Introduction to Machine Learning - CS725
Instructor: Prof. Ganesh Ramakrishnan
Lecture 12 - Support Vector Regression and its Dual

KKT conditions for the Constrained (Convex) Problem

- Here, $\mathbf{w} \in \mathbb{R}^n$ and the domain is the intersection of all functions. Lagrangian is:

$$L(\mathbf{w}, \lambda, \mu) = f(\mathbf{w}) + \sum_{i=1}^{m} \lambda_i g_i(\mathbf{w}) + \sum_{j=1}^{p} \mu_j h_j(\mathbf{w})$$

- KKT **necessary** conditions for all differentiable functions (i.e. f, g_i, h_j) with optimality points $\hat{\mathbf{w}}$ and $(\hat{\lambda}, \hat{\mu})$ are:
  - $\nabla f(\hat{\mathbf{w}}) + \sum_{i=1}^{m} \hat{\lambda}_i \nabla g_i(\hat{\mathbf{w}}) + \sum_{j=1}^{p} \hat{\mu}_j \nabla h_j(\hat{\mathbf{w}}) = 0$
  - $g_i(\hat{\mathbf{w}}) \leq 0; 1 \leq i \leq m$
  - $\hat{\lambda}_i \geq 0; 1 \leq i \leq m$
  - $\hat{\lambda}_i g_i(\hat{\mathbf{w}}) = 0; 1 \leq i \leq m$
  - $h_j(\hat{\mathbf{w}}) = 0; 1 \leq j \leq p$
- When f and $g_i, \forall i \in [1, m]$ are convex and $h_j, \forall j \in [1, p]$ are affine, KKT conditions are also **sufficient** for optimality at $\hat{\mathbf{w}}$ and $(\hat{\lambda}, \hat{\mu})$

KKT conditions for the Constrained (Convex) Problem
Application 2: SVR and its Dual

KKT conditions for SVR

$$L(\mathbf{w}, \alpha, \alpha^*, \mu, \mu^*) = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_i(\xi_i + \xi_i^*) + \sum_{i=1}^m \alpha_i\left(y_i - \mathbf{w}^\top\phi(\mathbf{x}_i) - b - \epsilon - \xi_i\right) +$$
$$\sum_{i=1}^m \alpha_i^*\left(b + \mathbf{w}^\top\phi(\mathbf{x}_i) - y_i - \epsilon - \xi_i^*\right) - \sum_{i=1}^m \mu_i\xi_i - \sum_{i=1}^m \mu_i^*\xi_i^*$$

- Differentiating the Lagrangian w.r.t. $\mathbf{w}$,
  $$\mathbf{w} - \alpha_i\phi(\mathbf{x}_i) + \alpha_i^*\phi(\mathbf{x}_i) = 0 \text{ i.e., } \mathbf{w} = \sum_{i=1}^m(\alpha_i - \alpha_i^*)\phi(\mathbf{x}_i)$$
- Differentiating the Lagrangian w.r.t. ξ_i,
  $C - \alpha_i - \mu_i = 0$ *i.e.*, $\alpha_i + \mu_i = C$
- Differentiating the Lagrangian w.r.t ξ_i^*,
  $\alpha_i^* + \mu_i^* = C$
- Differentiating the Lagrangian w.r.t b,
  $\sum_i(\alpha_i^* - \alpha_i) = 0$
- Complimentary slackness:
  $\alpha_i(y_i - \mathbf{w}^\top\phi(\mathbf{x}_i) - b - \epsilon - \xi_i) = 0$ AND $\mu_i\xi_i = 0$ AND
  $\alpha_i^*(b + \mathbf{w}^\top\phi(\mathbf{x}_i) - y_i - \epsilon - \xi_i^*) = 0$ AND $\mu_i^*\xi_i^* = 0$

