10-715 Advanced Introduction to Machine Learning

Homework 2 Solutions *October 26, 2014*

1 More Regression & Classification (Samy)

1.1 Optimal Classification & Regression

1. Let g be the Bayes Classifier and f be any other rule. Since $R(f)-R(g) = \mathbb{E}\left[\mathbb{P}(Y \neq f(X)|X) - \mathbb{P}(Y \neq g(X)|X)|X\right]$ it is sufficient to show that $\mathcal{R} = \mathbb{P}(Y \neq f(X)) - \mathbb{P}(Y \neq g(X)) \geq 0$.

$$\begin{aligned}\mathcal{R} &= f(X)\mathbb{P}(Y \neq 1|X) + (1 - f(X))\mathbb{P}(Y = 1|X) - (g(X)\mathbb{P}(Y \neq 1|X) + (1 - g(X))\mathbb{P}(Y = 1|X)) \\ &= 2\left(\mathbb{E}[Y|X] - 1/2\right)\left(g(X) - f(X)\right) \geq 0\end{aligned}$$

   The last step follows by noting that $\mathbb{E}[Y|X] = \mathbb{P}(Y = 1|X)$. The inequality follows by noting that $g(X) \geq 0$ iff $\mathbb{E}[Y|X] \geq 1/2$.

2. Let $g(X) = \mathbb{E}[Y|X]$ and $f : \mathcal{X} \to \mathcal{Y}$ be any other rule.

$$\begin{aligned}\mathbb{E}_{XY}[(f(X) - Y)^2] &= \mathbb{E}_{XY}\left[(f(X) - g(X))^2 + (g(X) - Y)^2 + 2(f(X) - g(X))(g(X) - Y)\right] \\ &= \mathbb{E}_X\left[(f(X) - g(X))^2\right] + \mathbb{E}_{XY}\left[(g(X) - Y)^2\right] + 2\mathbb{E}_X\left[(f(X) - g(X))\,\mathbb{E}_Y\left[(g(X) - Y)|X\right]\right] \\ &\geq \mathbb{E}_{XY}\left[(g(X) - Y)^2\right]\end{aligned}$$

   The last step follows by noting that $\mathbb{E}_Y\left[(g(X) - Y)|X\right] = g(X) - \mathbb{E}_Y[Y|X] = 0$ and that $\mathbb{E}_X\left[(f(X) - g(X))^2\right] \geq 0$.

1.2 Support Vector Regression

1. By introducing slack variables s_i s.t. $s_i = |y_i - f(x_i)| - \epsilon$ if $|y_i - f(x_i)| > \epsilon$ and 0 otherwise, we have the following problem

$$\begin{aligned}\underset{w,s}{\text{minimize}} \quad & \frac{1}{2}\|w\|^2 + c\sum_{i=1}^{n} s_i \\ \text{subject to} \quad & s_i \geq \mathbf{0} \qquad i = 1, \ldots, n \\ & |y_i - x_i^\top w| \leq s_i + \epsilon \qquad i = 1, \ldots, n\end{aligned}$$

   By writing $s \in \mathbb{R}^n$ and denoting $\succeq, \preceq$ to denote elementwise inequalities we obtain the following quadratic program.

$$\begin{aligned}\underset{w,s}{\text{minimize}} \quad & \frac{1}{2}w^\top w + c\mathbf{1}^\top s \\ \text{subject to} \quad & s \succeq \mathbf{0} \\ & -s - \epsilon\mathbf{1} \preceq y - Xw \preceq s + \epsilon\mathbf{1}\end{aligned}$$

   In the Lagrangian, we use $\lambda_1, \lambda_2, \lambda_3 \in \mathbb{R}^n$ to denote the dual variables for the three inequality constraints above.

$$\begin{aligned}\mathcal{L}(w, s, \lambda_1, \lambda_2, \lambda_3) &= \frac{1}{2}w^\top w + c\mathbf{1}^\top s - \lambda_1^\top s + \lambda_2^\top(y - Xw - s - \epsilon\mathbf{1}) + \lambda_3^\top(-s - \epsilon 1 - y + Xw) \\ &= \frac{1}{2}w^\top w + \left[X^\top(\lambda_3 - \lambda_2)\right]^\top w + (c\mathbf{1} - \lambda_1 - \lambda_2 - \lambda_3)^\top s + (\lambda_2 - \lambda_3)^\top y - \epsilon(\lambda_2 + \lambda_3)^\top\mathbf{1}\end{aligned}$$

