University of Amsterdam
Informatics Institute

AMLAB
Amsterdam
Machine Learning Lab

Machine Learning 1

Lecture 11.6 - Kernel Methods
Support Vector Machines - Soft Margin Classifier

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(Bishop 7.1.1)

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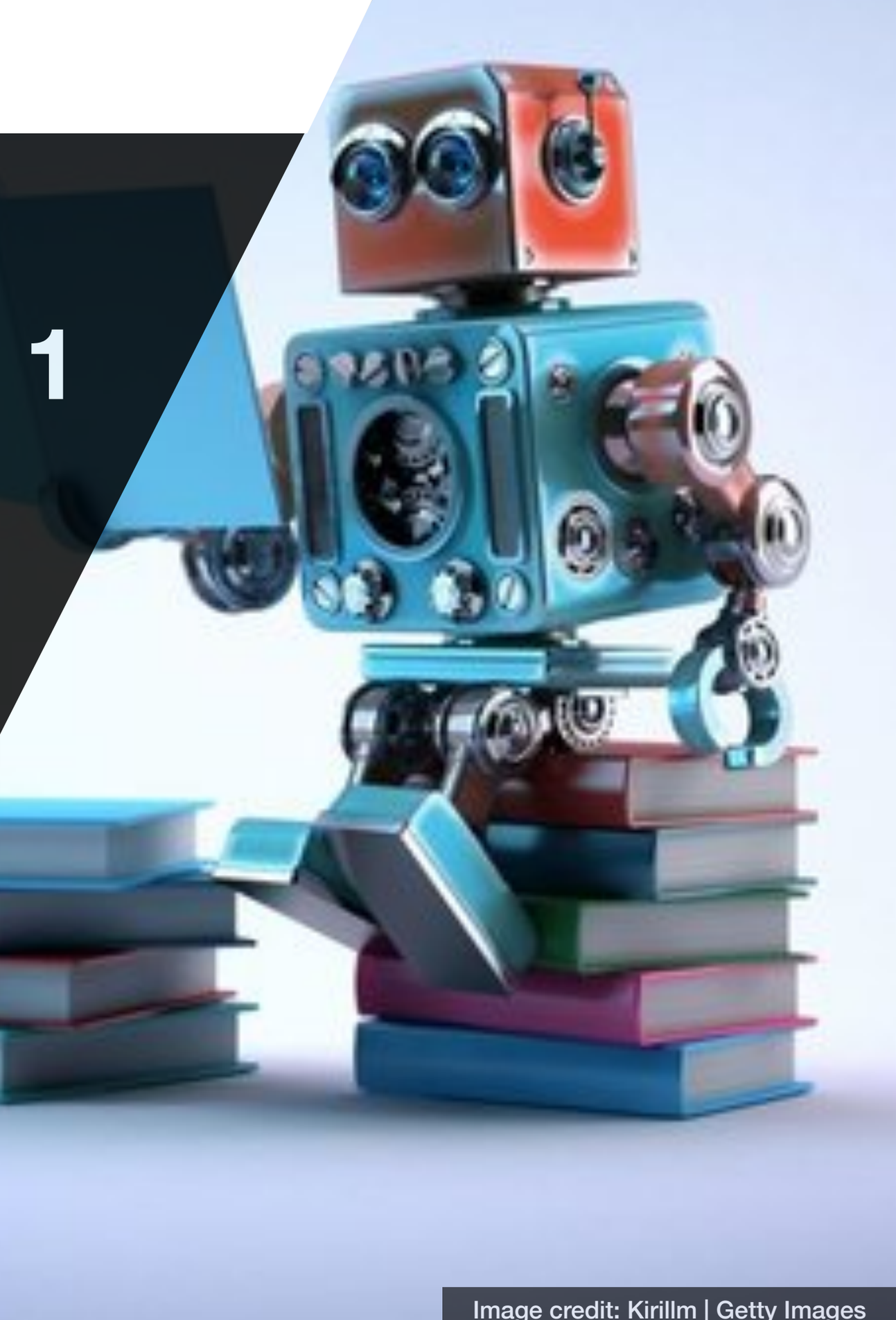

