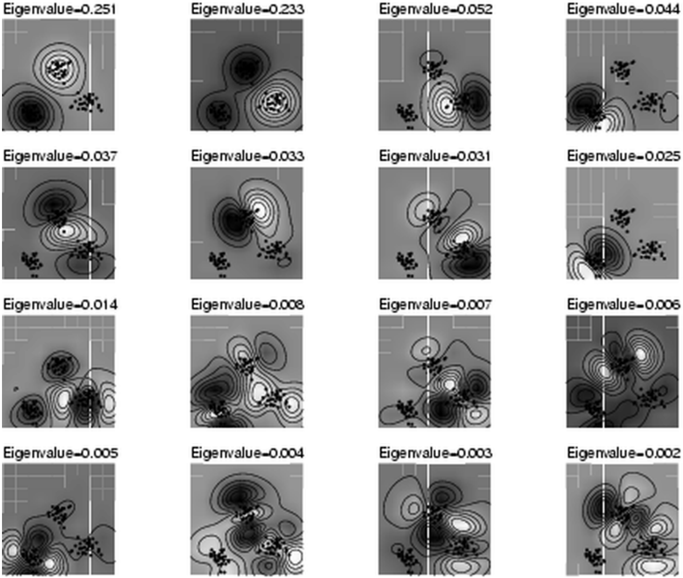
Plugging in $f = \sum_{\ell=1}^{m} \alpha_\ell \, \phi(x_\ell)$ and multiplying from the right by any $\phi(x_j)$ :

$$\frac{1}{m} \sum_{i=1}^{m} \sum_{\ell=1}^{m} \langle \phi(x_j), \phi(x_i) \rangle \langle \phi(x_i), \phi(x_\ell) \rangle \, \alpha_\ell = \lambda \sum_{\ell=1}^{m} \langle \phi(x_j), \phi(x_\ell) \rangle \, \alpha_\ell .$$

Using $\langle \phi(x_j), \phi(x_i) \rangle = k(x_i, x_j)$ and letting $K$ be the Gram matrix,

$$K^2 \boldsymbol{\alpha} = m \lambda K \alpha \qquad \Longrightarrow \qquad K \boldsymbol{\alpha} = m \lambda \boldsymbol{\alpha},$$

so kernel PCA reduces to just finding the first eigenvector of the Gram matrix!



Eigenvalue-0.251

Eigenvalue-0.233

Eigenvalue-0.052

Eigenvalue-0.044

Eigenvalue-0.037

Eigenvalue-0.033

Eigenvalue-0.031

Eigenvalue-0.025

Eigenvalue-0.014

Eigenvalue-0.008

Eigenvalue-0.007

Eigenvalue-0.006

Eigenvalue-0.005

Eigenvalue-0.004

Eigenvalue-0.003

Eigenvalue-0.002

# 3. Ridge Regression

# Ridge Regression

Using squared error loss and setting $\lambda = m/2C$ ,

$$\widehat{f} = \operatorname*{argmin}_{f \in \mathcal{H}_k} \Bigg[ \underbrace{\sum_{i=1}^{m} (f(x_i) - y_i)^2 + \lambda \, \|f\|_{\mathcal{H}_k}^2}_{\mathcal{R}[f]} \Bigg].$$

By the Representer Theorem, $f(x) = \sum_{i=1}^{m} \alpha_i k(x_i, x)$, so

$$\mathcal{R}[f] = \sum_{i=1}^{m} \Bigg( \sum_{j=1}^{m} \alpha_j \, k(x_i, x_j) - y_i \Bigg)^2 + \lambda \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_i \alpha_j \, k(x_i, x_j).$$

# Ridge Regression

Letting $\mathbf{y} = (y_1, \ldots, y_m)$ , $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_m)^\top$ and $K_{i,j} = k(x_i, x_j)$ ,

$$\mathcal{R}(\boldsymbol{\alpha}) = \| \boldsymbol{K}\boldsymbol{\alpha} - \mathbf{y} \|^2 + \lambda \boldsymbol{\alpha}^\top \boldsymbol{K}\boldsymbol{\alpha}.$$

At the optimum,

$$\frac{\partial R(\boldsymbol{\alpha})}{\partial \alpha_i} = [\boldsymbol{K}(\boldsymbol{K}\boldsymbol{\alpha} - \mathbf{y})]_i + \lambda [\boldsymbol{K}\boldsymbol{\alpha}]_i = 0,$$

so

$$\boldsymbol{K}(\boldsymbol{K}\boldsymbol{\alpha} - \mathbf{y}) + \lambda \boldsymbol{K}\boldsymbol{\alpha} = 0 \qquad \Longrightarrow \qquad \boldsymbol{\alpha} = (\boldsymbol{K} + \lambda \boldsymbol{I})^{-1}\mathbf{y}.$$

# Ridge Regression

Defining $\boldsymbol{k}_x = k(x_i, x)$ , the final solution is

$$\widehat{f}(x) = \boldsymbol{k}_x^\top (\boldsymbol{K} + \lambda \boldsymbol{I})^{-1} \mathbf{y}.$$

- In this case RRM reduced to just inverting a matrix.
- In fact, this is just **ridge regression**, which is a classical method in statistics, and the simplest non-linear regression/interpolation method possible.
- Ridge regression is the same as the MAP of a Gaussian Process with mean zero and covariance function $k$ .