We may derive the dual via the KKT Conditions. First compute the derivatives w.r.t to the primal variables.

$$\nabla_w \mathcal{L} = w + X^\top(\lambda_3 - \lambda_2) := 0$$
$$\nabla_s \mathcal{L} = c\mathbf{1} - \lambda_1 - \lambda_2 - \lambda_3 := 0$$

Write $\mu = \lambda_2 - \lambda_3$. By setting the above to 0 and observing dual feasibilty gives us,

$$\lambda_1 \succeq 0 \implies \lambda_2 + \lambda_3 \preceq c\mathbf{1} \implies 2\lambda_2 - \mu \preceq c\mathbf{1}$$
$$\lambda_3 \succeq 0 \implies \lambda_2 \succeq \mu$$

Accordingly, we have the following dual QP

$$\begin{aligned} \underset{\lambda_2,\mu}{\text{maximize}} \quad & -\frac{1}{2}\mu^\top X X^\top \mu + (y + \epsilon\mathbf{1})^\top \mu - 2\epsilon\lambda_2^\top \mathbf{1} \\ \text{subject to} \quad & 2\lambda_2 \preceq \mu + c\mathbf{1} \\ & \lambda_2 \succeq \mu \\ & \lambda_2 \succeq 0 \end{aligned}$$

2. To Kernelize the algorithm, we replace $XX^\top$ via a kernel matrix $K = (k(x_i, x_j))_{ij} \in \mathbb{R}^{n\times n}$ and solve,

$$\begin{aligned} \underset{\lambda_2,\mu}{\text{maximize}} \quad & -\frac{1}{2}\mu^\top K \mu + (y + \epsilon\mathbf{1})^\top \mu - 2\epsilon\lambda_2^\top \mathbf{1} \\ \text{subject to} \quad & 2\lambda_2 \preceq \mu + c\mathbf{1} \\ & \lambda_2 \succeq \mu \\ & \lambda_2 \succeq 0 \end{aligned}$$

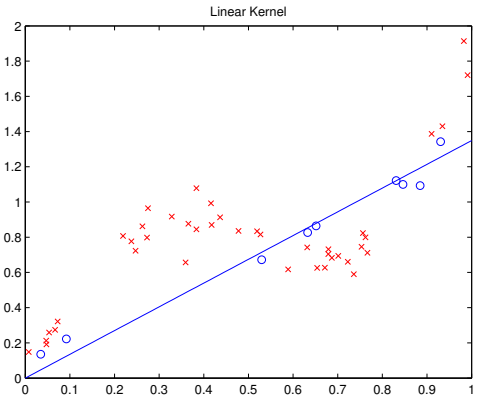
   The prediction at a new point x_* is $\hat{f}(x_*) = \sum_{i=1}^n \mu_i k(x_i, x_*)$.
   To see this, the prediction from the primal solution w is, $\hat{f}(x_*) = w^\top x_*$. If we solve the dual problem, then $\hat{f}(x) = \mu^\top X x_*$. In the kernelized version, denote the mapping of x_* by $\phi(x_*)$ and the mapping of the training data by Φ. Then $\hat{f}(x_*) = \mu^\top \Phi\phi(x_*)$ which can be computed using just the inner prducts as $\hat{f}(x_*) = \sum_{i=1}^n \mu_i k(x_i, x_*)$

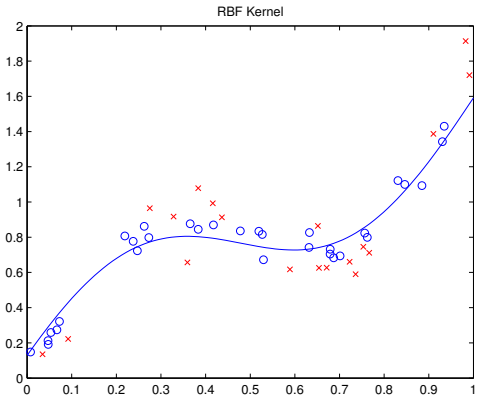
3. In classification, the support vectors are those points whose inequality constraints are active and are used in computing the prediction. Here, similarly they are the points for which $s_i > 0$ in the primal problem and hence by complementary slackness $\lambda_{1i} = 0 \Leftrightarrow 2\lambda_{2i} = \mu_i + c$ in the dual problem. Geometrically, these are the points that lie outside an ϵ-tube of the estimated function.