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Maximum Margin Classifiers

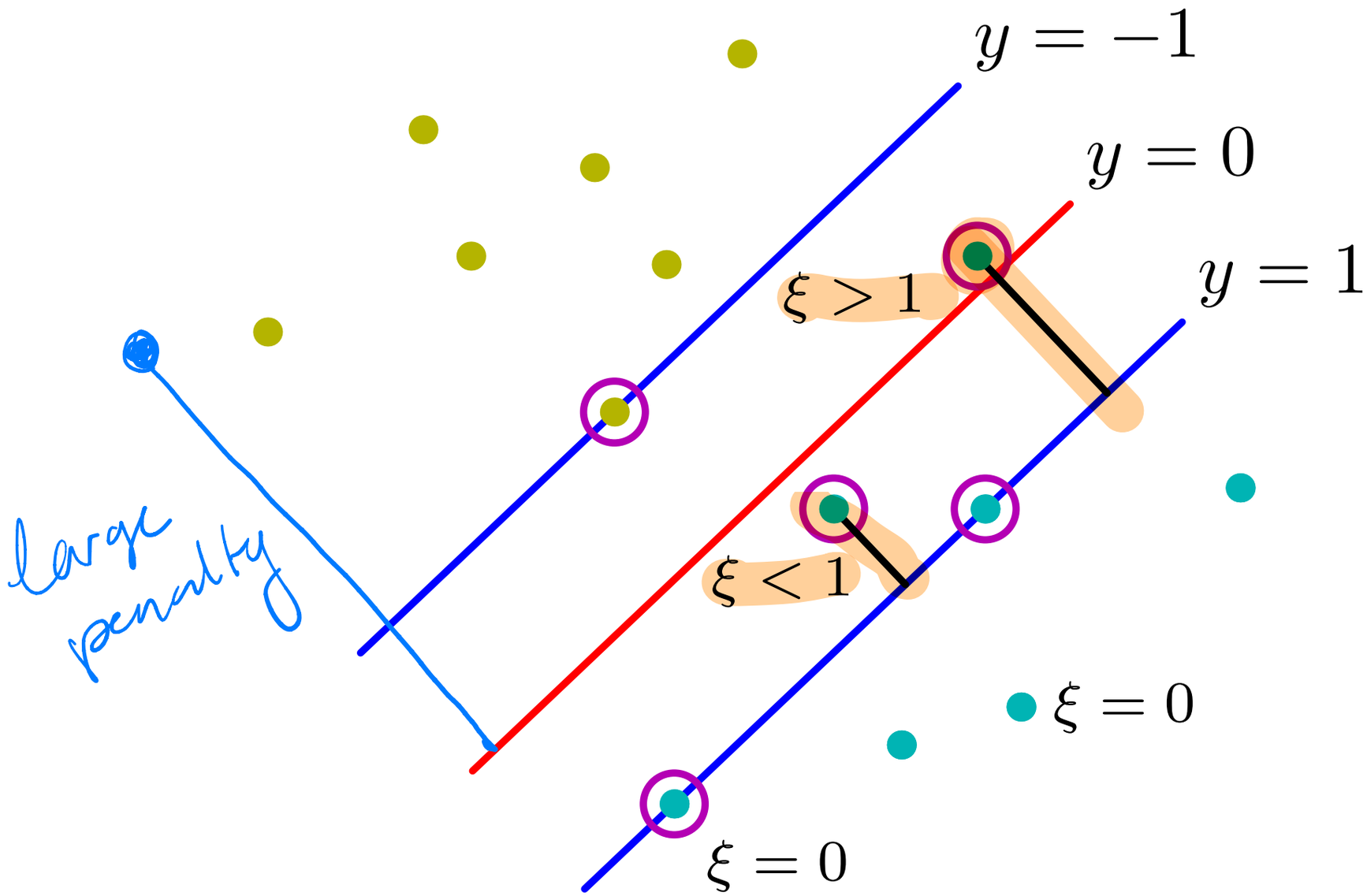
- So far we have assumed the data points are perfectly separable with a linear decision boundary, or with a nonlinear decision boundary by using a nonlinear kernel.

- Sometimes the class conditional distributions have overlap!

- We need to modify the Maximum Margin classifier to allow for some training points to be misclassified.

  - Datapoints are allowed to be on the “wrong” side of the margin boundary, but they have to pay a penalty proportional to the distance to the margin boundary.

Soft Margin Classifiers



- Allows datapoints to lie on the wrong side of the margin boundary.
- Those datapoints pay a penalty proportional to the distance to the margin boundary.