Support Vector Regression

Dual Objective

SVR Dual objective

- $L^*(\alpha, \alpha^*, \mu, \mu^*) = \min_{\mathbf{w}, b, \xi, \xi^*} L(\mathbf{w}, b, \xi, \xi^*, \alpha, \alpha^*, \mu, \mu^*)$
- Assume: In case of SVR, we have a strictly convex objective and linear constraints $\Rightarrow$ KKT conditions are necessary and sufficient and strong duality holds (for $\alpha, \alpha^* \geq 0$):

$$\min_{\mathbf{w}, b, \xi, \xi^*} \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^{m} (\xi_i + \xi_i^*) = \max_{\alpha, \alpha^*, \mu, \mu^*} L^*(\alpha, \alpha^*, \mu, \mu^*)$$

s.t. $y_i - \mathbf{w}^\top \phi(\mathbf{x}_i) - b \leq \epsilon - \xi_i$, and
$w^\top \phi(\mathbf{x}_i) + b - y_i \leq \epsilon - \xi_i^*$, and
$\xi_i, \xi^* \geq 0, \ \forall i = 1, \ldots, n$

- This value is precisely obtained at the $\left\{\hat{\mathbf{w}}, \hat{b}, \hat{\xi}, \hat{\xi}^*, \hat{\alpha}, \hat{\alpha}^*, \hat{\mu}, \hat{\mu}^*\right\}$ that satisfies the necessary (and sufficient) KKT optimality conditions [**KKT Constraint Set**]
- Given strong duality, we can equivalently solve: $\max_{\hat{\alpha}, \hat{\alpha}^*, \hat{\mu}, \hat{\mu}^*} L^*(\hat{\alpha}, \hat{\alpha}^*, \hat{\mu}, \hat{\mu}^*)$

- $L(\hat{\alpha}, \hat{\alpha}^*, \hat{\mu}, \hat{\mu}^*) = \frac{1}{2}\|\hat{\mathbf{w}}\|^2 + C\sum_{i=1}^{m}(\hat{\xi}_i + \hat{\xi}_i^*) + \sum_{i=1}^{m}\Big(\hat{\alpha}_i(y_i - \mathbf{w}^\top\phi(\mathbf{x}_i) - b - \epsilon - \hat{\xi}_i) + \hat{\alpha}_i^*(\mathbf{w}^\top\phi(\mathbf{x}_i) + b - y_i - \epsilon - \hat{\xi}_i^*)\Big) - \sum_{i=1}^{m}(\hat{\mu}_i\hat{\xi}_i + \hat{\mu}_i^*\hat{\xi}_i^*)$
- We obtain $\hat{\mathbf{w}}$, $\hat{b}$, $\hat{\xi}_i$, $\hat{\xi}_i^*$ in terms of $\hat{\alpha}$, $\hat{\alpha}^*$, $\hat{\mu}$ and $\hat{\mu}^*$ by using the KKT conditions derived earlier as $\hat{\mathbf{w}} = \sum_{i=1}^{m}(\hat{\alpha}_i - \hat{\alpha}_i^*)\phi(\mathbf{x}_i)$ and $\sum_{i=1}^{m}(\hat{\alpha}_i - \hat{\alpha}_i^*) = 0$ and $\hat{\alpha}_i + \hat{\mu}_i = C$ and $\hat{\alpha}_i^* + \hat{\mu}_i^* = C$
- Thus, we get (after dropping the messy $\hat{}$ hat notation):

- $L(\hat{\alpha}, \hat{\alpha}^*, \hat{\mu}, \hat{\mu}^*) = \frac{1}{2}\|\hat{\mathbf{w}}\|^2 + C\sum_{i=1}^m(\hat{\xi}_i + \hat{\xi}_i^*) +$
  $\sum_{i=1}^m \left(\hat{\alpha}_i(y_i - \mathbf{w}^\top\phi(\mathbf{x}_i) - b - \epsilon - \hat{\xi}_i) + \hat{\alpha}_i^*(\mathbf{w}^\top\phi(\mathbf{x}_i) + b - y_i - \epsilon - \hat{\xi}_i^*)\right) -$
  $\sum_{i=1}^m (\hat{\mu}_i\hat{\xi}_i + \hat{\mu}_i^*\hat{\xi}_i^*)$
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- Thus, we get (after dropping the messy $\hat{}$ hat notation):
  $L(\mathbf{w}, b, \xi, \xi^*, \alpha, \alpha^*, \mu, \mu^*)$
  $= \frac{1}{2}\sum_i\sum_j(\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*)\phi^\top(\mathbf{x}_i)\phi(\mathbf{x}_j) +$
  $\sum_i(\xi_i(C - \alpha_i - \mu_i) + \xi_i^*(C - \alpha_i^* - \mu_i^*)) - b\sum_i(\alpha_i - \alpha_i^*) - \epsilon\sum_i(\alpha_i + \alpha_i^*) +$
  $\sum_i y_i(\alpha_i - \alpha_i^*) - \sum_i\sum_j(\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*)\phi^\top(\mathbf{x}_i)\phi(\mathbf{x}_j)$

