SVM and Kernels

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Outline

- **Standard form problem** (not necessarily convex)

$$
\begin{aligned}
\text{minimize}_{\mathbf{x}} \quad & f_0(\mathbf{x}) \\
\text{subject to} \quad & f_i(\mathbf{x}) \leq 0, \quad i = 1, \ldots, m \\
& h_i(\mathbf{x}) = 0, \quad i = 1, \ldots, p
\end{aligned}
$$

  variable $\mathbf{x} \in X \subseteq \mathbb{R}^d$, optimal value f^*

- **Lagrangian**: $L : \mathbb{R}^d \times \mathbb{R}^m \times \mathbb{R}^p \to \mathbb{R}$, with $\mathrm{dom}(L) = X \times \mathbb{R}^m \times \mathbb{R}^p$

$$
L(\mathbf{x}, \lambda, \nu) = f_0(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i f_i(\mathbf{x}) + \sum_{i=1}^{p} \nu_i h_i(\mathbf{x})
$$

  — weighted sum of objective and constraint functions
  — λ_i is Lagramge multiplier associated with $f_i(\mathbf{x}) \leq 0$
  — ν_i is Lagrange multiplier associate with $h_i(\mathbf{x}) = 0$

- **Lagrange dual function** $g : \mathbb{R}^m \times \mathbb{R}^p \to \mathbb{R}$

$$\begin{aligned} g(\lambda, \nu) &= \inf_{\mathbf{x} \in X} L(\mathbf{x}, \lambda, \nu) \\ &= \inf_{\mathbf{x} \in X} \left(f_0(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i f_i(\mathbf{x}) + \sum_{i=1}^{p} \nu_i h_i(\mathbf{x}) \right), \end{aligned}$$

  g is concave, can be $-\infty$ for some λ, ν

- **Lower bound property**: if $\lambda \geq 0$, then $g(\lambda, \nu) \leq f^*$
- proof: if $\widetilde{\mathbf{x}}$ is feasible and $\lambda \geq 0$, then

$$f_0(\widetilde{\mathbf{x}}) \geq L(\widetilde{\mathbf{x}}, \lambda, \nu) \geq \inf_{\mathbf{x} \in X} L(\mathbf{x}, \lambda, \nu) = g(\lambda, \nu)$$

  minimizing over all feasible $\widetilde{\mathbf{x}}$ gives $f^* \geq g(\lambda, \nu)$

Lower bound property: if $\lambda \geq 0$, then $g(\lambda, \nu) \leq f^*$

Lagrange dual problem

$$\begin{aligned} \text{maximize}_{\lambda,\nu} \quad & g(\lambda, \nu) \\ \text{subject to} \quad & \lambda \geq 0 \end{aligned}$$

- finds best lower bound on f^*, obtained from Lagrange dual function
- a convex optimization problem; optimal value denoted g^*
- λ, ν are dual feasible if $\lambda \geq 0$, $(\lambda, \nu) \in \mathrm{dom}(g)$

Weak and strong duality

weak duality: $g^* \leq f^*$

- always holds (for convex and nonconvex problems)
- can be used to find nontrivial lower bounds for difficult problems

strong duality: $g^* = f^*$

- does not hold in general
- (usually) holds for convex problems
- conditions that guarantee strong duality in convex problems are called **constraint qualifications**

- Slater's condition (or Slater condition) is a sufficient condition for strong duality to hold for a convex optimization problem
- Strong duality holds for a convex problem

$$\begin{aligned} \text{minimize}_{\mathbf{x}} \quad & f_0(\mathbf{x}) \\ \text{subject to} \quad & f_i(\mathbf{x}) \leq 0, \;\; i = 1, \dots, m \\ & A\mathbf{x} = b \end{aligned}$$

  if it is strictly feasible, i.e.,

$$\exists \mathbf{x} \in \mathbf{int}(X): \;\; f_i(\mathbf{x}) < 0, \; i = 1, \dots, m, \; A\mathbf{x} = b$$

  - also guarantees that the dual optimum is attained (if $f^* > -\infty$)

