Artificial Intelligence and Machine Learning

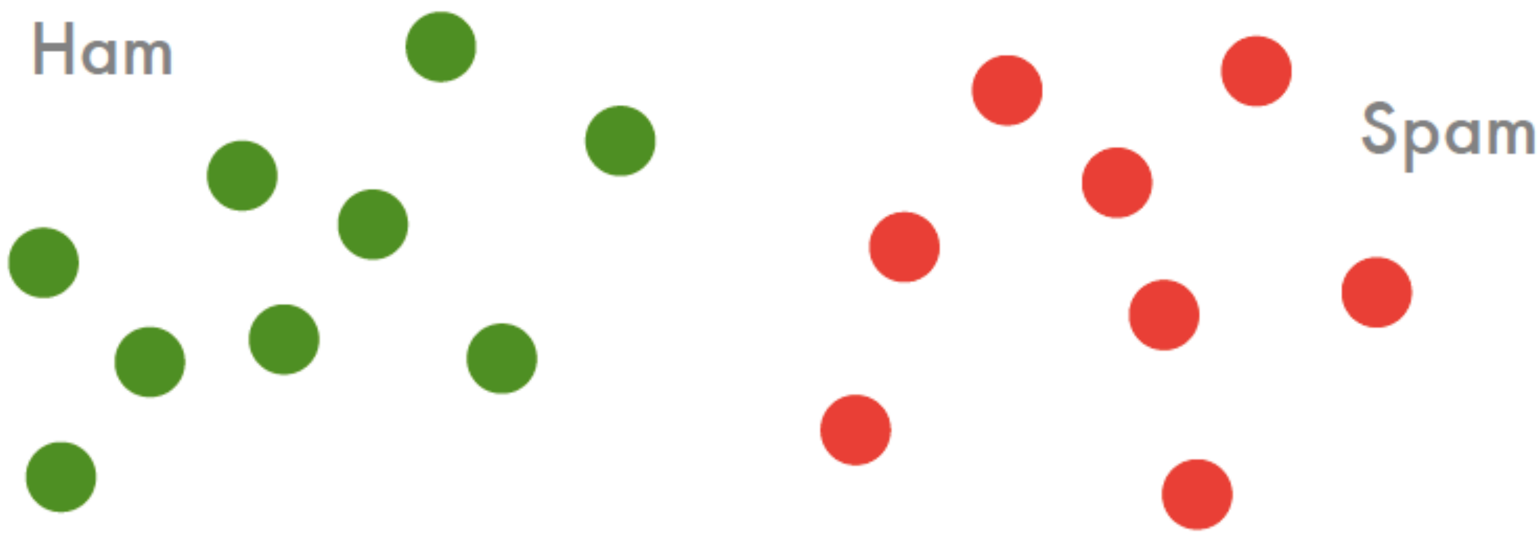
Barbara Caputo

Support Vector Machines

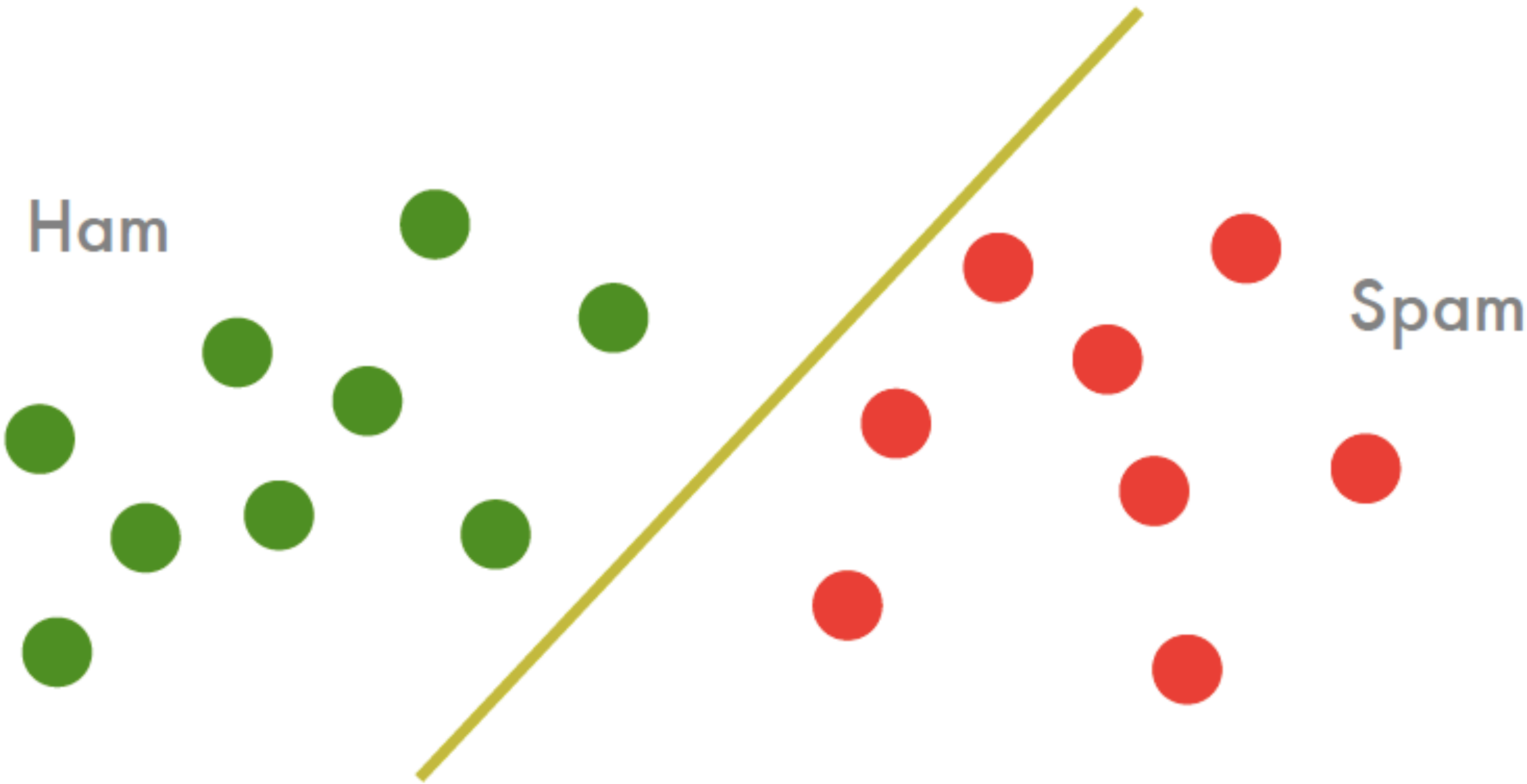
Outline

- Support Vector Classification
  Large Margin Separation, optimization problem
- Properties
  Support Vectors, kernel expansion
- Soft margin classifier
  Dual problem, robustness