# One-class SVM and Multiclass SVM

# The one-class SVM (outlier detection)

## RKHS primal form

$$\widehat{f} = \underset{f \in \mathcal{H}_k}{\operatorname{argmin}} \left[ \frac{1}{m} \sum_{i=1}^{m} (1 - f(x_i))_{\geq 0} + \frac{1}{2C} \| f \|_{\mathcal{H}_k}^2 \right].$$

Tries to peg $f(x_i) \geq 0$ for all points $x_1, \ldots, x_m$ in the training set
$\rightarrow$ outlier detector.

## Dual form

$$\text{maximize}_{\alpha_1, \ldots, \alpha_m} L(\boldsymbol{\alpha}) = \sum_i \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j k(x_i, x_j)$$

$$\text{subject to} \quad 0 \leq \alpha_i \leq \frac{C}{m} \ \forall i$$

# The Multiclass SVM

- Defining $f_z(x) = zf(x)/2$ for $z = \pm 1$,

$$\ell_{\text{hinge}}(f(x), y) = (1 - y\,f(x))_{\geq 0} = (1 - (f_y(x) - f_{-y}(x)))_{\geq 0},$$

i.e., the correct answer is supposed to beat the incorrect answer by at least a margin of 1.

- This inspires the **multiclass hinge loss**

$$\ell(f_1(x), \ldots f_k(x), y) = \sum_{y' \in \{1,2,\ldots,k\} \setminus \{y\}} \big(1 - (f_y(x) - f_{y'}(x))\big)_{\geq 0},$$

which is the basis of the $k$-class SVM ($f_j(x)$ is a bit like a “score”). This is essentially the same notion of multiclass margin as in the $k$-class perceptron. Predict $\widehat{y} = \operatorname{argmax}_{j \in \mathcal{Y}} f_j(x, j)$ .

# RKHS form of Multiclass SVM

The loss now depends on not just $f_y(x)$ , but also $f_{y'}(x)$ for all $y' \neq y$ , so the RKHS form also needs to be generalized slightly:

$$\widehat{f} = \operatorname*{argmin}_{f \in \mathcal{H}_k} \left[ \underbrace{\frac{1}{m} \sum_{i=1}^{m} \ell(f_1(x_i), f_2(x_i), \ldots, f_k(x_i), y_i)}_{\text{training error}} + \underbrace{\Omega(\|f\|_{\mathcal{H}})}_{\text{regularizer}} \right].$$

The corresponding generalized Representer Theorem will say that

$$f_j(x) = \sum_{i=1}^{m} \alpha_{i,j} k(x_i, x)$$

for all $j \in \{1, \ldots, k\}$ , so now we have many more coefficients to optimize.

# Structured prediction

# Multiclass to Structured Prediction

What if we combine $f_1, \dots, f_k \colon \mathcal{X} \to \mathbb{R}$ in the $k$-class SVM into a single function $f \colon \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$ where $\mathcal{Y} = \{1, \dots, k\}$ ? The loss becomes

$$\ell(f, x, y) = \sum_{y' \in \mathcal{Y} \setminus \{y\}} \big(1 - (f(x, y) - f(x, y'))\big)_{\geq 0}.$$

IDEA: Use this to search for $f$ in a **joint RKHS** of functions $f \colon \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$ :

- Kernel becomes $k((x, y), (x', y'))$ .
- We can now put structure on $\mathcal{Y}$ as well as $\mathcal{X}$ .
- We are now learning a single mapping $f \colon \mathcal{X} \to \mathcal{Y}$ directly.
- At the extreme, the distinction between $\mathcal{X}$ and $\mathcal{Y}$ is blurred.

$\rightarrow$ **structured prediction**

# RRM form of Structured Prediction

Let $k$ be a psd kernel $k\colon (\mathcal{X}\times\mathcal{Y})\times(\mathcal{X}\times\mathcal{Y})\to\mathbb{R}$, let $\mathcal{H}_k$ be the corresponding RKHS, and $\Omega$ a monotonically increasing function. Solve

$$\widehat{f} = \arg\min_{f\in\mathcal{H}_k}\Big[\underbrace{\frac{1}{m}\sum_{i=1}^{m}\ell((f(x_i,y))_{y\in\mathcal{Y}},y_i)}_{\text{training error}} + \underbrace{\Omega\|f\|_{\mathcal{F}}}_{\text{regularizer}}\Big],$$

and predict $\widehat{y} = \mathrm{argmax}_{y\in\mathcal{Y}}\,\widehat{f}(x,y)$ .

The loss (in principle) now depends on $f(x_i,y)$ for all possible $y$. Therefore, the Representer Theorem says that $f$ is of the form

$$f(x,y) = \sum_{i=1}^{m}\sum_{y^*\in\mathcal{Y}}\alpha_{i,y^*}\,k((x_i,y^*),(x,y)).$$

In practice, this is usually unfeasible, so only add $\alpha_{i,y^*}$ coefficients to the optimization on the fly “as needed”.

# Kernels for Structured Learning

The simplest way to get a kernel $k\colon (\mathcal{X} \times \mathcal{Y}) \times (\mathcal{X} \times \mathcal{Y}) \to \mathbb{R}$ :

- Get a kernel $k_{\mathcal{X}}$ that quantifies similarity between the $x$ 's.
- Get a kernel $k_{\mathcal{Y}}$ that quantifies similarity between the $y$ 's.
- Define

$$k((x,y),(x',y')) = k_{\mathcal{X}}(x,x') \cdot k_{\mathcal{Y}}(y,y').$$

Question: Is this a valid kernel? What is its RKHS?