Assume strong duality holds, $\mathbf{x}^*$ is primal optimal, (λ^*, ν^*) is dual optimal

$$
\begin{aligned}
f_0(\mathbf{x}^*) = g(\lambda^*, \nu^*) = \inf_{\mathbf{x} \in X} L(\mathbf{x}, \lambda^*, \nu^*) = \\
\inf_{\mathbf{x}} \left(f_0(\mathbf{x}) + \sum_{i=1}^m \lambda_i^* f_i(\mathbf{x}) + \sum_{i=1}^p \nu_i^* h_i(\mathbf{x}) \right) \\
\leq f_0(\mathbf{x}^*) + \sum_{i=1}^m \lambda_i^* f_i(\mathbf{x}^*) + \sum_{i=1}^p \nu_i^* h_i(\mathbf{x}^*) \\
\leq f_0(\mathbf{x}^*)
\end{aligned}
$$

hence, the two inequlities hold with equality

- $\mathbf{x}^*$ minimizes $L(\mathbf{x}, \lambda^*, \nu^*)$
- $\lambda_i^* f_i(\mathbf{x}^*) = 0$ for $i = 1, 2, \ldots, m$ (known as complementary slackness):

$$
\lambda_i^* > 0 \Rightarrow f_i(\mathbf{x}^*) = 0, \;\; f_i(\mathbf{x}^*) < 0 \Rightarrow \lambda_i^* = 0
$$

The following four conditions are called KKT conditions (for a problem with differentiable f_i, h_i)

- Primal constraints: $f_i(\mathbf{x}) \leq 0$, $i = 1, 2, \ldots, m$, $h_i(\mathbf{x}) = 0$, $i = 1, 2, \ldots, p$
- Dual constraints: $\lambda \geq 0$
- Complementary slackness: $\lambda_i f_i(\mathbf{x}) = 0$, $i = 1, 2, \ldots, m$
- Gradient of Lagrangian with respect to $\mathbf{x}$ vanishes:

$$\nabla f_0(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i \nabla f_i(\mathbf{x}) + \sum_{i=1}^{p} \nu_i \nabla h_i(\mathbf{x}) = 0$$

- If strong duality holds and $\mathbf{x}, \lambda, \nu$ are optimal, then they must satisfy the KKT conditions

KKT conditions for convex problem

If $\widetilde{\mathbf{x}}, \widetilde{\lambda}, \widetilde{\nu}$ satisfy KKT for a convex problem, then they are optimal:

- from slackness: $f_0(\widetilde{\mathbf{x}}) = L(\widetilde{\mathbf{x}}, \widetilde{\lambda}, \widetilde{\nu})$
- from 4th condition (and convexity): $g(\widetilde{\lambda}, \widetilde{\nu}) = L(\widetilde{\mathbf{x}}, \widetilde{\lambda}, \widetilde{\nu})$

hence, $f_0(\widetilde{\mathbf{x}}) = g(\widetilde{\lambda}, \widetilde{\nu})$

If **Slater's condition** is satisfied:

- $\mathbf{x}$ is optimal if and only if there exist λ, ν that satisfy KKT conditions
- recall that Slater implies strong duality, and dual optimum is attained
- generalizes optimality condition $\nabla f_0(\mathbf{x}) = 0$ for unconstrained problem

Binary Classification: Problem Statement

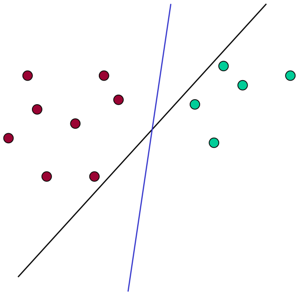
- **Training data**: sample drawn i.i.d. w.r.t. D on $X \subseteq \mathbb{R}^d$

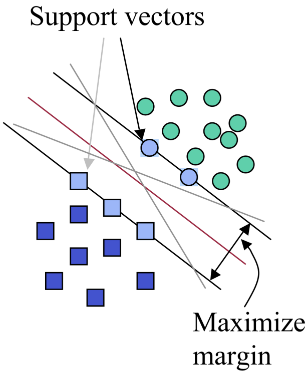
$$S_m = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\} \in \{X \times \{-1, +1\}\}^m$$

- **Problem**: find hypothesis $h : X \to \{-1, +1\}$ in H (classifier) with small generalization error $R(h)$

- First we consider linear classification (hyperplanes) if dimension d is not too large

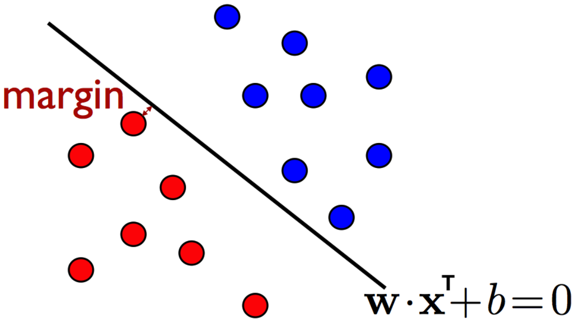
- Support vectors are the data points that lie closest to the decision surface (or hyperplane)
- Support vectors are the elements of the training set that would change the position of the dividing hyperplane if removed
- They are the data points most difficult to classify
- In general, lots of possible solutions for a hyperplane