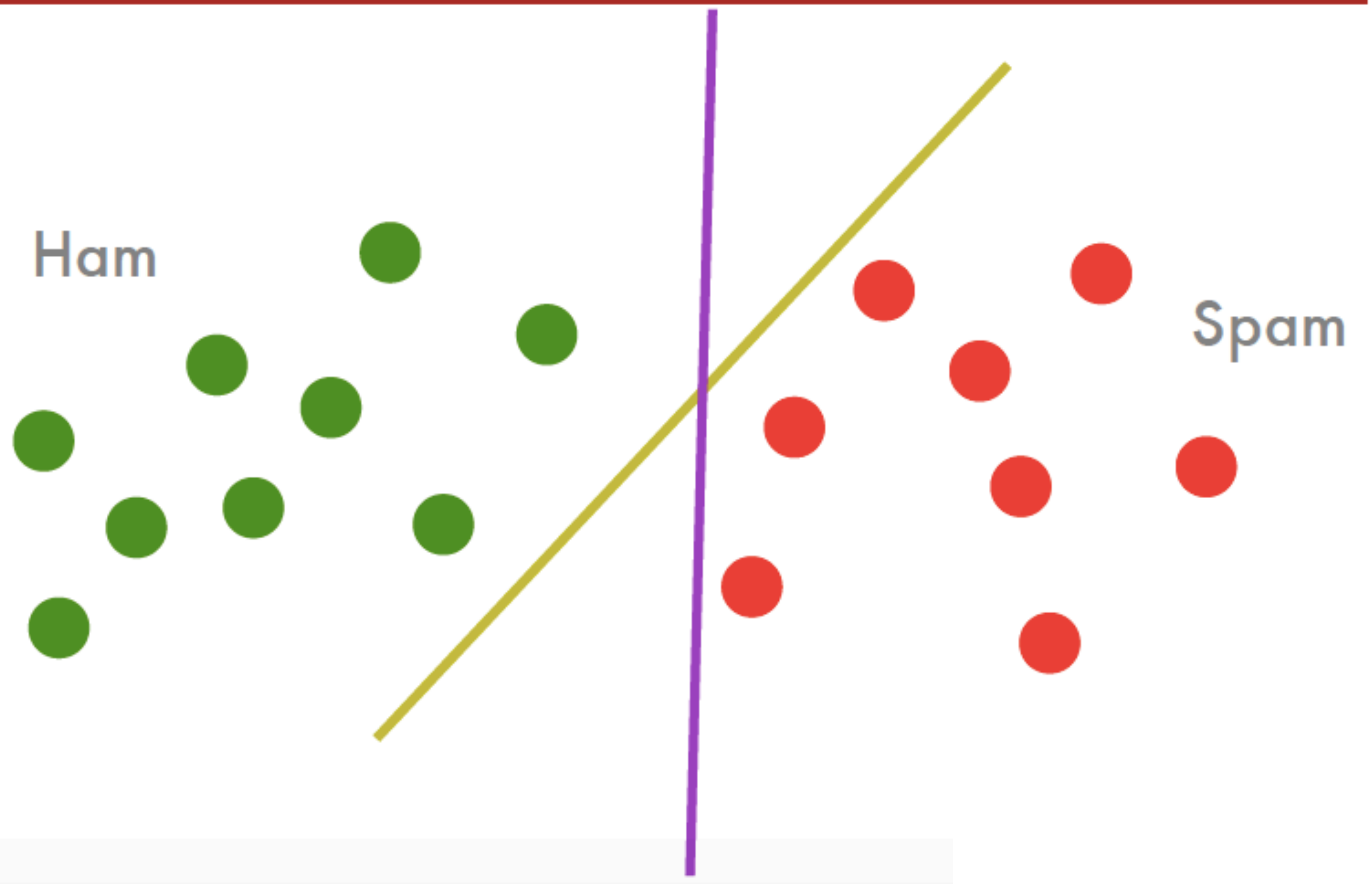
Linear Separator



Linear Separator



Linear Separator