- $L(\hat{\alpha}, \hat{\alpha}^*, \hat{\mu}, \hat{\mu}^*) = \frac{1}{2}\|\hat{\mathbf{w}}\|^2 + C\sum_{i=1}^{m}(\hat{\xi}_i + \hat{\xi}_i^*) + \sum_{i=1}^{m}\left(\hat{\alpha}_i(y_i - \mathbf{w}^\top\phi(\mathbf{x}_i) - b - \epsilon - \hat{\xi}_i) + \hat{\alpha}_i^*(\mathbf{w}^\top\phi(\mathbf{x}_i) + b - y_i - \epsilon - \hat{\xi}_i^*)\right) - \sum_{i=1}^{m}(\hat{\mu}_i\hat{\xi}_i + \hat{\mu}_i^*\hat{\xi}_i^*)$
- We obtain $\hat{\mathbf{w}}$, $\hat{b}$, $\hat{\xi}_i$, $\hat{\xi}_i^*$ in terms of $\hat{\alpha}$, $\hat{\alpha}^*$, $\hat{\mu}$ and $\hat{\mu}^*$ by using the KKT conditions derived earlier as $\hat{\mathbf{w}} = \sum_{i=1}^{m}(\hat{\alpha}_i - \hat{\alpha}_i^*)\phi(\mathbf{x}_i)$ and $\sum_{i=1}^{m}(\hat{\alpha}_i - \hat{\alpha}_i^*) = 0$ and $\hat{\alpha}_i + \hat{\mu}_i = C$ and $\hat{\alpha}_i^* + \hat{\mu}_i^* = C$
- Thus, we get (after dropping the messy $\hat{}$ hat notation):
  $L(\mathbf{w}, b, \xi, \xi^*, \alpha, \alpha^*, \mu, \mu^*)$
  $= \frac{1}{2}\sum_i\sum_j(\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*)\phi^\top(\mathbf{x}_i)\phi(\mathbf{x}_j) + \sum_i\left(\xi_i(C - \alpha_i - \mu_i) + \xi_i^*(C - \alpha_i^* - \mu_i^*)\right) - b\sum_i(\alpha_i - \alpha_i^*) - \epsilon\sum_i(\alpha_i + \alpha_i^*) + \sum_i y_i(\alpha_i - \alpha_i^*) - \sum_i\sum_j(\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*)\phi^\top(\mathbf{x}_i)\phi(\mathbf{x}_j)$
  $= -\frac{1}{2}\sum_i\sum_j(\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*)\phi^\top(\mathbf{x}_i)\phi(\mathbf{x}_j) - \epsilon\sum_i(\alpha_i + \alpha_i^*) + \sum_i y_i(\alpha_i - \alpha_i^*)$

SVR Dual Formulation using only dot products $\phi^T(\mathbf{x}_i)\phi(\mathbf{x}_j)$

- $\mathbf{w} = \sum_{i=1}^{m}(\alpha_i - \alpha_i^*)\phi(x_i) \Rightarrow$ the final decision function $f(\mathbf{x}) = \mathbf{w}^T\phi(\mathbf{x})+b = \sum_{i=1}^{m}(\alpha_i-\alpha_i^*)\phi^T(\mathbf{x}_i)\phi(\mathbf{x})+y_j-\sum_{i=1}^{m}(\alpha_i-\alpha_i^*)\phi^T(\mathbf{x}_i)\phi(\mathbf{x}_j)-\epsilon$ $\mathbf{x}_j$ is any point with $\alpha_j \in (0, C)$. **Tutorial 5: Derive kernelized expression for Ridge Regression**
- The dual optimization problem to compute the α's for SVR is:

SVR Dual Formulation using only dot products $\phi^T(\mathbf{x}_i)\phi(\mathbf{x}_j)$

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  $\mathbf{x}_j$ is any point with $\alpha_j \in (0, C)$. **Tutorial 5: Derive kernelized expression for Ridge Regression**
- The dual optimization problem to compute the α's for SVR is:

$$max_{\alpha_i,\alpha_i^*} - \frac{1}{2}\sum_i\sum_j(\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*)\phi^\top(\mathbf{x}_i)\phi(\mathbf{x}_j)$$

$$-\epsilon\sum_i(\alpha_i + \alpha_i^*) + \sum_i y_i(\alpha_i - \alpha_i^*)$$

s.t.