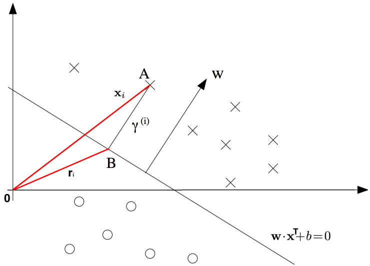
- Support Vector Machine (SVM) finds an optimal solution
- SVMs maximize the margin (the “street”) around the separating hyperplane
- The decision function is fully specified by a (usually very small) subset of training samples, the support vectors

SVM: Linear separable case



- classifiers: $H = \{\mathbf{x} \to \mathrm{sgn}(\mathbf{w} \cdot \mathbf{x}^\top + b), \mathbf{w} \in \mathbb{R}^d, b \in \mathbb{R}\}$

SVM: Linear separable case



- $\gamma^{(i)}$ is a distance from $\mathbf{x}_i$ to the hyperplane $\mathbf{w} \cdot \mathbf{x}^\top + b = 0$
- $\mathbf{w}/\|\mathbf{w}\|$ is a unit perpendicular to the hyperplane
- Vector $\mathbf{r}_i$ of a point B is equal to

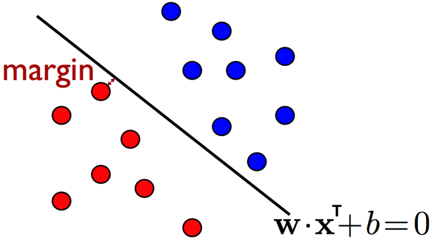
$$\mathbf{r}_i = \mathbf{x}_i - \gamma^{(i)} \mathbf{w}/\|\mathbf{w}\|$$

- Since point B belongs to the hyperplane: $\mathbf{w} \cdot \mathbf{r}_i^\top + b = 0$, i.e.

$$\mathbf{w} \left(\mathbf{x}_i^\top - \gamma^{(i)} \frac{\mathbf{w}^\top}{\|\mathbf{w}\|} \right) + b = 0$$

- Thus we get that $\gamma^{(i)} = \frac{\mathbf{w}}{\|\mathbf{w}\|} \mathbf{x}_i^\top + \frac{b}{\|\mathbf{w}\|}$

Optimal Hyperplane (V.& C., 1965)



- In general case

$$\gamma^{(i)} = \left|\frac{\mathbf{w}}{\|\mathbf{w}\|}\mathbf{x}_i^{\top} + \frac{b}{\|\mathbf{w}\|}\right| = \frac{|\mathbf{w}\cdot\mathbf{x}_i^{\top} + b|}{\|\mathbf{w}\|} \to \min_{i\in[1,m]} \text{ (worst case!)}$$

- The margin is

$$\rho = \max_{\mathbf{w},b:\, y_i(\mathbf{w}\cdot\mathbf{x}_i^{\top}+b)\geq 0}\left[\min_{i\in[1,m]}\gamma^{(i)}\right]$$

- Optimization problem

$$\rho = \max_{\mathbf{w},b:\, y_i(\mathbf{w}\cdot\mathbf{x}_i^\top + b)\geq 0} \left[\min_{i\in[1,m]} \frac{|\mathbf{w}\cdot\mathbf{x}_i^\top + b|}{\|\mathbf{w}\|}\right]$$

- Target $\min_{i\in[1,m]} \frac{|\mathbf{w}\cdot\mathbf{x}_i^\top + b|}{\|\mathbf{w}\|}$ is scale-invariant, i.e.

$$\min_{i\in[1,m]} \frac{|\mathbf{w}\cdot\mathbf{x}_i^\top + b|}{\|\mathbf{w}\|} = \frac{\min_{i\in[1,m]} |\mathbf{w}\cdot\mathbf{x}_i^\top + b|\cdot\mathrm{const}}{\|\mathbf{w}\|\cdot\mathrm{const}} =$$

$$= \frac{\min_{i\in[1,m]} |\widetilde{\mathbf{w}}\cdot\mathbf{x}_i^\top + \widetilde{b}|}{\|\widetilde{\mathbf{w}}\|} \ (\widetilde{\mathbf{w}} = \mathbf{w}\cdot\mathrm{const},\, \widetilde{b} = b\cdot\mathrm{const})$$