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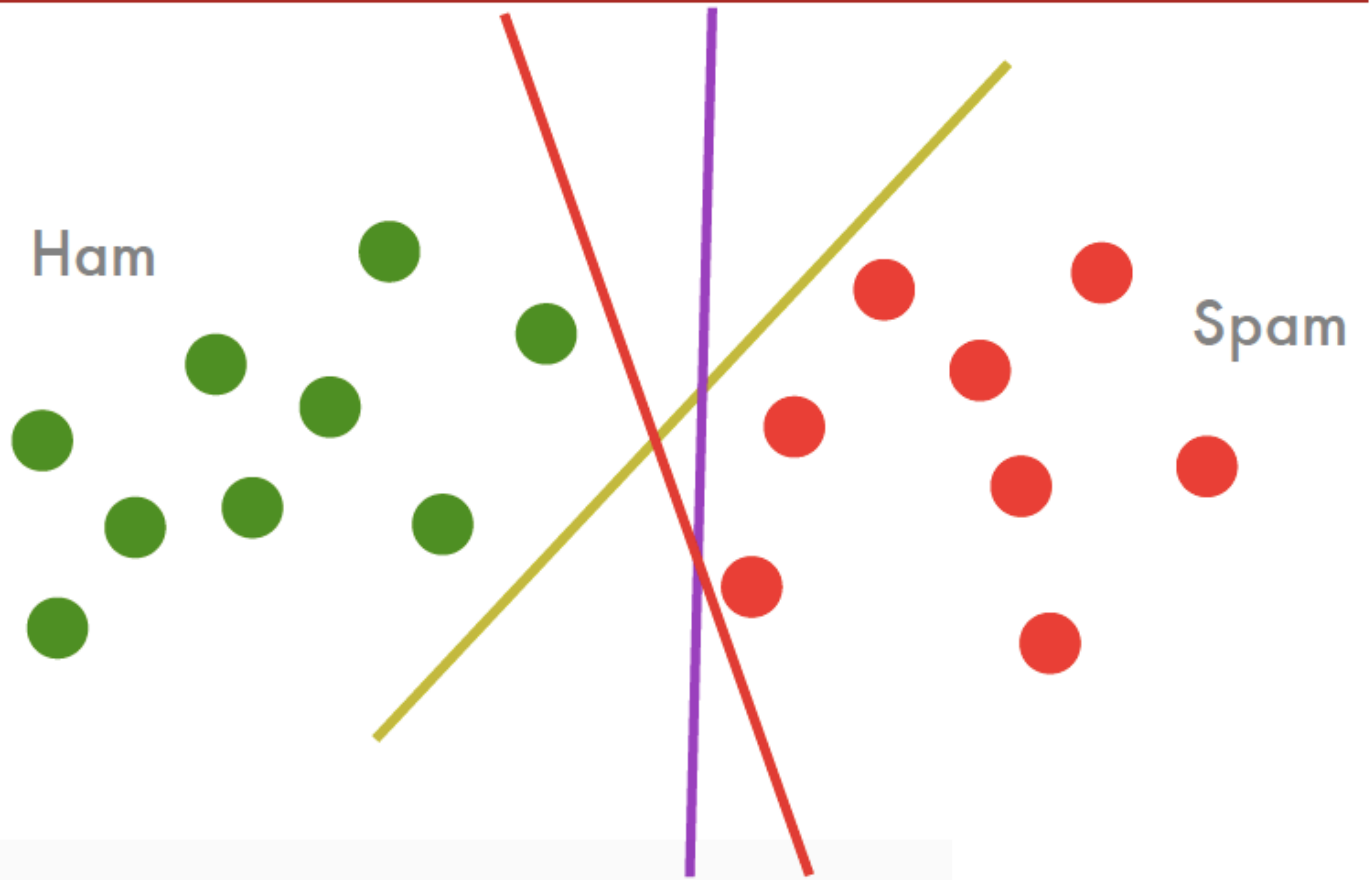

