SVM and Kernels

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Outline

1. Convex optimization and Duality: Basics
2. Support Vector Machine
3. SVMs with kernels
4. Support Vector Regression

1 Convex optimization and Duality: Basics

2 Support Vector Machine

3 SVMs with kernels

4 Support Vector Regression

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

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

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 $f_i(\mathbf{x}) \le 0$
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- **Lagrange dual function** $g : \mathbb{R}^m \times \mathbb{R}^p \to \mathbb{R}$

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

  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

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

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

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- (usually) holds for convex problems
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- 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

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if it is strictly feasible, i.e.,

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

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

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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):

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

- Primal constraints: $f_i(\mathbf{x}) \leq 0$, $i = 1, 2, \ldots, m$, $h_i(\mathbf{x}) = 0$, $i = 1, 2, \ldots, p$
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- If strong duality holds and $\mathbf{x}, \lambda, \nu$ are optimal, then they must satisfy the KKT conditions

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

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3 SVMs with kernels

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

- **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

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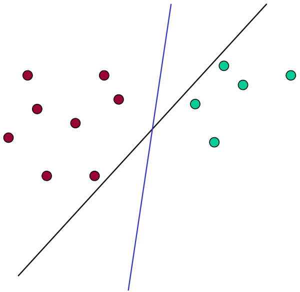
Support Vectors

- 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



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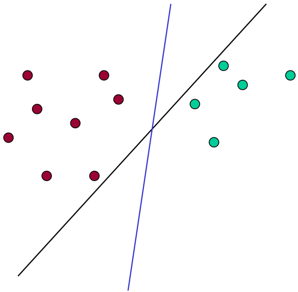

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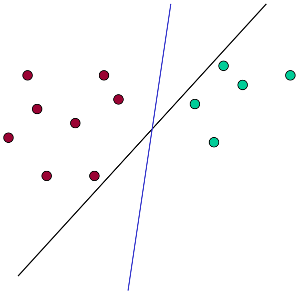

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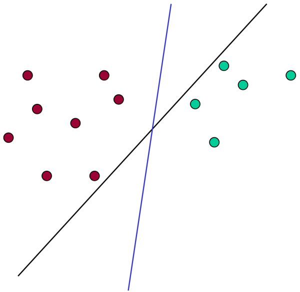
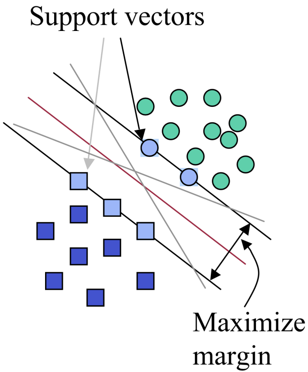
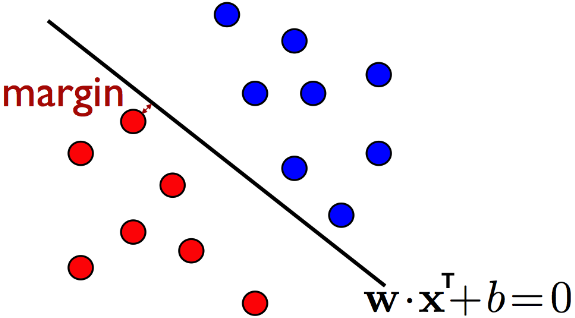
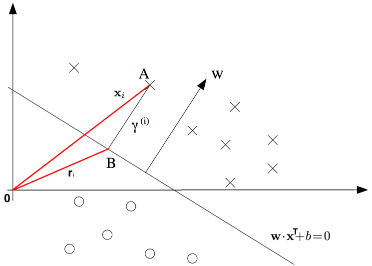




- Support Vector Machine (SVM) finds an optimal solution
- SVMs maximize the margin (the "street") around the separating hyperplane
- The decision function is fully specified by a (usually very small) subset of training samples, the support vectors