- Inequality $y_i(\mathbf{w}\cdot\mathbf{x}_i^\top + b)\geq 0 \Leftrightarrow y_i(\widetilde{\mathbf{w}}\cdot\mathbf{x}_i^\top + \widetilde{b})\geq 0$
- We can always re-normalize $\mathbf{w}$ and b such that
  - it holds: $\min_{i\in[1,m]} |\mathbf{w}\cdot\mathbf{x}_i^\top + b| = 1$
  - inequality $y_i(\mathbf{w}\cdot\mathbf{x}_i^\top + b)\geq 0$ does not change
  - target function $\min_{i\in[1,m]} \frac{|\mathbf{w}\cdot\mathbf{x}_i^\top + b|}{\|\mathbf{w}\|}$ does not change

$$\rho = \max_{\mathbf{w}, b \colon y_i(\mathbf{w} \cdot \mathbf{x}_i^\top + b) \geq 0} \left[\min_{i \in [1,m]} \frac{|\mathbf{w} \cdot \mathbf{x}_i^\top + b|}{\|\mathbf{w}\|} \right]$$

$$= \max_{\substack{\mathbf{w}, b \colon \; y_i(\mathbf{w} \cdot \mathbf{x}_i^\top + b) \geq 0 \\ \min_{i \in [1,m]} |\mathbf{w} \cdot \mathbf{x}_i^\top + b| = 1}} \left[\min_{i \in [1,m]} \frac{|\mathbf{w} \cdot \mathbf{x}_i^\top + b|}{\|\mathbf{w}\|} \right] \text{ (scale-invar.)}$$

$$= \max_{\substack{\mathbf{w}, b \colon \; y_i(\mathbf{w} \cdot \mathbf{x}_i^\top + b) \geq 0 \\ \min_{i \in [1,m]} |\mathbf{w} \cdot \mathbf{x}_i^\top + b| = 1}} \left[\frac{1}{\|\mathbf{w}\|} \right]$$

$$= \max_{\mathbf{w}, b \colon y_i(\mathbf{w} \cdot \mathbf{x}_i^\top + b) \geq 1} \left[\frac{1}{\|\mathbf{w}\|} \right]$$

- Optimization problem

$$\max_{\mathbf{w},b:\, y_i(\mathbf{w}\cdot\mathbf{x}_i^\top + b)\geq 1} \left[\frac{1}{\|\mathbf{w}\|}\right]$$

- **Constrained Optimization**:

$$\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2$$

$$\text{s.t. } y_i(\mathbf{w}\cdot\mathbf{x}_i^\top + b) \geq 1,\ i \in [1,m]$$

- **Properties**:
  - Convex optimization
  - Unique solution for linearly separable case

- **Lagrangian**: for all $\mathbf{w}, b, \alpha_i \geq 0$

$$L(\mathbf{w}, b, \alpha) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{m} \alpha_i [y_i(\mathbf{w} \cdot \mathbf{x}_i^\top + b) - 1]$$

- **KKT conditions**:

$$\nabla_{\mathbf{w}} L = \mathbf{w} - \textstyle\sum_{i=1}^{m} \alpha_i y_i \mathbf{x}_i^\top = 0 \Leftrightarrow \mathbf{w} = \textstyle\sum_{i=1}^{m} \alpha_i y_i \mathbf{x}_i$$

$$\nabla_b L = -\textstyle\sum_{i=1}^{m} \alpha_i y_i = 0 \Leftrightarrow \textstyle\sum_{i=1}^{m} \alpha_i y_i = 0$$

$$\forall i \in [1, m],\ \alpha_i [y_i(\mathbf{w} \cdot \mathbf{x}_i^\top + b) - 1] = 0$$

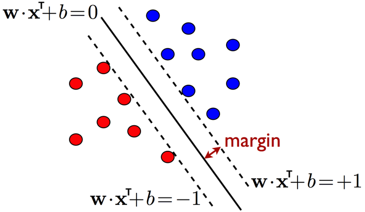
- **Complementary conditions**:

$$\alpha_i[y_i(\mathbf{w} \cdot \mathbf{x}_i^\top + b) - 1] = 0 \Rightarrow \ \alpha_i = 0 \text{ or } y_i(\mathbf{w} \cdot \mathbf{x}_i^\top + b) = 1$$

- **Support vectors**: vectors $\mathbf{x}_i$ such that

$$\alpha_i \neq 0 \ \text{ and } \ y_i(\mathbf{w} \cdot \mathbf{x}_i^\top + b) = 1$$

