Support Vector Machines (SVM) and Sequential Minimal Optimization (SMO)

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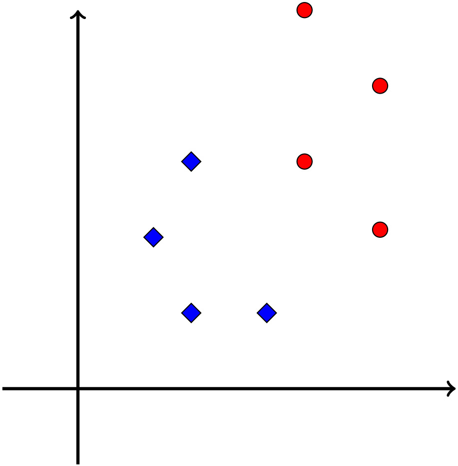
Support Vector Machines (SVM)



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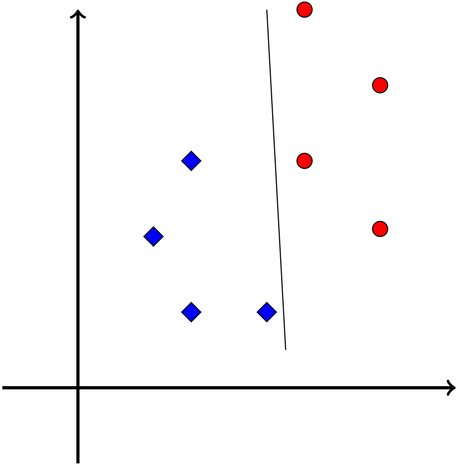

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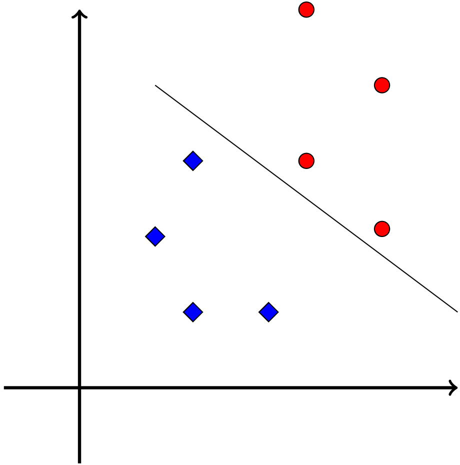

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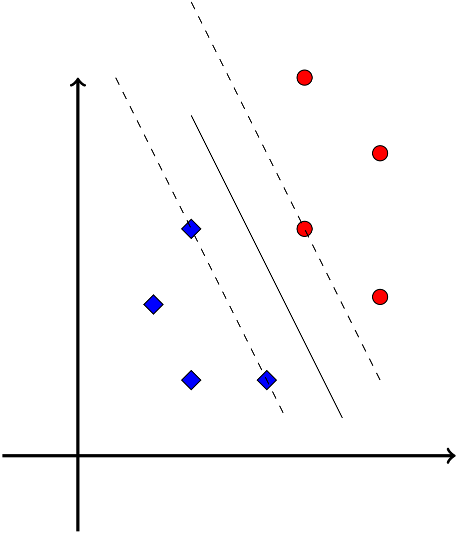
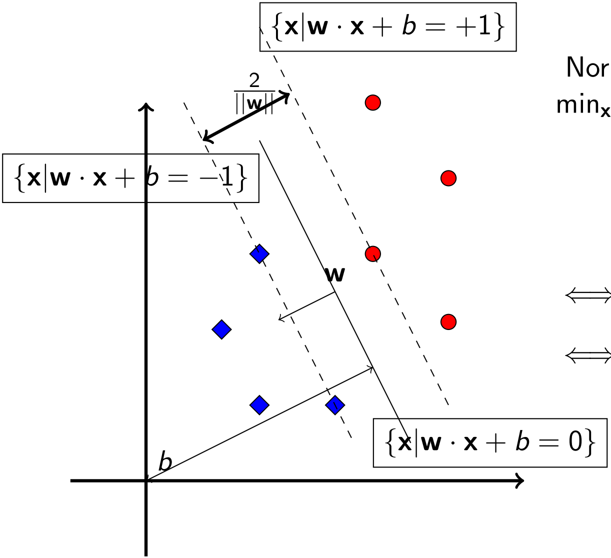
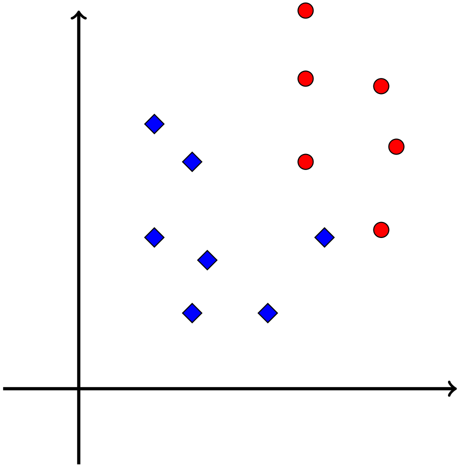