4. This is our implementation.

```
function [params, svs] = dualSVMRegression(K, y, c, eps)

  N = size(y, 1);

  cvx_begin
    variables muu(N) lambda2(N)
    maximize( -0.5* muu' * K * muu + (y + eps)'*muu - 2*eps * sum(lambda2) );
    subject to
      2*lambda2 <= muu + c;
      lambda2 >= muu;
      lambda2 >= 0;
  cvx_end

  params.muu = muu;
```

```
  params.lambda2 = lambda2;
  svs = abs(2*lambda2 - muu -c) < 1e-5;

end


function K = rbfKernel(X, Y, h)
  D = dist2(X, Y);
  K = exp(-D/(2*h^2));
end


function preds = dualSVMPredict(params, k)
  preds = params.muu' * k;
end
```





2 Expectation Maximization (Samy)

2.1 EM Basics

The solutions are straightforward. Please see the slides.

2.2 Pólya Mixture Model

2.2.1 Model

Conditioned on $z_i = k, m_i$ the distribuiton of x corresponds to a Dirichlet Multinomial with parameters m_i, α_k. Its mass function and the logarithm is

$$p_{dm}(x_i; \alpha_k) = \frac{\Gamma(A_k)}{\Gamma(m_i + A_k)} \prod_{s=1}^{V} \frac{\Gamma(x_i^{(s)} + \alpha_k^{(s)})}{\Gamma(\alpha_k^{(s)})}$$

$$\log p_{dm}(x_i; \alpha_k) = \log \Gamma(A_k) - \log \Gamma(m_i + A_k) + \sum_{s=1}^{V} \left(\log \Gamma(x_i^{(s)} + \alpha_k^{(s)}) - \log \Gamma(\alpha_k^{(s)}) \right)$$

where $A_k = \sum_{s=1}^{V} \alpha_k^{(s)}$ and $m_i = \sum_{s=1}^{V} x_i^{(s)}$.

Let $\Theta = \theta, \alpha_1, \ldots, \alpha_K$. The likelihood and log likelihood of the data $\mathcal{D} = (x_i)_{i=1}^n$ is given by,

$$p(\mathcal{D}|\Theta) = \prod_{i=1}^{n} \sum_{k=1}^{K} p(x_i, z_k; \Theta)$$
$$\tilde{\ell}(\Theta|\mathcal{D}) = \sum_{i=1}^{n} \log \sum_{k=1}^{K} p(x_i, z_k; \Theta)$$

where, $p(x_i, z_k; \Theta) = p(z_k; \Theta)p(x_i|z_k; \Theta) = \theta^{(k)} p_{dm}(x_i; \alpha_k)$

Accordingly, the joint probability of the parameters and the data and its log are given by,

$$\begin{aligned} p(\mathcal{D}, \Theta) &= p(\theta) \left(\prod_{k=1}^{K} p(\alpha_k) \right) p(\mathcal{D}|\Theta) \\ &= \left(\frac{\Gamma(\sum_k \theta_0^{(k)})}{\prod_k \Gamma(\theta_0^{(k)})} \prod_{k=1}^{K} {\theta^{(k)}}^{\theta_0^{(k)}-1} \right) \left(\prod_{k=1}^{K} \frac{1}{(2\pi)^{K/2}(1/2\lambda)^{K/2}} \exp\left(-\lambda \|\alpha_k\|^2\right) \right) p(\mathcal{D}|\Theta) \\ \ell(\Theta, \mathcal{D}) &= \sum_{k=1}^{K} (\theta_0^{(k)} - 1) \log \theta^{(k)} + \sum_{k=1}^{K} -\lambda \|\alpha_k\|^2 + \ell(\Theta|\mathcal{D}) + C(\theta_0, \lambda) \end{aligned}$$