- Support Vectors: Input vectors that just touch the boundary of the margin (street)



Dual Optimization Problem (I)

- From KKT we get that optimal

$$\mathbf{w} = \sum_{i=1}^{m} \alpha_i y_i \mathbf{x}_i$$

- Plugging $\mathbf{w}$ in $L = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{m} \alpha_i [y_i(\mathbf{w} \cdot \mathbf{x}_i^\top + b) - 1]$ we get

$$L = \underbrace{\frac{1}{2}\left\|\sum_{i=1}^{m} \alpha_i y_i \mathbf{x}_i\right\|^2 - \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j^\top)}_{-\frac{1}{2}\sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j^\top)}$$

$$- \underbrace{\sum_{i=1}^{m} \alpha_i y_i}_{=0} b + \sum_{i=1}^{m} \alpha_i$$

- Thus

$$L = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j^\top)$$

- **Constrained Optimization**:

$$\max_{\alpha} \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j}^{m} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j^\top)$$

$$\text{s.t. } \alpha_i \geq 0 \text{ and } \sum_{i=1}^{m} \alpha_i y_i = 0, \; i \in [1, m]$$

- Optimal

$$\mathbf{w} = \sum_{i=1}^{m} \alpha_i y_i \mathbf{x}_i$$

- **Solution**: classifier based on the separating hyperplane $\mathbf{w} \cdot \mathbf{x}^\top + b = 0$ has the form $h(\mathbf{x}) = \operatorname{sign}(\mathbf{w} \cdot \mathbf{x}^\top + b)$, i.e.

$$h(\mathbf{x}) = \operatorname{sign}\left(\sum_{i=1}^{m} \alpha_i y_i (\mathbf{x}_i \cdot \mathbf{x}^\top) + b \right),$$

with $b = y_i - \sum_{j=1}^{m} \alpha_j y_j (\mathbf{x}_j \cdot \mathbf{x}_i^\top)$ for any SV $\mathbf{x}_i$

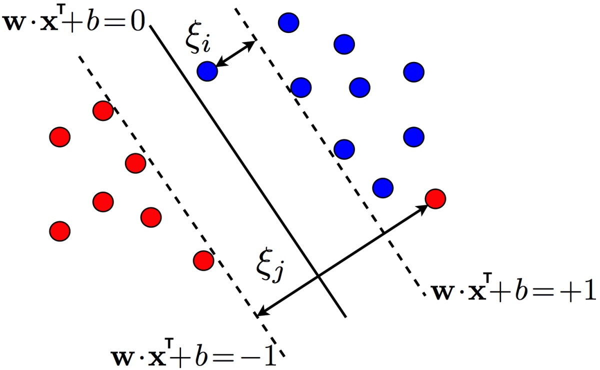
- **Problem**: data often not linearly separable in practice. For any hyperplane there exists $\mathbf{x}_i$, such that

$$y_i[\mathbf{w} \cdot \mathbf{x}_i^\top + b] \not\geq 1$$

- **Approach**: relax constraints using slack variables $\xi_i \geq 0$

$$y_i[\mathbf{w} \cdot \mathbf{x}_i^\top + b] \geq 1 - \xi_i$$

Soft-margin hyperplane



- **Support vectors**: points along the margin or outliers
- **Soft margin**: $\rho = \frac{1}{\|\mathbf{w}\|}$

- **Constrained Optimization**:

$$\min_{\mathbf{w},b,\xi} \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{m}\xi_i$$

$$\text{s.t. } y_i(\mathbf{w}\cdot\mathbf{x}_i^\top + b) \geq 1 - \xi_i \text{ and } \xi_i \geq 0,\ i \in [1, m]$$

- **Properties**:
  - Convex optimization
  - Unique solution
  - $C \geq 0$ is a trade-off parameter

Comments

- How to determine C?
- The problem of determining a hyperplane minimizing the train error is NP-complete (as a function of dimension)
- Other convex functions of the slack variables can be used

- **Lagrangian**: for all $\mathbf{w}, b, \alpha_i \geq 0, \beta_i \geq 0$

$$L(\mathbf{w}, b, \xi, \alpha, \beta) = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{m}\xi_i$$
$$- \sum_{i=1}^{m}\alpha_i[y_i(\mathbf{w}\cdot\mathbf{x}_i^\top + b) - 1 + \xi_i] - \sum_{i=1}^{m}\beta_i\xi_i$$