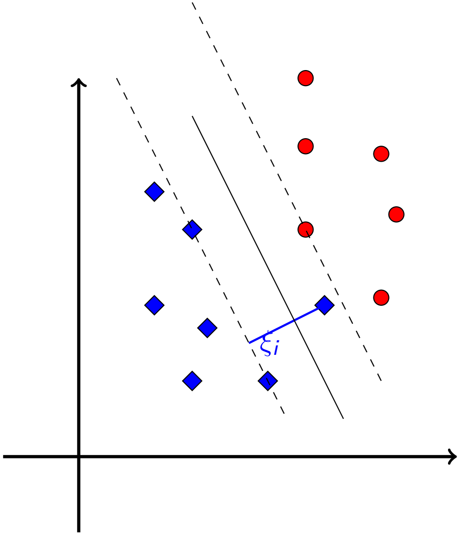
Normalize $\mathbf{w}$ so that
$\min_{\mathbf{x}_i} \mathbf{w} \cdot \mathbf{x}_i + b = 1.$

$$
\begin{aligned}
& \mathbf{w} \cdot \mathbf{x}_1 + b = +1 \\
& \mathbf{w} \cdot \mathbf{x}_2 + b = -1 \\
\iff & \mathbf{w} \cdot (\mathbf{x}_1 - \mathbf{x}_2) = 2 \\
\iff & \frac{\mathbf{w}}{||\mathbf{w}||} \cdot (\mathbf{x}_1 - \mathbf{x}_2) = \frac{2}{||\mathbf{w}||}
\end{aligned}
$$

Slack variables



Slack variables



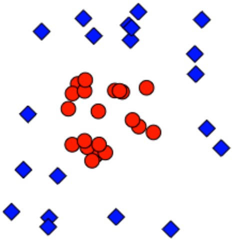
Introduce slack variables ξ_i:

$$\min_{\mathbf{w},b,\xi_i} \quad ||\mathbf{w}||^2 + C\sum_{i=1}^{N} \xi_i$$

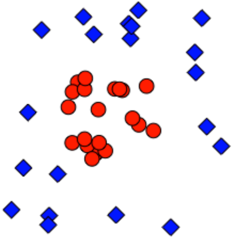
$$\text{subject to} \quad y_i(\mathbf{w} \cdot \mathbf{x_i} + b) \geq 1 - \xi_i$$

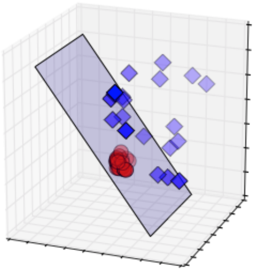
$$\xi_i \geq 0$$

Non-linear hyperplanes



Non-linear hyperplanes





Map into a higher dimensional feature space:

$$\begin{aligned} \Phi : \quad \mathbb{R}^2 &\rightarrow \mathbb{R}^3 \\ (x_1, x_2) &\mapsto (x_1^2, \sqrt{2}x_1x_2, x_2^2) \end{aligned}$$

Dual SVM

Primal

$$\min_{\mathbf{w},b,\xi_i} \quad ||\mathbf{w}||^2 + C\sum_{i=1}^{N}\xi_i$$

$$\text{subject to} \quad y_i(\mathbf{w}\cdot\Phi(\mathbf{x_i})+b) \geq 1-\xi_i \;\text{ and }\; \xi_i \geq 0 \quad \text{for } i = 1\ldots N$$

Dual

$$\max_{\alpha} \quad \sum_{i=1}^{N}\alpha_i - \frac{1}{2}\sum_{i,j=1}^{N}\alpha_i\alpha_j y_i y_j\left(\Phi(\mathbf{x_i})\cdot\Phi(\mathbf{x_j})\right)$$

$$\text{subject to} \quad \sum_{i=1}^{N}\alpha_i y_i = 0 \;\text{ and }\; C \geq \alpha_i \geq 0 \quad \text{for } i = 1\ldots N$$

Data points x_i only appear in scalar products $(\Phi(\mathbf{x_i})\cdot\Phi(\mathbf{x_j}))$.

The Kernel Trick

Replace scalar products with kernel function (**?**):

$$k(x, y) = \Phi(x) \cdot \Phi(y)$$

- Compute kernel matrix $K_{ij} = k(x_i, x_j)$, i.e. never use Φ directly
- Underlying mapping Φ can be unknown
- Kernels can be adopted to specific task, e.g. using prior knowledge (kernels for graphs, trees, strings, ...)