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



- $\gamma^{(i)}$ 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.
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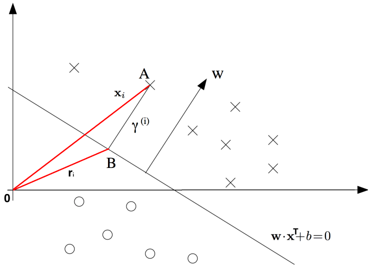
SVM: Linear separable case



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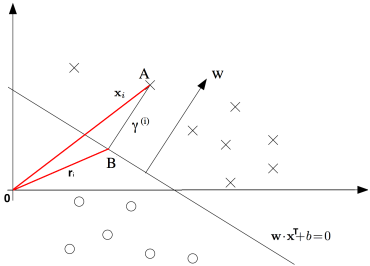

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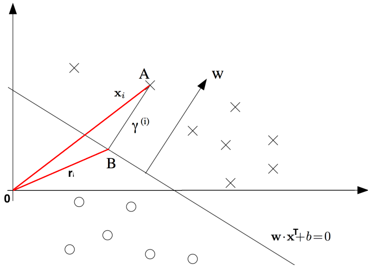

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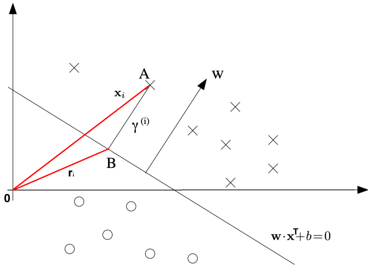

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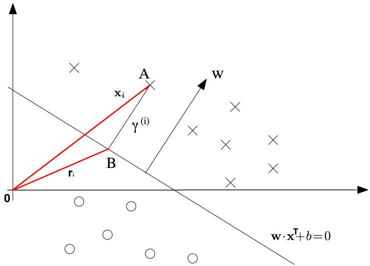

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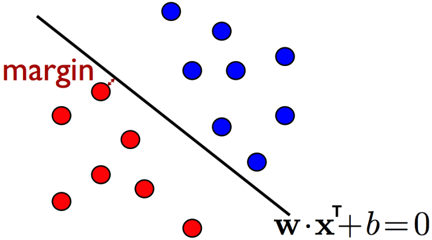
Optimal Hyperplane (V.& C., 1965)

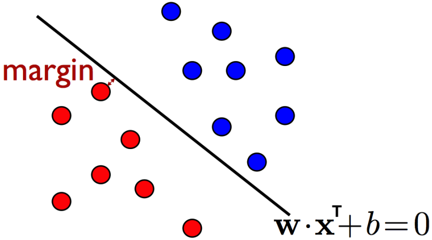


- In general case

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

- The margin is

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



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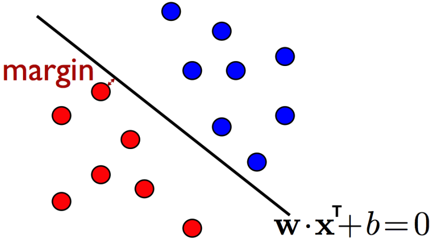

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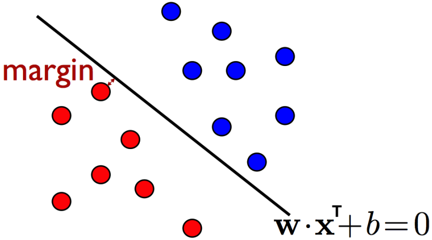

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Optimal Hyperplane (Vapnik & Chervonenkis, 1965)

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

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

- Inequality $y_i(\mathbf{w}\cdot\mathbf{x}_i^\top + b) \geq 0 \Leftrightarrow y_i(\widetilde{\mathbf{w}}\cdot\mathbf{x}_i^\top + \widetilde{b}) \geq 0$
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$$\max_{\mathbf{w},b:\, y_i(\mathbf{w}\cdot\mathbf{x}_i^\top+b)\geq 1}\left[\frac{1}{\|\mathbf{w}\|}\right]$$