The log joint probability can be bounded via $\ell(\Theta, \mathcal{D}) \geq \ell_b(\Theta; \mathcal{D})$ where,

$$\ell_b(\Theta; \mathcal{D}) = \sum_{k=1}^{K} (\theta_0^{(k)} - 1) \log \theta^{(k)} - \lambda \sum_{k=1}^{K} \|\alpha_k\|^2 + \sum_{i=1}^{n} \sum_{k=1}^{K} R(z_k|x_i) \log \left(\frac{p(x_i, z_k; \Theta)}{R(z_k|x_i)} \right) + C(\theta_0, \lambda)$$

Here $R(z_k|x_i)$ is any distribution on the z_k's. In E step we set it to $R(z_k|x_i) = p(z_k|x_i; \Theta)$ where the class posterior probabilities are computed using the current estimates for Θ. Let $S_k = \sum_{i=1}^{n} R(z_k|x_i)$.

In the M-step we maximize the above w.r.t Θ. We can write $\ell_b(\Theta; \mathcal{D}) = \ell_0(\theta) + \sum_{k=1}^{K} \ell_k(\alpha_k) + C_1$ where C_1 is a constant that does not affect the optimization and

$$\begin{aligned} \ell_0(\theta) &= \sum_{k=1}^{K} (\theta_0^{(k)} - 1 + S_k) \log \theta^{(k)} \\ \ell_k(\alpha_k) &= -\lambda \|\alpha_k\|^2 + \sum_{i=1}^{n} R(z_k|x_i) \left(\log \Gamma(A_k) - \log \Gamma(m_i + A_k) + \sum_{s=1}^{V} \left(\log \Gamma(x_i^{(s)} + \alpha_k^{(s)}) - \log \Gamma(\alpha_k^{(s)}) \right) \right) \\ &= -\lambda \|\alpha_k\|^2 + S_k \log \Gamma(A_k) - \sum_{i=1}^{n} R(z_k|x_i) \log \Gamma(m_i + A_k) + \sum_{i=1}^{n} R(z_k|x_i) \sum_{s=1}^{V} \log \Gamma(x_i^{(s)} + \alpha_k^{(s)}) - S_k \sum_{s=1}^{V} \log \Gamma(\alpha_k^{(s)}) \end{aligned}$$

To optimize w.r.t θ we write out the Lagrangian and obtain the derivatives. The maximum can be found to be,

$$\hat{\theta}^{(k)} := \frac{S_k + \theta_0^{(k)} - 1}{n + \sum_j \theta_0^{(j)} - K}$$

To maximize w.r.t α_k we use a Newton scheme as before. The first and second derivatives of ℓ_k are,

$$\begin{aligned} \frac{\partial \ell_k}{\partial \alpha_k^{(s)}} &= -2\lambda \alpha_k^{(s)} + S_k \Psi(A_k) - \sum_{i=1}^{n} R(z_k|x_i) \Psi(m_i + A_k) + \sum_{i=1}^{n} R(z_k|x_i) \Psi(x_i^{(s)} + \alpha_k^{(s)}) - S_k \Psi(\alpha_k^{(s)}) \\ \frac{\partial^2 \ell_k}{\partial {\alpha_k^{(s)}}^2} &= -2\lambda + S_k \Psi'(A_k) - \sum_{i=1}^{n} R(z_k|x_i) \Psi'(m_i + A_k) + \sum_{i=1}^{n} R(z_k|x_i) \Psi'(x_i^{(s)} + \alpha_k^{(s)}) - S_k \Psi'(\alpha_k^{(s)}) \\ \frac{\partial^2 \ell_k}{\partial \alpha_k^{(s)} \partial \alpha_k^{(t)}} &= S_k \Psi'(A_k) - \sum_{i=1}^{n} R(z_k|x_i) \Psi'(m_i + A_k) \end{aligned}$$