- **KKT conditions**:

$$\nabla_{\mathbf{w}} L = \mathbf{w} - \sum_{i=1}^{m}\alpha_i y_i \mathbf{x}_i = 0 \Leftrightarrow \mathbf{w} = \sum_{i=1}^{m}\alpha_i y_i \mathbf{x}_i$$

$$\nabla_b L = -\sum_{i=1}^{m}\alpha_i y_i = 0 \Leftrightarrow \sum_{i=1}^{m}\alpha_i y_i = 0$$

$$\nabla_{\xi_i} L = C - \alpha_i - \beta_i = 0 \Leftrightarrow \alpha_i + \beta_i = C$$

$$\forall i \in [1, m],\ \alpha_i[y_i(\mathbf{w}\cdot\mathbf{x}_i^\top + b) - 1 + \xi_i] = 0 \text{ and } \beta_i\xi_i = 0$$

- **Complementary conditions**:

  $\alpha_i[y_i(\mathbf{w} \cdot \mathbf{x}_i^\top + b) - 1 + \xi_i] = 0 \Rightarrow \ \alpha_i = 0$ or $y_i(\mathbf{w} \cdot \mathbf{x}_i^\top + b) = 1 - \xi_i$

- **Support vectors**: vectors $\mathbf{x}_i$ such that

$$\alpha_i \neq 0 \ \text{ and } \ y_i(\mathbf{w} \cdot \mathbf{x}_i^\top + b) = 1 - \xi_i$$

Dual Optimization Problem (I)

- Plugging optimal $\mathbf{w} = \sum_{i=1}^{m} \alpha_i y_i \mathbf{x}_i$ in L we get

$$L = \underbrace{\frac{1}{2}\left\|\sum_{i=1}^{m} \alpha_i y_i \mathbf{x}_i\right\|^2 - \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j^\top)}_{-\frac{1}{2}\sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j^\top)}$$

$$\underbrace{-\sum_{i=1}^{m} \alpha_i y_i}_{=0} b + \sum_{i=1}^{m} \alpha_i$$

- Thus

$$L = \sum_{i=1}^{m} \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j^\top)$$

- Since $\beta_i = C - \alpha_i$, the condition $\beta_i \geq 0$ is equivalent to $\alpha_i \leq C$

- **Constrained Optimization**:

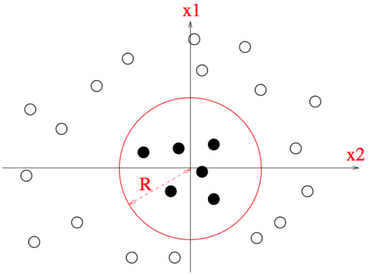
$$\max_{\alpha} \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j}^{m} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j^\top)$$

$$\text{s.t. } 0 \leq \alpha_i \leq C \text{ and } \sum_{i=1}^{m} \alpha_i y_i = 0,\ i \in [1, m]$$

- **Solution**: separating hyperplane $\mathbf{w} \cdot \mathbf{x}^\top + b = 0$

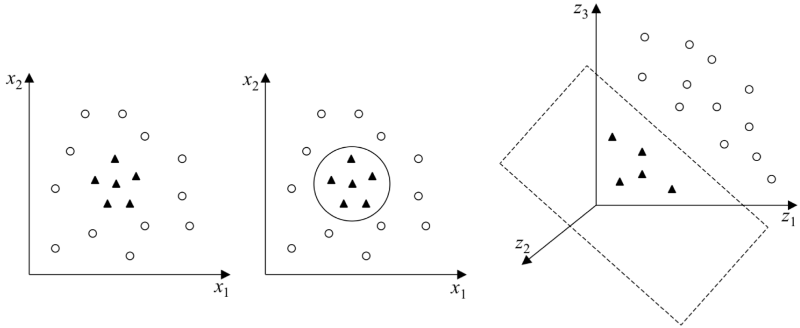
$$h(\mathbf{x}) = \operatorname{sgn}\left(\sum_{i=1}^{m} \alpha_i y_i (\mathbf{x}_i \cdot \mathbf{x}^\top) + b \right),$$

with $b = y_i - \sum_{j=1}^{m} \alpha_j y_j (\mathbf{x}_j \cdot \mathbf{x}_i^\top)$ for any SV $\mathbf{x}_i$ with $0 < \alpha_i < C$



- Linear separation impossible in most problems
- Non-linear mapping $\Phi : X \to \mathbb{H}$ from input space to high-dimensional feature space
- Generalization ability: independent of $\dim(\mathbb{H})$, depends only on d and m