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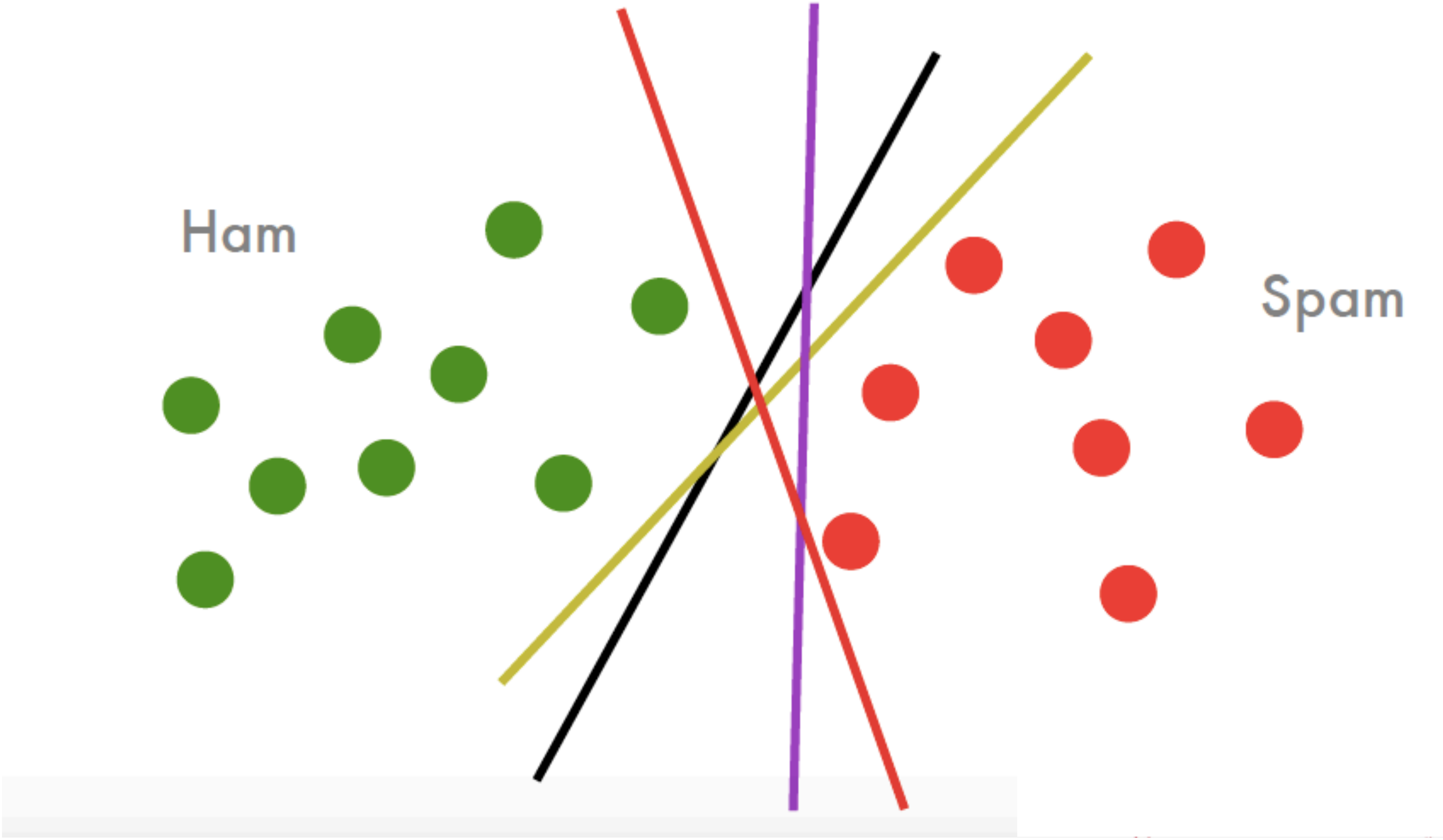
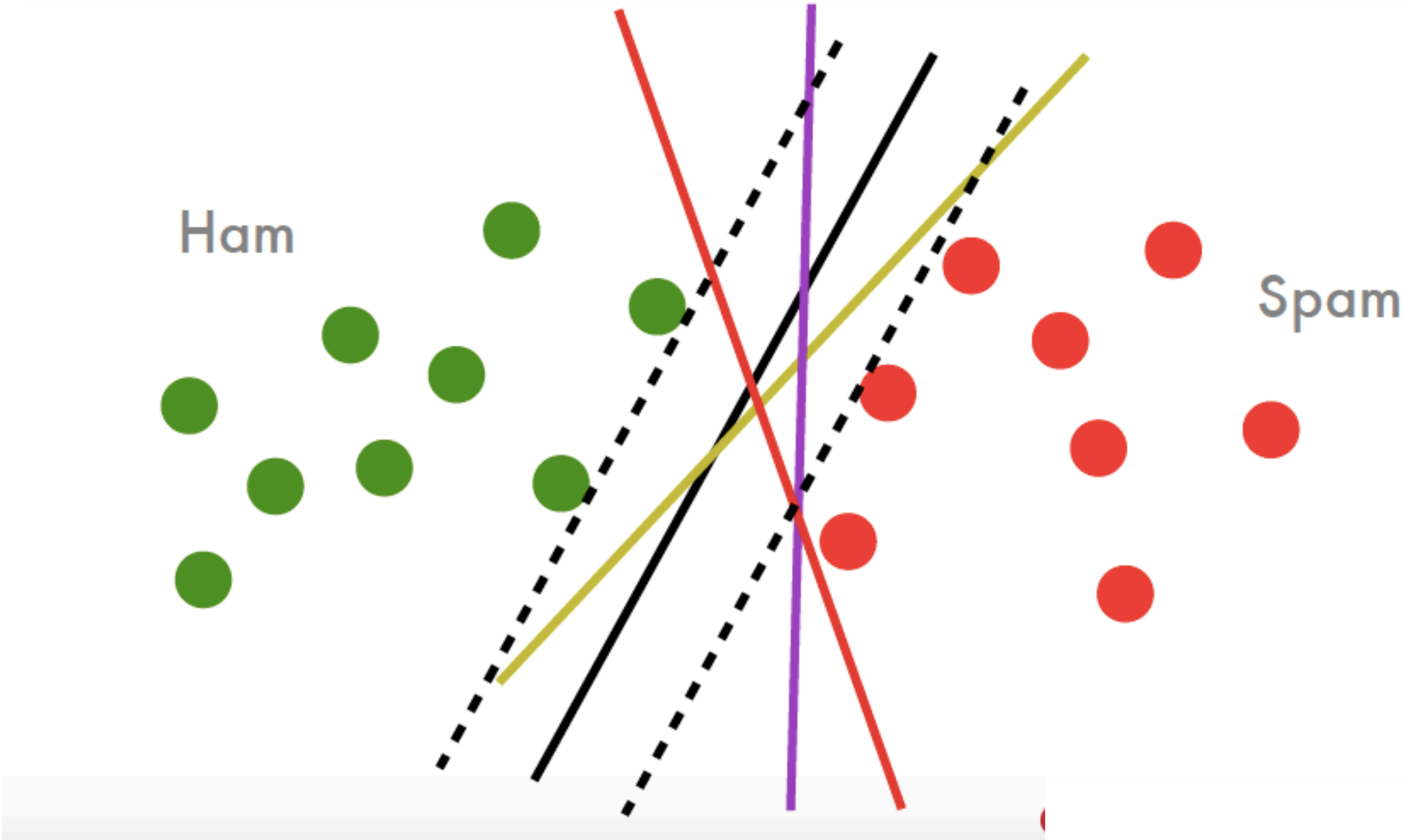