  - $\sum_i(\alpha_i - \alpha_i^*) = 0$
  - $\alpha_i, \alpha_i^* \in [0, C]$
- **We notice that the only way these three expressions involve ϕ is through $\phi^\top(\mathbf{x}_i)\phi(\mathbf{x}_j) = K(\mathbf{x}_i, \mathbf{x}_j)$, for some i, j**

Support Vectors: Non-zero contribution $\alpha_i - \alpha_i^*$ outside ϵ-band

- **For any point $(\mathbf{x}_i, y_i)$, the product $\alpha_i \alpha_i^* = 0$.**

Support Vectors: Non-zero contribution $\alpha_i - \alpha_i^*$ outside ϵ-band

- **For any point $(\mathbf{x}_i, y_i)$, the product $\alpha_i \alpha_i^* = 0$.**
  - Let $\alpha_i > 0$ and $\alpha_i^* > 0$. This leads to a contradiction.
  - By Complimentary slackness, $y_i - \mathbf{w}^\top \phi(\mathbf{x}_i) - b - \epsilon - \xi_i = 0$ AND $b + \mathbf{w}^\top \phi(\mathbf{x}_i) - y_i - \epsilon - \xi_i^* = 0$. Adding up the two equalities gives us: $\xi_i + \xi_i^* = -2\epsilon$.
  - Since only one of ξ_i and ξ_i^* can be non-zero,$\Longrightarrow$ the non-zero component is negative, which is a contradiction since $\xi_i, \xi_i^* \geq 0$
  - Thus, $\alpha_i - \alpha_i^* \propto \max\{\alpha_i, \alpha_i^*\}$
- **For points within the ϵ-insensitive tube $\alpha_i = 0$ and $\alpha_i^* = 0$:**

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- **For points within the ϵ-insensitive tube $\alpha_i = 0$ and $\alpha_i^* = 0$:**
  - If $y_i - \mathbf{w}^\top \phi(\mathbf{x}_i) - b - \epsilon - \xi_i < 0$, then $\alpha_i = 0$, $\mu_i = C$ and $\xi_i = 0$. Similarly, $b + \mathbf{w}^\top \phi(\mathbf{x}_i) - y_i - \epsilon < 0$ leading to $\alpha_i^* = 0$.
- **$\alpha_i = C$ and $\alpha_i^* = C$ correspond to points lying either outside or on the $\epsilon-$tube:**

Support Vectors: Non-zero contribution $\alpha_i - \alpha_i^*$ outside ϵ-band

- **For any point $(\mathbf{x}_i, y_i)$, the product $\alpha_i \alpha_i^* = 0$.**
  - Let $\alpha_i > 0$ and $\alpha_i^* > 0$. This leads to a contradiction.
  - By Complimentary slackness, $y_i - \mathbf{w}^\top \phi(\mathbf{x}_i) - b - \epsilon - \xi_i = 0$ AND $b + \mathbf{w}^\top \phi(\mathbf{x}_i) - y_i - \epsilon - \xi_i^* = 0$. Adding up the two equalities gives us: $\xi_i + \xi_i^* = -2\epsilon$.
  - Since only one of ξ_i and ξ_i^* can be non-zero,$\Longrightarrow$ the non-zero component is negative, which is a contradiction since $\xi_i, \xi_i^* \geq 0$
  - Thus, $\alpha_i - \alpha_i^* \propto \max\{\alpha_i, \alpha_i^*\}$
- **For points within the ϵ-insensitive tube $\alpha_i = 0$ and $\alpha_i^* = 0$:**
  - If $y_i - \mathbf{w}^\top \phi(\mathbf{x}_i) - b - \epsilon - \xi_i < 0$, then $\alpha_i = 0$, $\mu_i = C$ and $\xi_i = 0$. Similarly, $b + \mathbf{w}^\top \phi(\mathbf{x}_i) - y_i - \epsilon < 0$ leading to $\alpha_i^* = 0$.
- **$\alpha_i = C$ and $\alpha_i^* = C$ correspond to points lying either outside or on the $\epsilon-$tube:**
  - If $\alpha_i = C$, then $\mu_i = 0$ and $y_i - \mathbf{w}^\top \phi(\mathbf{x}_i) - b - \epsilon = \xi_i \geq 0$.
  - Similarly, $\alpha_i^* = C$ corresponds to points lying below (or beyond) the lower $\epsilon-$band.
- **For points on boundary of the ϵ-insensitive tube $\alpha_i \in [0, C]$:**