Example: polynomial kernel



For $\mathbf{x} = (x_1, x_2) \in \mathbb{R}^2$, let $\Phi(\mathbf{x}) = (x_1^2, \sqrt{2}x_1x_2, x_2^2) \in \mathbb{R}^3$. Then

$$
\begin{aligned}
K(\mathbf{x}', \mathbf{x}) &= \Phi(\mathbf{x}') \cdot \Phi(\mathbf{x})^\top \quad \text{[dot product of features]} \\
&= x_1^2(x_1')^2 + 2x_1x_2x_1'x_2' + x_2^2(x_2')^2 \\
&= (x_1x_1' + x_2x_2')^2 = (\mathbf{x}' \cdot \mathbf{x}^\top)^2
\end{aligned}
$$

- **Idea**:
  - Define $K : X \times X \to \mathbb{R}$ called kernel, such that
$$\Phi(\mathbf{x}) \cdot \Phi(\mathbf{x}')^\top = K(\mathbf{x}, \mathbf{x}')$$
  - K is often interpreted as a similarity measure

- **Benefits**:
  - Efficiency: K is often more efficient to compute than Φ and the dot product
  - Flexibility: K can be chosen arbitrarily so long as the existence of Φ is guaranteed (PDS condition or Mercer's condition)

- **Gaussian kernel**:

$$K(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2\sigma^2}\right),\ \sigma \neq 0$$

- **Constrained Dual Optimization** problem:

$$\max_{\alpha} \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j}^{m} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j^\top)$$

$$\text{s.t. } 0 \leq \alpha_i \leq C \text{ and } \sum_{i=1}^{m} \alpha_i y_i = 0,\ i \in [1, m]$$

- **Decision function** $h(\mathbf{x}) = \mathrm{sgn}(\mathbf{w} \cdot \mathbf{x}^\top + b)$ has the form

$$h(\mathbf{x}) = \mathrm{sgn}\left(\sum_{i=1}^{m} \alpha_i y_i (\mathbf{x}_i \cdot \mathbf{x}^\top) + b \right),$$

with

$$\mathbf{w} = \sum_{i=1}^{m} \alpha_i y_i \mathbf{x}_i,\ b = y_i - \sum_{j=1}^{m} \alpha_j y_j (\mathbf{x}_i \cdot \mathbf{x}_j^\top)$$

for any SV $\mathbf{x}_i$ with $0 < \alpha_i < C$

- **Constrained Dual Optimization** problem:

$$\max_{\alpha} \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j}^{m} \alpha_i \alpha_j y_i y_j \underbrace{\Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x}_j)^\top}_{K(\mathbf{x}_i, \mathbf{x}_j)}$$

$$\text{s.t. } 0 \leq \alpha_i \leq C \text{ and } \sum_{i=1}^{m} \alpha_i y_i = 0,\ i \in [1, m]$$

- **Decision function** $h(\mathbf{x}) = \mathrm{sgn}(\mathbf{w} \cdot \Phi(\mathbf{x})^\top + b)$ has the form

$$h(\mathbf{x}) = \mathrm{sgn}\left(\sum_{i=1}^{m} \alpha_i y_i \underbrace{\Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x})^\top}_{K(\mathbf{x}_i, \mathbf{x})} + b \right),$$

with

$$\mathbf{w} = \sum_{i=1}^{m} \alpha_i y_i \Phi(\mathbf{x}_i),\ b = y_i - \sum_{j=1}^{m} \alpha_j y_j \underbrace{\Phi(\mathbf{x}_j) \cdot \Phi(\mathbf{x}_i)^\top}_{K(\mathbf{x}_j, \mathbf{x}_i)}$$

for any SV $\mathbf{x}_i$ with $0 < \alpha_i < C$

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- Hypothesis set

$$\{x \to \mathbf{w} \cdot \Phi(\mathbf{x})^\top + b : \mathbf{w} \in \mathbb{R}^p,\, b \in \mathbb{R}\}$$

- Loss function: ϵ-insensitive loss

$$L(y, y') = |y - y'|_\epsilon = \max\left(0, |y' - y| - \epsilon\right)$$

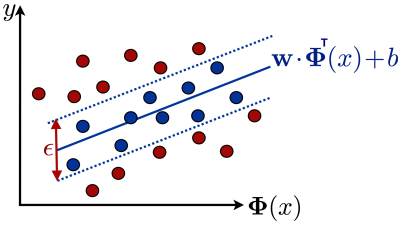


Figure – Fit “tube” with width ϵ to data

- **Optimization problem**: similar to that of SVM

$$\frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{m} |y_i - (\mathbf{w}\cdot\varPhi(\mathbf{x}_i)^\top + b)|_\epsilon \to \min_{\mathbf{w},b}$$