The Newton step update is given by $\alpha_k^{new} \leftarrow \alpha_k^{old} - \mathbf{H}_k^{-1}\mathbf{g}_k$ where $\mathbf{g}_k^{(s)} = \frac{\partial \ell_k}{\partial \alpha_k^{(s)}}$ and $\mathbf{H}_k^{(s,t)} = \frac{\partial^2 \ell_k}{\partial \alpha_k^{(s)} \partial \alpha_k^{(t)}}$. As before, we can use the Sherman Morrison formula to compute the Newton step in $\tilde{O}(V)$ time. We can write $\mathbf{H}_k = \mathbf{D}_k + z\mathbf{1}\mathbf{1}^\top$ where,

$$\mathbf{D}_k^{(s,s)} = -2\lambda + \sum_{i=1}^{n} R(z_k|x_i)\Psi'(x_i^{(s)} + \alpha_k^{(s)}) - S_k\Psi'(\alpha_k^{(s)})$$

$$z = S_k\Psi'(A_k) - \sum_{i=1}^{n} R(z_k|x_i)\Psi'(m_i + A_k)$$

and then, $[\mathbf{H}_k^{-1}\mathbf{g}_k]^{(i)} = \mathbf{g}_k^{(i)}/\mathbf{D}^{(i,i)} - \frac{\sum_j \mathbf{g}_k^{(j)}/\mathbf{D}^{(j,j)}}{1/z + \sum_j 1/\mathbf{D}^{(j,j)}} \left(1/\mathbf{D}^{(i,i)}\right)$.

To summarize, our learning algorithm is as follows:

- Initialize: $t = 0$, Set $\theta[0], \alpha_k[0]$ to reasonable values.
- Repeat until convergence:
  - $t = t + 1$
  - **E-step**
    - Compute
    $$R(z_k|x_i) = p(z_k|x_i; \Theta[t]) = \frac{\theta[t]^{(k)} p_{dm}(x_i; \alpha_k[t])}{\sum_{j=1}^{K} \theta[t]^{(j)} p_{dm}(x_i; \alpha_j[t])}$$
    - Compute $S_k = \sum_{i=1}^{n} R(z_k|x_i)$.
  - **M-step**
    - Set
    $$\hat{\theta}^{(k)} := \frac{S_k + \theta_0^{(k)} - 1}{n + \sum_j \theta_0^{(j)} - K}$$
    - Maximize w.r.t the α_k's as outlined above.

Finally, to obtain the prediction at a new point we choose the class that maximizes the posterior $p(z|x) = \frac{p(x|z)p(z)}{p(x)}$,

$$z_* = \underset{k \in \{1,\ldots,K\}}{\operatorname{argmax}}\ p(z = k|x_*) = \underset{k \in \{1,\ldots,K\}}{\operatorname{argmax}}\ p(x_*|z = k)p(z = k) = \underset{k \in \{1,\ldots,K\}}{\operatorname{argmax}}\ p_{dm}(x_*; \alpha_k)\theta^{(k)}$$