Support Vectors: Non-zero contribution $\alpha_i - \alpha_i^*$ outside ϵ-band

- **For any point $(\mathbf{x}_i, y_i)$, the product $\alpha_i\alpha_i^* = 0$.**
    - Let $\alpha_i > 0$ and $\alpha_i^* > 0$. This leads to a contradiction.
    - By Complimentary slackness, $y_i - \mathbf{w}^\top\phi(\mathbf{x}_i) - b - \epsilon - \xi_i = 0$ AND $b + \mathbf{w}^\top\phi(\mathbf{x}_i) - y_i - \epsilon - \xi_i^* = 0$. Adding up the two equalities gives us: $\xi_i + \xi_i^* = -2\epsilon$.
    - Since only one of ξ_i and ξ_i^* can be non-zero,$\Longrightarrow$ the non-zero component is negative, which is a contradiction since $\xi_i, \xi_i^* \geq 0$
    - Thus, $\alpha_i - \alpha_i^* \propto \max\{\alpha_i, \alpha_i^*\}$
- **For points within the ϵ-insensitive tube $\alpha_i = 0$ and $\alpha_i^* = 0$:**
    - If $y_i - \mathbf{w}^\top\phi(\mathbf{x}_i) - b - \epsilon - \xi_i < 0$, then $\alpha_i = 0$, $\mu_i = C$ and $\xi_i = 0$. Similarly, $b + \mathbf{w}^\top\phi(\mathbf{x}_i) - y_i - \epsilon < 0$ leading to $\alpha_i^* = 0$.
- **$\alpha_i = C$ and $\alpha_i^* = C$ correspond to points lying either outside or on the $\epsilon-$tube:**
    - If $\alpha_i = C$, then $\mu_i = 0$ and $y_i - \mathbf{w}^\top\phi(\mathbf{x}_i) - b - \epsilon = \xi_i \geq 0$.
    - Similarly, $\alpha_i^* = C$ corresponds to points lying below (or beyond) the lower $\epsilon-$band.
- **For points on boundary of the ϵ-insensitive tube $\alpha_i \in [0, C]$:**
    - For any point on the upper margin, $y_i - \mathbf{w}^\top\phi(\mathbf{x}_i) - b - \epsilon = 0$ and $\xi_i = 0 \Longrightarrow \mu_i \geq 0$ $\Longrightarrow \alpha_i \in [0, C]$. Similarly, $\alpha_i^* \in [0, C]$ for points lying on the margin of the lower $\epsilon-$band.

Kernel function: $K(\mathbf{x}_i, \mathbf{x}_j) = \phi^T(\mathbf{x}_i)\phi(\mathbf{x}_j)$

- We call $\phi^\top(\mathbf{x}_i)\phi(\mathbf{x}_j)$ a **kernel function**:
  $K(\mathbf{x}_i, \mathbf{x}_j) = \phi^\top(\mathbf{x}_i)\phi(\mathbf{x}_j)$
- The Kernel Trick: For some important choices of ϕ, compute $K(\mathbf{x}_i, \mathbf{x}_j)$ directly and more efficiently than having to explicitly compute/enumerate $\phi(\mathbf{x}_i)$ and $\phi(\mathbf{x}_j)$
- The expression for decision function becomes $f(x) = \sum_{i=1}^{m} \alpha_i K(\mathbf{x}, \mathbf{x}_i)$
- Computation of α_i is specific to the objective function being minimized: Closed form exists for Ridge regression but NOT for SVR