- Equivalent formulation

$$\begin{aligned} & \min_{\mathbf{w},b,\xi,\xi'} \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{m}(\xi_i + \xi_i') \\ \text{subject to} \quad & (\mathbf{w}\cdot\varPhi(\mathbf{x}_i)^\top + b) - y_i \leq \epsilon + \xi_i \\ & y_i - (\mathbf{w}\cdot\varPhi(\mathbf{x}_i)^\top + b) \leq \epsilon + \xi_i' \\ & \xi_i \geq 0,\ \xi_i' \geq 0 \end{aligned}$$

- **Optimization problem**:

$$\max_{\boldsymbol{\alpha},\boldsymbol{\alpha}'} -\epsilon(\boldsymbol{\alpha}'+\boldsymbol{\alpha})^\top \mathbf{1} + (\boldsymbol{\alpha}'-\boldsymbol{\alpha})^\top \mathbf{Y}$$
$$-\frac{1}{2}(\boldsymbol{\alpha}'-\boldsymbol{\alpha})^\top \mathrm{K}(\boldsymbol{\alpha}'-\boldsymbol{\alpha})$$
$$\text{s.t. } (\mathbf{0}\le\boldsymbol{\alpha}\le\mathbf{C}) \text{ or } (\mathbf{0}\le\boldsymbol{\alpha}'\le\mathbf{C}) \text{ or } ((\boldsymbol{\alpha}'-\boldsymbol{\alpha})^\top\mathbf{1}=0)$$

Here $\mathrm{K} = \{\Phi(\mathbf{x}_i)\cdot\Phi(\mathbf{x}_j)^\top\}_{i,j=1}^m = \{K(\mathbf{x}_i,\mathbf{x}_j)\}_{i,j=1}^m \in \mathbb{R}^{m\times m}$

- **Solution**

$$h(\mathbf{x}) = \sum_{i=1}^m (\alpha_i'-\alpha_i)\underbrace{K(\mathbf{x}_i,\mathbf{x})}_{\Phi(\mathbf{x}_i)\cdot\Phi(\mathbf{x})^\top} + b$$

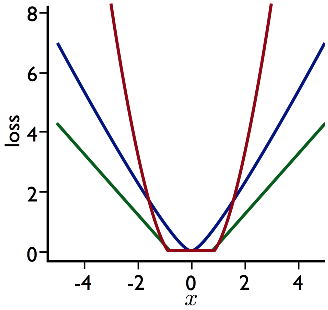
with

$$b = \begin{cases} -\sum_{i=1}^m(\alpha_j'-\alpha_j)K(\mathbf{x}_j,\mathbf{x}_i)+y_i+\epsilon, & \text{when } 0<\alpha_i<C \\ -\sum_{i=1}^m(\alpha_j'-\alpha_j)K(\mathbf{x}_j,\mathbf{x}_i)+y_i-\epsilon, & \text{when } 0<\alpha_i'<C \end{cases}$$

- Support vectors: points strictly outside the tube

- Advantages
  - strong theoretical guarantees (for that loss)
  - sparser solution
  - use of kernels
- Disadvantages
  - selection of two parameters: C and ϵ. Heuristics for that:
    * search C near maximum y, ϵ near average difference of y-s, measure of no. of SVs
  - large matrices: low-rank approximations of kernel matrix

Alternative Loss Functions (similar formulations and results)



- quadratic ϵ-insensitive

$$x \to \max(0, |x| - \epsilon)^2$$

- Huber

$$x \to \begin{cases} x^2, & \text{if } |x| \le c \\ 2c|x| - c^2, & \text{otherwise} \end{cases}$$

- ϵ-insensitive

$$x \to \max(0, |x| - \epsilon)$$

- SVR in case of quadratic ϵ-insensitive for $\epsilon = 0$ coincides with Kernel Ridge Regression (see lecture 2)

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

where

$$\boldsymbol{\alpha} = (\Phi(\mathbf{X}) \cdot \Phi(\mathbf{X})^{\top} + \lambda \mathbf{I})^{-1} \mathbf{Y} = (\mathrm{K} + \lambda \mathbf{I})^{-1} \mathbf{Y},$$

where

$$\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_m\} \in \mathbb{R}^{m \times d},\ \mathbf{Y} = (y_1, \ldots, y_m) \in \mathbb{R}^{m \times 1}$$

- In case of $\epsilon > 0$ SVR allows to reduce a number of terms in (*) above thanks to the support vector concept: explicit solution vs. sparsity!