2.2.2 Experiment

Our Implementation is as follows,

```
function [theta, alpha] = trainPMM(X, K, theta0, lambda, thetaInit, alphaInit)
% X is an nxV matrix, y is an nx1 vector
% This function returns
% theta: a Kx1 vector indicating the class probabilities
% alpha: a KxV matrix

  % Prelims
  V = size(X, 2);
  numData = size(X, 1);
  numEMIters = 10;
```

```
  % Perform EM
  theta = thetaInit;
  alpha = alphaInit;
  for emIter = 1:numEMIters
    fprintf('EM Iter: %d\n', emIter);
    [theta, alpha] = emPMM(X, K, theta0, lambda, theta, alpha);
  end

end


% This function performs EM
function [theta, alpha] = emPMM(X, K, theta0, lambda, thetaPrev, alphaPrev)

  % prelims
  n = size(X, 1);
  V = size(X, 2);

  % E-step
  %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
  % First obtain the class log likelihoods
  classLogLs = zeros(n, K);
  for k = 1:K
    classLogLs(:, k) = classLogLikelihoods(X, alphaPrev(k, :));
  end
  % Add the prior to obtain the joint
  classLogJoints = bsxfun(@plus, classLogLs, log(thetaPrev'));
  shiftClassLogJoints = ...
    bsxfun(@minus, classLogJoints, max(classLogJoints, [], 2));
  shiftLogJoints = exp(shiftClassLogJoints);
  R = bsxfun(@rdivide, shiftLogJoints, sum(shiftLogJoints, 2));
%   logJoints = log_sum_exp(classLogJoints')';
%   R = exp( bsxfun(@minus, classLogJoints, logJoints) );
  S = sum(R);

  % M-step
  %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
  % First theta
  theta = theta0 + S' -1;
  theta = theta / sum(theta);
  % Then alpha
  alpha = zeros(K, V);
  for k = 1:K
  % Iterate through each class and obtain the alpha_k's
    alpha(k, :) = newtonRaphsonPMM(X, R(:,k), S(k), lambda);
  end

end


% This function implements Newton's Method.
function [alphak] = newtonRaphsonPMM(X, Rk, Sk, lambda)
```

```
  % Prelims
  numNRIters = 10; % Just use 10 iterations of NR
  V = size(X, 2); % size of vocabulary
  n = size(X, 1); % number of training data in this class
  m = sum(X, 2); % number of words in each documents

  % Set up initializations
  initPt = sum( bsxfun(@times, X, Rk) );
  initPt = initPt / sum(initPt);

    nrProgress = zeros(numNRIters, 1);
    alphak = initPt; % alphak in the current iteration
    for nrIter = 1:numNRIters
      % Compute the following
      Ak = sum(alphak);
      XplusAlpha = bsxfun(@plus, X, alphak);
      % The gradient
      g = Sk * psi(Ak) - Rk' * psi(m + Ak) + Rk' * psi(XplusAlpha) ...
          - Sk * psi(alphak) - 2 * lambda * alphak;
      % The value z ( see solutions)
      z = Sk * psi(1, Ak) - Rk' * psi(1, m + Ak);
      % The diagonal of the Hessian
      D = Rk' * psi(1, XplusAlpha) - Sk * psi(1, alphak) - 2*lambda;
      % Newton's step update
      Hinvg = g./D - (1./D) * sum(g./D) / (1/z + sum(1./D));
      alphak = alphak - 1*Hinvg;

      % DEBUG
      nrProgress(nrIter) = Rk' * classLogLikelihoods(X, alphak);

    end
%     nrProgress,

end


function logP = classLogJointProb(X, alphak, lambda)
% Computes the log joint probability for one class (ignoring the constants).

  logL = classLogLikelihoods(X, alphak);
  logP = sum(logL) - lambda * norm(alphak)^2;
end


function logL = classLogLikelihoods(X, alphak)
% X is an nxV matrix, alphak is the class Dirichlet parameter. logL is a nx1
% vector with the log likelihood of each point

  % Prelims
  Ak = sum(alphak);
  V = size(X, 2); % size of vocabulary
  n = size(X, 1); % number of training data in this class
  m = sum(X, 2); % number of words in each documents
  XplusAlpha = bsxfun(@plus, X, alphak);
```

```
  % Compute the log likelihood
  logL = gammaln(Ak) - gammaln(m + Ak) + ...
    sum(gammaln(XplusAlpha), 2) - sum( gammaln(alphak) );

end


function [preds, classLogJoints] = predictPMM(X, theta, alpha)
% X is an nxV matrix. theta, alpha are the learned parameters.
% preds (nx1) is the predictions for X
% post (nxK) is the posterior for each class

  % prelims
  n = size(X, 1);
  V = size(X, 2);
  K = numel(theta);

  % First obtain the class log likelihoods
  classLogLs = zeros(n, K);
  for k = 1:K
    classLogLs(:, k) = classLogLikelihoods(X, alpha(k, :));
  end
  % Add the prior to obtain the joint
  classLogJoints = bsxfun(@plus, classLogLs, log(theta'));

  % Finally obtain the predictions
  [~, preds] = max(classLogJoints, [], 2);

end
```

3 Kernels and RKHS (Veeru)

3.1 Image similarity functions

1. Let d denote the number of possible 16×16 pixel patches. As each pixel can take 256 values, $d = 256^{16\times16}$. Define feature map ϕ from the space of arbitrary rectangular pictures to $\{0,1\}^d$ by setting 1 in a position if the corresponding patch is present in the picture, 0 otherwise. It is easy to see that $k_1(x,x') = \langle\phi(x), \phi(x')\rangle$ for this ϕ.
2. Let A, B denote a two patches with all 0's and all 1's respectively. Let x_1, x_2, x_3 be three pictures with $x_1 = A, x_2 = B, x_3 = [AB](A, B$ horizontally concatenated. Then the Gram matix is K is not positive semi-definite.