The Kernelized version of SVR

- The kernelized dual problem:

$$max_{\alpha_i,\alpha_i^*} -\frac{1}{2}\sum_i\sum_j(\alpha_i-\alpha_i^*)(\alpha_j-\alpha_j^*)K(\mathbf{x}_i,\mathbf{x}_j)$$

$$-\epsilon\sum_i(\alpha_i+\alpha_i^*)+\sum_i y_i(\alpha_i-\alpha_i^*)$$

  s.t.
  - $\sum_i(\alpha_i-\alpha_i^*)=0$
  - $\alpha_i,\alpha_i^*\in[0,C]$
- The kernelized decision function:
  $f(\mathbf{x})=\sum_i(\alpha_i-\alpha_i^*)K(\mathbf{x}_i,\mathbf{x})+b$
- Using any point x_j with $\alpha_j\in(0,C)$:
  $b=y_j-\sum_i(\alpha_i-\alpha_i^*)K(\mathbf{x}_i,\mathbf{x}_j)$
- Computing $K(\mathbf{x}_1,\mathbf{x}_2)$ often does not even require computing $\phi(\mathbf{x}_1)$ or $\phi(\mathbf{x}_2)$ explicitly

Basis function expansion and the Kernel trick

- We started off with the functional form[1]

$$f(\mathbf{x}) = \sum_{j=1}^{p} w_j \phi_j(\mathbf{x})$$

  Each ϕ_j is called a *basis function* and this representation is called *basis function expansion*[2]

- And we landed up with an equivalent

$$f(\mathbf{x}) = \sum_{i=1}^{m} \alpha_i K(\mathbf{x}, \mathbf{x}_i)$$

  for Ridge regression and Support Vector Regression

- Aside: For $p \in [0, \infty)$, with what K, kind of regularizers, loss functions, *etc.*, will these dual representations hold?[3]

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[1] The additional b term can be either absorbed in ϕ or kept separate as discussed on several occasions.

[2] Section 2.8.3 of Tibshi

[3] Section 5.8.1 of Tibshi

Tutorial 5: Kernelizing Ridge Regression

- Given $w = (\Phi^T\Phi + \lambda I)^{-1}\Phi^T y$ and using the identity $(P^{-1} + B^T R^{-1} B)^{-1} B^T R^{-1} = PB^T(BPB^T + R)^{-1}$
  - $\Rightarrow w = \Phi^T(\Phi\Phi^T + \lambda I)^{-1} y = \sum_{i=1}^{m} \alpha_i \phi(x_i)$ where $\alpha_i = \left((\Phi\Phi^T + \lambda I)^{-1} y\right)_i$
  - $\Rightarrow$ the final decision function $f(\mathbf{x}) = \phi^T(\mathbf{x})\mathbf{w} = \sum_{i=1}^{m} \alpha_i \phi^T(\mathbf{x})\phi(\mathbf{x}_i)$
- Again, **We notice that the only way the decision function $f(\mathbf{x})$ involves ϕ is through $\phi^\top(\mathbf{x}_i)\phi(\mathbf{x}_j)$, for some i, j**

The Representer Theorem & Reproducing Kernel Hilbert Space (RKHS)

1. The solution $f^* \in \mathcal{H}$ (Hilbert space) to the following problem

$$f^* = \arg\min_{f \in \mathcal{H}} \sum_{i=1}^{m} \mathbf{E}\left(f\left(\mathbf{x}^{(i)}\right), y^{(i)}\right) + \Omega(\|f\|_K)$$

can be always written as $f^*(\mathbf{x}) = \sum_{i=1}^{m} \alpha_i K(\mathbf{x}, \mathbf{x}^{(i)})$, provided $\Omega(\|f\|_K)$ is a ....

2. More specifically, if $f(\mathbf{x}) = \mathbf{w}^T\phi(\mathbf{x}) + b$ and $K(\mathbf{x}', \mathbf{x}) = \phi^T(\mathbf{x})\phi(\mathbf{x}')$ then the solution $\mathbf{w}^* \in \Re^n$ to the following problem

$$(\mathbf{w}^*, b^*) = \arg\min_{\mathbf{w}, b} \sum_{i=1}^{m} \mathbf{E}\left(f\left(\mathbf{x}^{(i)}\right), y^{(i)}\right) + \Omega(\|\mathbf{w}\|_2)$$

can be always written as $\phi^T(\mathbf{x})\mathbf{w}^* + b = \sum_{i=1}^{m} \alpha_i K(\mathbf{x}, \mathbf{x}^{(i)})$, provided $\Omega(\|\mathbf{w}\|_2)$ is a monotonically increasing function of $\|\mathbf{w}\|_2$. $\Re^n$ is the Hilbert space and $K(., \mathbf{x}) : \mathcal{X} \rightarrow \Re$ is the **Reproducing (RKHS) Kernel**