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

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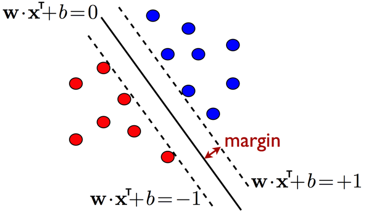

Dual Optimization Problem (I)

- From KKT we get that optimal

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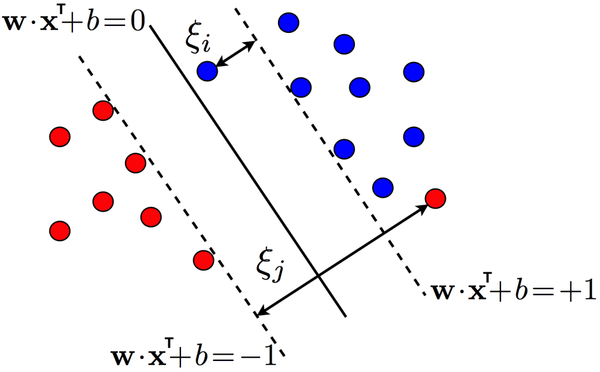
with $b = y_i - \sum_{j=1}^{m} \alpha_j y_j (\mathbf{x}_j \cdot \mathbf{x}_i^\top)$ for any SV $\mathbf{x}_i$

- **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 $\xi_i \geq 0$

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



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

- **Constrained Optimization**:

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

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

- 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 $\mathbf{w}, b, \alpha_i \geq 0, \beta_i \geq 0$

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

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

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- **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 $0 < \alpha_i < C$

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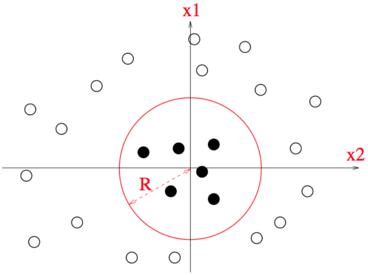
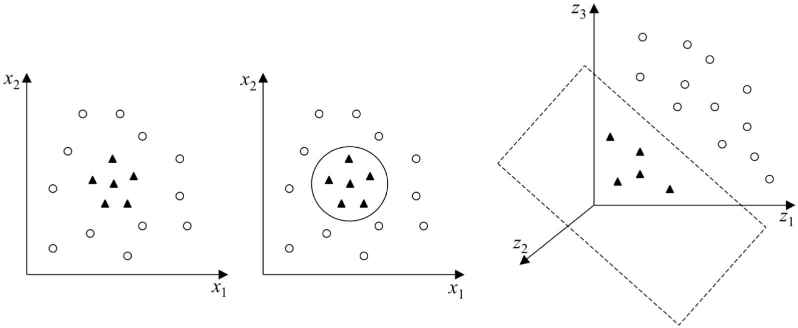
Recall: Non-linear separation



- 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



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

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

- **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)

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- **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:

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

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

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

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

Recall: Linear SVM

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

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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

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

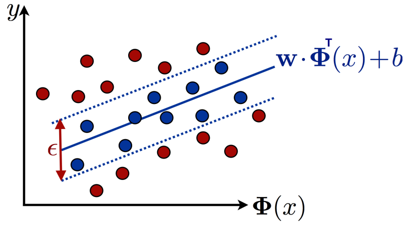

Figure – Fit "tube" with width ϵ to data

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

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

- Equivalent formulation

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

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

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- **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

- **Optimization problem**:

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

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- 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

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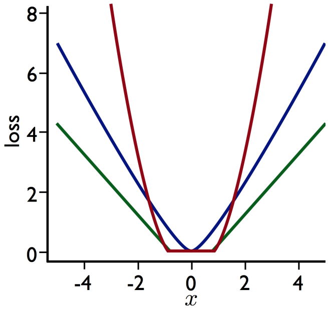
Alternative Loss Functions (similar formulations and results)



- 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!