3.2 Positive definiteness of Gaussian Kernel

1. Let x_1, x_2, x_n be arbitrary points in $\mathbb{R}^d$. Let K_1, K_2 be the Gram matrices of k_1, k_2 for these points. Then the Gram matrix of k is $\alpha K_1 + \beta K_2$ which is $\succeq 0$ because $K_1, K_2 \succeq 0$ and $\alpha, \beta \geq 0$.
2. Let K_1, K_2 be the Gram matrices of k_1, k_2. Then their element-wise product $K = K_1 \circ K_2$ is the Gram matrix of k. Let U, V be independent zero-mean Gaussian random variables with covariance matrices

K_1, K_2. Then the covariance matrix of $U \circ V$ is $K_1 \circ K_2$ as its ijth element is

$$\mathbb{E}[U_i V_i U_j V_j] = \mathbb{E}[U_i U_j]\mathbb{E}[V_i V_j] = (K_1)_{ij}(K_2)_{ij}$$

which means $K \succeq 0$.

3. Let the partial sums in the Taylor expansion of $\exp(k)$ be

$$k_m = \sum_{i=1}^{m} \frac{k^i}{i!} \text{ , so that } \exp(k) = \lim_{m\to\infty} k_m.$$

k_m is a valid kernel for $m \in \mathbb{N}$. Let $x_i, i \in [n]$ be n arbitrary points in $\mathbb{R}^d$. Let $u \in \mathbb{R}^n$. Let $\epsilon > 0$. $\exists m_0 \in \mathbb{N} \ni m \geq m_0 \Rightarrow |k(x_i, x_j) - k_m(x_i, x_j)| < \epsilon$. Let $m \geq m_0$ and let K, K_m be the Gram matrices of k, k_m respectively for $x_1, \cdots, x_n$.

$$|u^T K u - u_m^K u| = |\sum_{i,j} u_i u_j (K - K_m)_{ij}| \leq \epsilon u^T u \Rightarrow u^T K u \geq u_m^K u - \epsilon u^T u \geq -\epsilon u^T u$$

Thus, given any $u \in \mathbb{R}^n$, and $\epsilon > 0$, we can show $u^K u \geq -\epsilon u^T u$, which means $u^T K u \geq 0$. This shows that $K \succeq 0$ and hence $exp(k)$ is a positive definite kernel.

4. Let $psi(x) = \exp(-\delta\|x\|^2)$. Write

$$k(x, x') = \exp(-\delta\|x - x'\|^2) = \psi(x)\psi(x')\exp(\delta\langle x, x'\rangle)$$

Let $k_1(x, x') = \psi(x)\psi(x')$. Then for arbitrary points $x_1, x_2, \cdots, x_n$, the Gram matrix constructed from k_1 would be the outer product

$$[\psi(x_1), \cdots, \psi(x_n)][\psi(x_1), \cdots, \psi(x_n)]^T$$

which is $\succeq 0$, and hence k_1 is a positive definite kernel. Now using parts 3 and 2 of this subproblem, k is a positive definite kernel.

5. Let $k_1 = \exp(-k)$ and let x, y be two distint points. We will show that $k_1^2(x, y) > k_1(x, x)k_1(y, y)$ which means k_1 is not a positive definite kernel.

$$\begin{aligned}
&k_1^2(x, y) > k_1(x, x)k_1(y, y) \\
&\Leftrightarrow e^{-2k(x,y)} > e^{-k(x,x)}e^{-k(y,y)} \\
&\Leftrightarrow -2k(x, y) > -k(x, x) - k(y, y) \\
&\Leftrightarrow \|k(x, .) - k(y, .)\|^2 > 0
\end{aligned}$$

which is true.