The Representer Theorem and SVR

1. The SVR Objective

$$(\mathbf{w}^*, b^*, \xi_i^*) = \arg\min_{\mathbf{w}, b, \xi_i} C \sum_{i=1}^{m} (\xi_i + \xi_i^*) + \frac{1}{2} \|\mathbf{w}\|_2^2$$

s.t. $y_i - \mathbf{w}^\top \phi(\mathbf{x}_i) - b \leq \epsilon - \xi_i$, and
$w^\top \phi(\mathbf{x}_i) + b - y_i \leq \epsilon - \xi_i^*$, and
$\xi_i, \xi^* \geq 0, \forall i = 1, \ldots, n$

2. Can be rewritten as

The Representer Theorem and SVR

1. The SVR Objective

$$(\mathbf{w}^*, b^*, \xi_i^*) = \arg\min_{\mathbf{w}, b, \xi_i} C \sum_{i=1}^{m} (\xi_i + \xi_i^*) + \frac{1}{2} \|\mathbf{w}\|_2^2$$

s.t. $y_i - \mathbf{w}^\top \phi(\mathbf{x}_i) - b \leq \epsilon - \xi_i$, and
$w^\top \phi(\mathbf{x}_i) + b - y_i \leq \epsilon - \xi_i^*$, and
$\xi_i, \xi^* \geq 0, \; \forall i = 1, \ldots, n$

2. Can be rewritten as

$$(\mathbf{w}^*, b^*, \xi_i^*) = \arg\min_{\mathbf{w}, b, \xi_i} C \sum_{i=1}^{m} \max \left\{ \epsilon \pm \left(y_i - \mathbf{w}^\top \phi(\mathbf{x}_i) - b \right), 0 \right\} + \frac{1}{2} \|\mathbf{w}\|_2^2$$

The Representer Theorem and SVR (contd.)

1. If $f(\mathbf{x}) = \mathbf{w}^T\phi(\mathbf{x}) + b$ and $K(\mathbf{x}', \mathbf{x}) = \phi^T(\mathbf{x})\phi(\mathbf{x}')$ and given the SVR objective

$$(\mathbf{w}^*, b^*, \xi_i^*) = \underset{\mathbf{w}, b, \xi_i}{\arg\min}\; C\sum_{i=1}^{m} \max\left\{\epsilon \pm \left(y_i - \mathbf{w}^\top\phi(\mathbf{x}_i) - b\right), 0\right\} + \frac{1}{2}\|\mathbf{w}\|_2^2$$

2. Setting $\mathbf{E}\left(f\left(\mathbf{x}^{(i)}\right), y^{(i)}\right) = C\max\left\{\epsilon \pm \left(y_i - \mathbf{w}^\top\phi(\mathbf{x}_i) - b\right), 0\right\}$ and $\Omega(\|\mathbf{w}\|_2) = \frac{1}{2}\|\mathbf{w}\|_2^2$, we can apply the Representer theorem to SVR, so that $\phi^T(\mathbf{x})\mathbf{w}^* + b = \sum_{i=1}^{m}\alpha_i K(\mathbf{x}, \mathbf{x}^{(i)})$

An Example Kernel

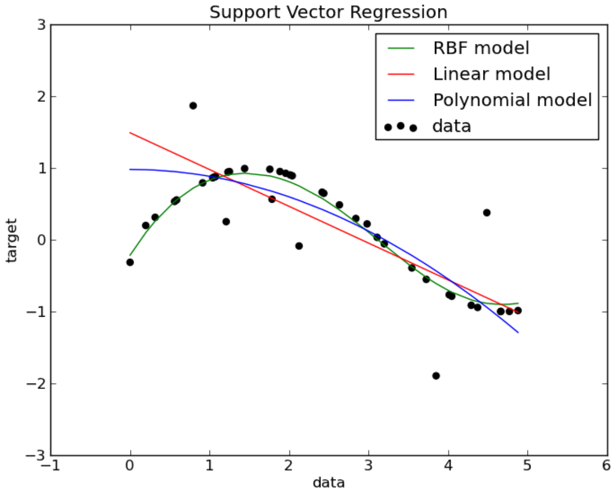
- Let $K(\mathbf{x}_1, \mathbf{x}_2) = (1 + \mathbf{x}_1^\top \mathbf{x}_2)^2$
- Which value of $\phi(\mathbf{x})$ will yield $\phi^\top(\mathbf{x}_1)\phi(\mathbf{x}_2) = K(\mathbf{x}_1, \mathbf{x}_2) = (1 + \mathbf{x}_1^\top \mathbf{x}_2)^2$
- Is such a ϕ guaranteed to exist?
- Is there a unique ϕ for given K?