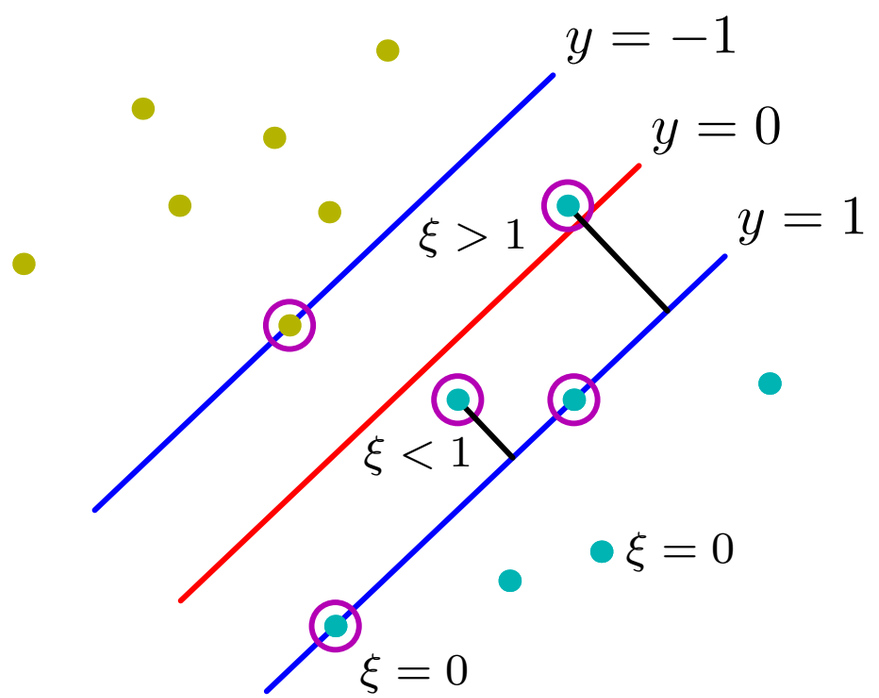
Maximum Margin Classifiers: Soft Margins!

- Introduce slack variables: $\xi_n \geq 0$ for $n = 1, \ldots, N$
- If on the correct side of the margin: $\xi_n = 0$
- If on the wrong side of the margin: $\xi_n = |t_n - y(\mathbf{x}_n)|$
- Previously: hard constraints/hard margin

$$t_n y(\mathbf{x}_n) \geq 1, \quad n = 1, \ldots, N$$

- Now: Soft constraint/soft margin

$$t_n y(\mathbf{x}_n) \geq 1 - \xi_n, \; n = 1, \ldots, N$$



Maximum Margin Classifiers: Soft Margins!

- Goal: maximize margin, give a penalty to points that lie on the wrong side of the boundary!

- We minimize $\underset{\mathbf{w},b,\xi_n}{\arg\min} \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{n=1}^{N}\xi_n$

subject to constraints

$$t_n y(\mathbf{x}_n) \geq 1 - \xi_n, \quad \text{for} \quad n = 1,\ldots,N$$

$$\xi_n \geq 0, \quad \text{for} \quad n = 1,\ldots,N$$

- Corresponding Lagrangian:

$$L(\mathbf{w}, b, \boldsymbol{\xi}, \mathbf{a}, \boldsymbol{\mu}) = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{n=1}^{N}\xi_n - \sum_{n=1}^{N} a_n\{t_n(\mathbf{w}^T\mathbf{x}_n + b) - 1 + \xi_n\} - \sum_{n=1}^{N}\mu_n\xi_n$$

- Lagrange multipliers

$$a_n \geq 0, \quad \mu_n \geq 0$$

1. Lagrangian
2. KKT
3. Solve primal variables
4. Obtain dual Lagrangian
5. Solve for duals

Maximum Margin Classifiers: Soft Margins!

- Lagrangian function

$$L(\mathbf{w}, b, \boldsymbol{\xi}, \mathbf{a}, \boldsymbol{\mu}) = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{n=1}^{N}\xi_n - \sum_{n=1}^{N} a_n\{t_n(\mathbf{w}^T\mathbf{x}_n + b) - 1 + \xi_n\} - \sum_{n=1}^{N}\mu_n\xi_n$$

- Lagrange multipliers. $a_n \geq 0, \quad \mu_n \geq 0$

- KKT conditions:

$$a_n \geq 0 \qquad \mu_n \geq 0$$

$$t_n y(\mathbf{x}_n) - 1 + \xi_n \geq 0 \qquad \xi_n \geq 0$$

$$a_n\{t_n y(\mathbf{x}_n) - 1 + \xi_n\} = 0 \qquad \mu_n\xi_n = 0$$

3 N 3 N

- How many KKT conditions?