Linear Separator



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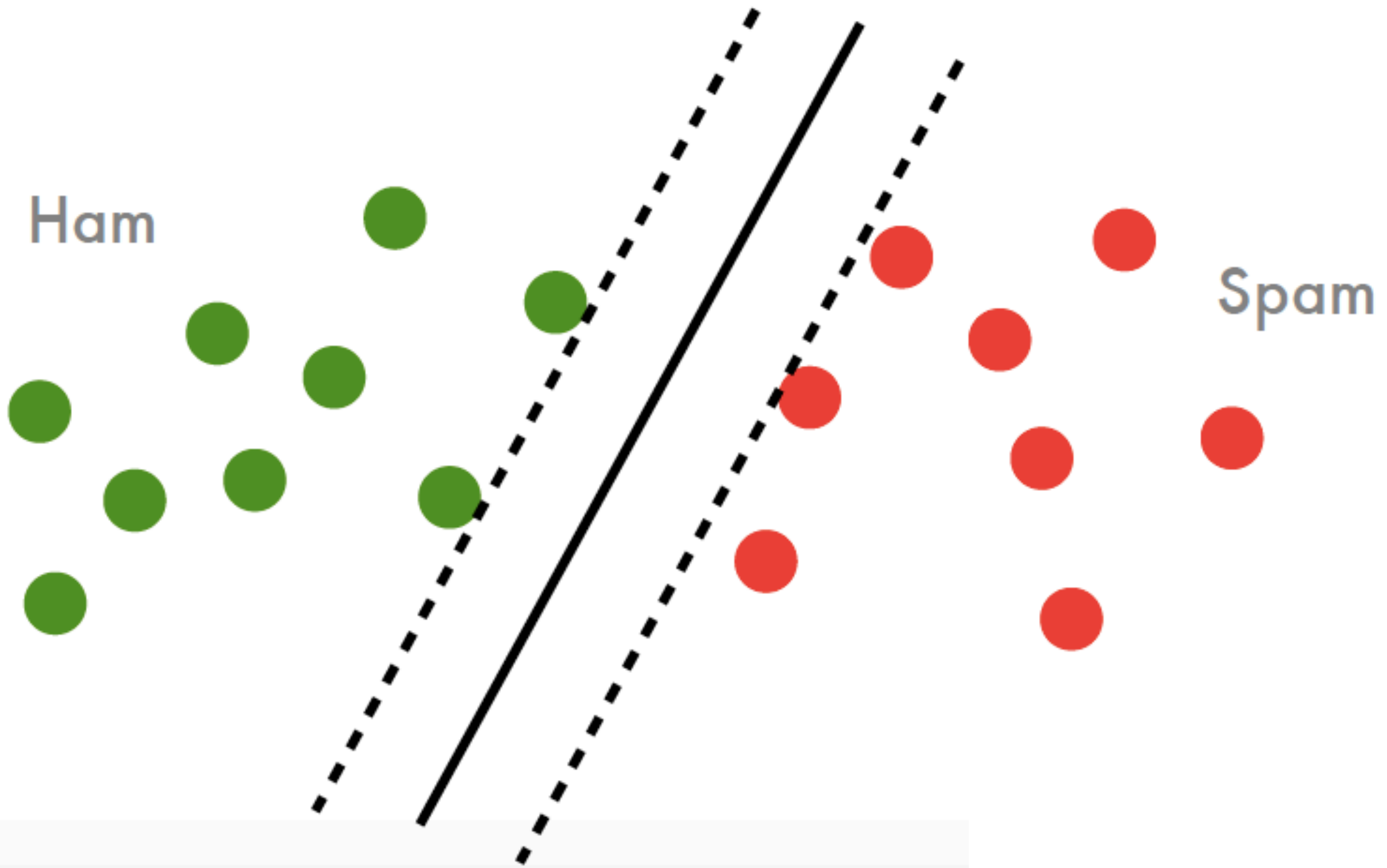
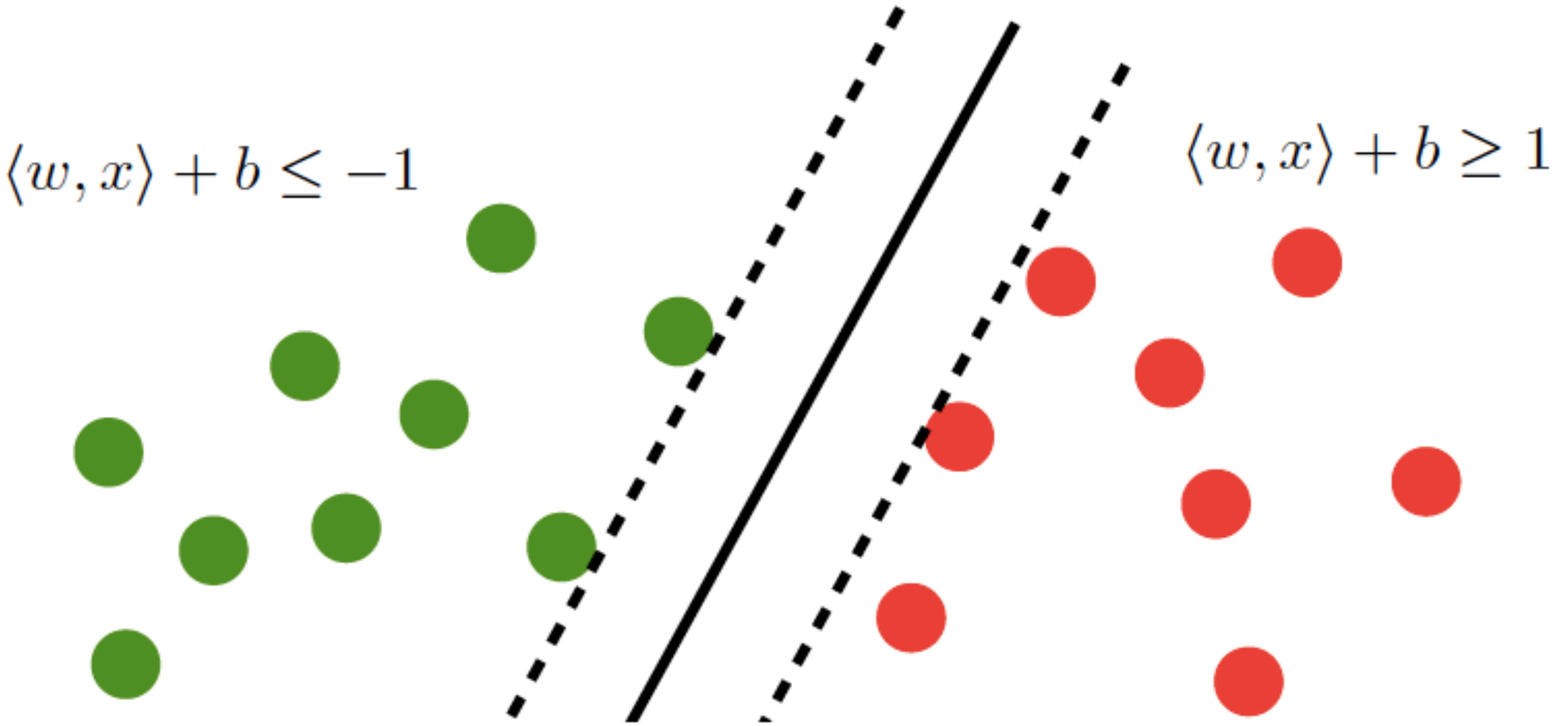