Common kernels

Gaussian Kernel: $k(x, y) = \exp\left(-\frac{||x-y||^2}{2\sigma^2}\right)$

Linear Kernel: $k(x, y) = x \cdot y$

Polynomial Kernel: $k(x, y) = (x \cdot y + c)^d$

The Support Vectors in SVM

$$\max_{\alpha} \quad \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} \alpha_i \alpha_j y_i y_j \left(\Phi(\mathbf{x_i}) \cdot \Phi(\mathbf{x_j}) \right)$$

$$\text{subject to} \quad \sum_{i=1}^{N} \alpha_i y_i = 0 \;\text{ and }\; C \geq \alpha_i \geq 0 \quad \text{for } i = 1 \dots N$$

KKT conditions

$$y_i \left[\mathbf{w}\Phi(\mathbf{x_i})) + b\right] > 1 \Longrightarrow \qquad a_i = 0 \longrightarrow \qquad x_i \text{ irrelevant}$$

$$y_i \left[\mathbf{w}\Phi(\mathbf{x_i})) + b\right] = 1 \Longrightarrow \qquad \text{on/in margin} \longrightarrow \qquad x_i \text{ Support Vector}$$

Old model $f(x) = w \cdot \Phi(x_i) + b$ becomes via $w = \sum_{i=1}^{N} \alpha_i y_i \Phi(x_i)$:

$$f(x) = \sum_{i=1}^{N} \alpha_i y_i k(x_i, x) + b \quad \longrightarrow \quad f(x) = \sum_{x_i \in SV} \alpha_i y_i k(x_i, x) + b$$

Quadratic Programming (QP)

Reminder: The SVM optimization problem

$$\max_{\alpha} \quad \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} \alpha_i \alpha_j y_i y_j k(x_i, x_j)$$

$$\text{subject to} \quad \sum_{i=1}^{N} \alpha_i y_i = 0 \ \text{ and } \ C \geq \alpha_i \geq 0 \quad \text{for } i = 1 \ldots N$$

Quadratic Programming

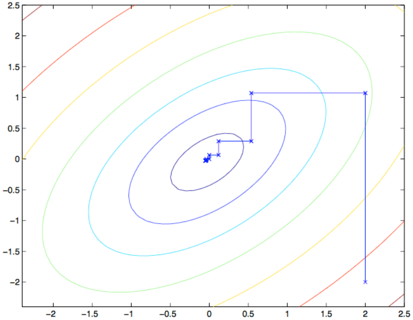
$$\begin{aligned} \min_{x} \quad & \frac{1}{2} x^{\intercal} P x + q^{\intercal} x \\ \text{s.t.} \quad & Gx \preceq h \\ & Ax = b \end{aligned}$$

$\Longrightarrow$ We can solve the SVM problem with a QP solver.

Coordinate Descent

Imagine a multivariate function $W(x_1, x_2, \ldots, x_N)$ and the problem

$$\operatorname{argmax}_{\mathbf{x}} W(x_1, x_2, \ldots, x_N)$$



Coordinate Descent Algorithm

while not converged **do**

  for $i = 1 \ldots N$ **do**

    $x_i \leftarrow \operatorname{argmax}_{x_i} W(x_1, \ldots, x_i, \ldots, x_N)$

  end for

end while

Sequential Minimal Optimization (SMO) Idea

We have to solve the SVM optimization problem subject to the condition

$$\sum_{i=1}^{N} \alpha_i y_i = 0.$$

I.e. we can *not* optimize one single variable individually.

Solution: Optimize two variables α_i and α_j with $y_i \neq y_j$ while keeping the other α fixed.

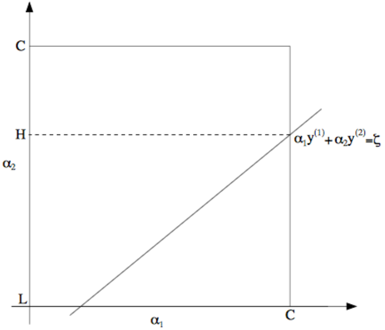
From KKT conditions, we get (optimizing α_1 and α_2 WLOG)

$$\alpha_1 y_1 + \alpha_2 y_2 = -\sum_{i=3}^{N} \alpha_i y_i$$

where the right handside is fixed $\zeta = -\sum_{i=3}^{N} \alpha_i y_i$.

Box constraints

- From the second contraint $0 \leq \alpha_i \leq C$, we know that α_1 and α_2 have to lie inside the pictured box:
- We can see, that there exists a upper and lower bound for α_2: $L \leq \alpha_2 \leq H$.



- If we write $\alpha_1 = (\zeta - \alpha_2 y_2) y_1$, we have to solve a quadratic function in one variable (α_2).
- The new α_2 then has to be clipped to the box constraints L and H (!)
- Find α_1 via $\alpha_1 = (\zeta - \alpha_2 y_2) y_1$. Then pick two new α and repeat.