6 N

Maximum Margin Classifiers: Soft Margins!

- Lagrangian function

$$L(\mathbf{w}, b, \boldsymbol{\xi}, \mathbf{a}, \boldsymbol{\mu}) = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{n=1}^{N}\xi_n - \sum_{n=1}^{N} a_n\{t_n(\mathbf{w}^T\mathbf{x}_n + b) - 1 + \xi_n\} - \sum_{n=1}^{N}\mu_n\xi_n$$

- Minimize L w.r.t. primal variables $\mathbf{w}, b, \xi_n$ and use the KKT conditions to eliminate $\mathbf{w}, b, \xi_n$ from Lagrangian to obtain dual formulation!

$$\frac{\partial L}{\partial \mathbf{w}} = \mathbf{w}^T - \sum_{n=1}^{N} a_n t_n \mathbf{x}_n^T = 0 \quad \rightarrow \quad \mathbf{w} = \sum_{n=1}^{N} a_n t_n \mathbf{x}_n$$

$$\frac{\partial L}{\partial b} = -\sum_{n=1}^{N} a_n t_n = 0 \quad \rightarrow \quad \sum_{n=1}^{N} a_n t_n = 0$$

$$\frac{\partial L}{\partial \xi_n} = C - a_n - \mu_n = 0 \quad \rightarrow \quad a_n = C - \mu_n$$

same as before!

new constraint!

- Use this to eliminate $\mathbf{w}, b, \xi_n$, dual Lagrangian:

$$\tilde{L}(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m t_n t_m \mathbf{x}_n^T \mathbf{x}_m$$

Maximum Margin Classifiers: Soft Margins!

- Minimization of primal variables gave these conditions:

$$\mathbf{w} = \sum_{n=1}^{N} a_n t_n \mathbf{x}_n \,, \qquad \sum_{n=1}^{N} a_n t_n = 0 \,, \qquad a_n = C - \mu_n \quad (*)$$

- KKT conditions:

$$a_n \geq 0 \quad (**) \qquad \mu_n \geq 0$$

$$t_n y(\mathbf{x}_n) - 1 + \xi_n \geq 0 \qquad \xi_n \geq 0$$

$$a_n \{ t_n y(\mathbf{x}_n) - 1 + \xi_n \} = 0 \qquad \mu_n \xi_n = 0$$

- Dual lagrangian:

$$\tilde{L}(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} a_n a_m t_n t_m \mathbf{x}_n^T \mathbf{x}_m$$

- Remaining constraints:

$$0 \leq a_n \leq C \quad \text{Box constraints} \qquad (**) \quad (*)$$

$$\sum_{n=1}^{N} a_n t_n = 0$$

Maximum Margin Classifiers: Soft Margins!

- Dual problem: Maximize w.r.t an

$$\tilde{L}(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} a_n a_m t_n t_m \mathbf{x}_n^T \mathbf{x}_m$$

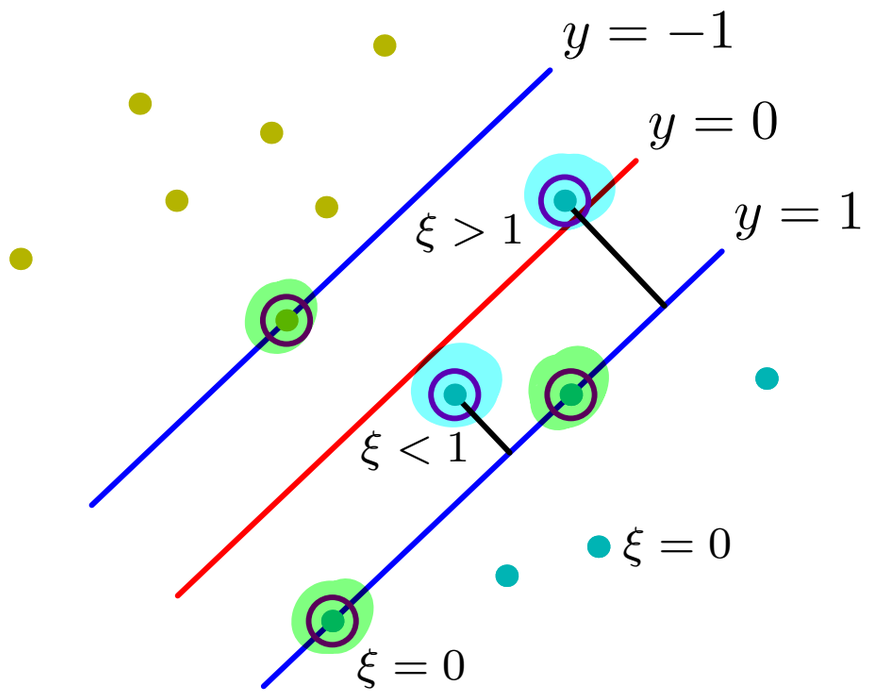
subject to $\quad 0 \leq a_n \leq C\,, \qquad \sum_{n=1}^{N} a_n t_n = 0$