3.3 Checking validity by Fourier transforms

1. Define $f : \mathbb{R} \to \mathbb{R}$ by $f(x) = \exp(-\delta x^2)$. Its Fourier transform $\tilde{f}\mathbb{R} \to \mathbb{R}$ can be lookedup up from Wikipedia:

$$\tilde{f}(a) = \int_{\mathbb{R}} e^{2\pi a x} e^{-\delta x^2/2}\, dx = \sqrt{\pi/\delta} e^{-\pi^2 a^2}/\delta > 0$$

The Fourier transform of k' is

$$\tilde{k}'(w) = \int_{\mathbb{R}^d} e^{2\pi i\langle w,x\rangle} e^{-\delta\|x\|^2}\, dx = \int_{\mathbb{R}^d} \prod_{i=1}^{d} e^{2\pi w_i x_i} e^{-\delta x_i^2}\, dx = \prod_{i=1}^{d} \int_{\mathbb{R}} e^{2\pi w_i x_i} e^{-\delta x_i^2}\, dx_i = \prod_{i=1}^{d} \tilde{f}(w_i)$$

which is positive and so k' is positive definite.

2. Define $f : \mathbb{R} \to \mathbb{R}$ by $f(x) = \frac{1}{1+x^2}$. Its Fourier transform $\tilde{f}\mathbb{R} \to \mathbb{R}$ can be lookedup up from Wikipedia(characterstic function of univariate Cauchy distribution):

$$\tilde{f}(a) = \int_{\mathbb{R}} e^{2\pi a x} \frac{1}{1+x^2}\, dx = \pi e^{-2\pi|a|} > 0$$

The Fourier transform of k' is

$$\tilde{k'}(w) = \int_{\mathbb{R}^d} e^{2\pi i\langle w,x\rangle} \prod_{i=1}^{d} \frac{1}{1+x_i^2}\, dx = \int_{\mathbb{R}^d} \prod_{i=1}^{d} e^{2\pi w_i x_i} \frac{1}{1+x_i^2}\, dx = \prod_{i=1}^{d} \int_{\mathbb{R}} e^{2\pi w_i x_i} \frac{1}{1+x_i^2}\, dx_i = \prod_{i=1}^{d} \tilde{f}(w_i)$$

which is positive and so k' is positive definite.

3.4 RKHS from the eigen functions of the kernels integral operator

Let $f \in \mathcal{H}$. Then f can be written as $f = \sum_{j=1}^{\infty} a_j \phi_j$, for some reals a_j.

$$\langle f, k(x,.)\rangle = \left\langle \sum_{j=1}^{\infty} a_j \phi_j, \sum_{i=1}^{\infty} \lambda_i \phi_i(x)\phi_i \right\rangle = \sum_{j=1}^{\infty} a_j \lambda_j \phi(x)/lambda a_j = \sum_{j=1}^{\infty} a_j \phi(x) = f(x)$$

3.5 Optimizing over an RKHS

Let f^* be a minimizer. By Representer theorem, there exists $\alpha_i \in \mathbb{R}, i \in [n]$ such that $f^* = \sum_{i=1}^{n} \alpha_i k(x_i,.)$. Let K denote the Gram matrix for the data points $x_i, i \in [n]$. Note that $f^*(x_i) = (K\alpha)_i$ and $\|f^*\|^2 = \alpha^T K \alpha$. f^* is an optimizer for the given problem

$$\begin{aligned}
&\Leftrightarrow \alpha \text{ minimizes } \|y - K\alpha\|^2 + \lambda \alpha^T K \alpha \\
&\Leftrightarrow K(K\alpha - y) + \lambda K\alpha = 0 \\
&\Leftrightarrow (K + \lambda I)(K\alpha) = Ky \\
&\Leftrightarrow K\alpha = (K + \lambda I)^{-1} Ky
\end{aligned}$$

Notice that $K + \lambda I \succ 0$ and hence invertible because $K \succeq 0$ and $\lambda I \succ 0$. For the fitted values,

$$\widehat{y} = f^*(x) = K\alpha = (K + \lambda I)^{-1} Ky,$$

which of the form $\widehat{y} = Sy$ with $S = (K + \lambda I)^{-1} K$.

3.6 Some computational considerations for SVM

1. $O(m^2)$
2. $O(md)$
3. $O(n \log d$ where n is the number of random projections used.