An Example Kernel

- We can prove that such a ϕ exists
- For example, for a 2-dimensional $\mathbf{x}_i$:

$$\phi(\mathbf{x}_i) = \begin{bmatrix} 1 \\ x_{i1}\sqrt{2} \\ x_{i2}\sqrt{2} \\ x_{i1}x_{i2}\sqrt{2} \\ x_{i1}^2 \\ x_{i2}^2 \end{bmatrix}$$

- $\phi(\mathbf{x}_i)$ exists in a 6-dimensional space
- But, to compute $K(\mathbf{x}_1, \mathbf{x}_2)$, all we need is $x_1^\top x_2$ without having to enumerate $\phi(\mathbf{x}_i)$



Support Vector Regression
RBF model
Linear model
Polynomial model
data
target
data
3
2
1
0
−1
−2
−3
−1
0
1
2
3
4
5
6

More on the Kernel Trick

- **Kernels** operate in a *high-dimensional*, *implicit* feature space without necessarily computing the coordinates of the data in that space, but rather by simply computing the Kernel function
- This approach is called the "*kernel trick*" and will subsequently talk about *valid kernels*
- This operation is often computationally cheaper than the explicit computation of the coordinates
- Claim: If $\mathcal{K}_{ij} = K(x_i, x_j) = \langle \phi(x_i), \phi(x_j) \rangle$ are entries of an $n \times n$ **Gram Matrix** $\mathcal{K}$ then
  - $\mathcal{K}$ must be positive semi-definite
  - Proof: $\mathbf{b}^T \mathcal{K} \mathbf{b} = \sum_{i,j} b_i \mathcal{K}_{ij} b_j = \sum_{i,j} b_i b_j \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle$
    $= \langle \sum_i b_i \phi(\mathbf{x}_i), \sum_j b_j \phi(\mathbf{x}_j) \rangle = || \sum_i b_i \phi(\mathbf{x}_i) ||_2^2 \geq 0$

Existence of basis expansion ϕ for symmetric K?

- *Positive-definite kernel:* For any dataset $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_m\}$ and for any m, the Gram matrix $\mathcal{K}$ must be positive definite

$$\mathcal{K} = \begin{bmatrix} K(\mathbf{x}_1, \mathbf{x}_1) & \ldots & K(\mathbf{x}_1, \mathbf{x}_n) \\ \ldots & K(\mathbf{x}_i, \mathbf{x}_j) & \ldots \\ K(\mathbf{x}_m, \mathbf{x}_1) & \ldots & K(\mathbf{x}_m, \mathbf{x}_m) \end{bmatrix}$$

so that $\mathcal{K} = U\Sigma U^T = (U\Sigma^{\frac{1}{2}})(U\Sigma^{\frac{1}{2}})^T = RR^T$ where rows of U are linearly independent and Σ is a positive diagonal matrix

[4]Eigen-decomposition wrt linear operators. See
`https://en.wikipedia.org/wiki/Mercer%27s_theorem`

[5]That is, if every Cauchy sequence is convergent.

Existence of basis expansion ϕ for symmetric K?

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  so that $\mathcal{K} = U\Sigma U^T = (U\Sigma^{\frac{1}{2}})(U\Sigma^{\frac{1}{2}})^T = RR^T$ where rows of U are linearly independent and Σ is a positive diagonal matrix
- *Mercer kernel:* Extending to eigenfunction decomposition[4]:

$$K(\mathbf{x}_1, \mathbf{x}_2) = \sum_{j=1}^{\infty} \alpha_j \phi_j(\mathbf{x}_1)\phi_j(\mathbf{x}_2) \text{ where } \alpha_j \geq 0 \text{ and } \sum_{j=1}^{\infty} \alpha_j^2 < \infty$$

- *Mercer kernel* and *Positive-definite kernel* turn out to be equivalent if the input space $\{x\}$ is *compact*[5]

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