- Kernel trick:

$$\tilde{L}(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} a_n a_m t_n t_m k(\mathbf{x}_n, \mathbf{x}_m)$$

- Prediction

$$y(\mathbf{x}) = \sum_{n=1}^{N} a_n t_n k(\mathbf{x}_n, \mathbf{x}) + b$$



Maximum Margin Classifiers: Soft Margins!

- Prediction: $y(\mathbf{x}) = \sum_{n=1}^{N} a_n t_n k(\mathbf{x}_n, \mathbf{x}) + b$ (with $0 \leq a_n \leq C$ and $\sum_{n=1}^{N} a_n t_n = 0$)

- Remember $a_n \geq 0$ $\mu_n \geq 0$

  $t_n y(\mathbf{x}_n) - 1 + \xi_n \geq 0$ $\xi_n \geq 0$

  $a_n\{t_n y(\mathbf{x}_n) - 1 + \xi_n\} = 0$ $\mu_n \xi_n = 0$

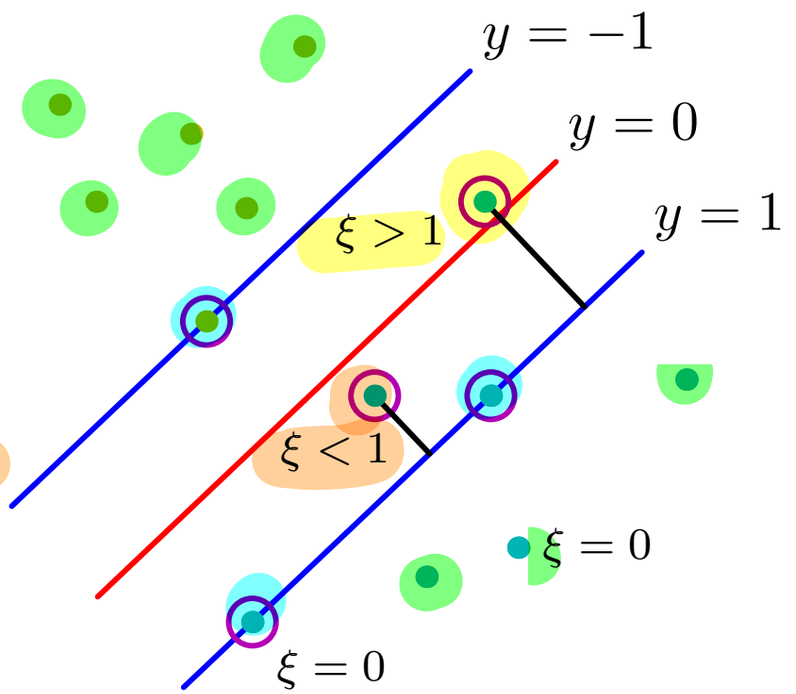
3 types of SV's

1. $a_n = 0$
2. $0 < a_n < C$
3. $a_n = C$

- **Support vectors** (If $a_n > 0$ then $t_n y(\mathbf{x}_n) = 1 - \xi_n$):

($a_n = C - \mu_n$)

  - If also $a_n < C$ then $\mu_n > 0$ so $\xi_n = 0$:
    - Points on margin
  - If $a_n = C$ then $\mu_n = 0$ so $\xi_n \geq 0$:
    - Correctly classified but within margin: $\xi_n \leq 1$
    - Misclassified $\xi_n > 1$



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$$\text{subject to} \quad t_n y(\mathbf{x}_n) \geq 1 - \xi_n\,, \quad \text{for} \quad n = 1,\ldots,N$$
$$\xi_n \geq 0\,, \quad \text{for} \quad n = 1,\ldots,N$$

- What happens in the limit: $C \to \infty$

– Hard margin Classifier

- What happens when $C \to 0$

Possibly
– Infinite margin
every point becomes a SV