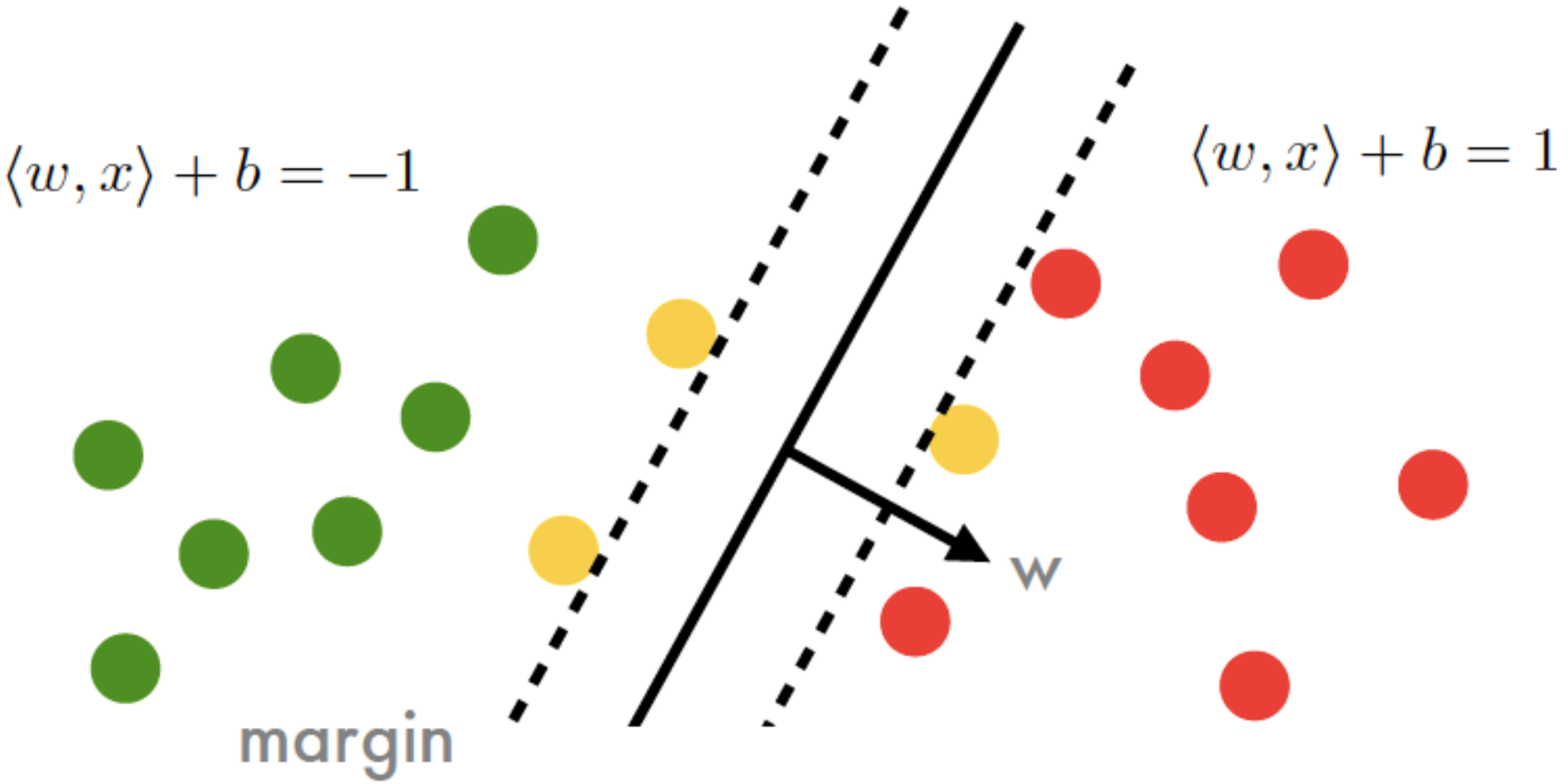
Large Margin Classifier



linear function

$$f(x) = \langle w, x \rangle + b$$

Large Margin Classifier



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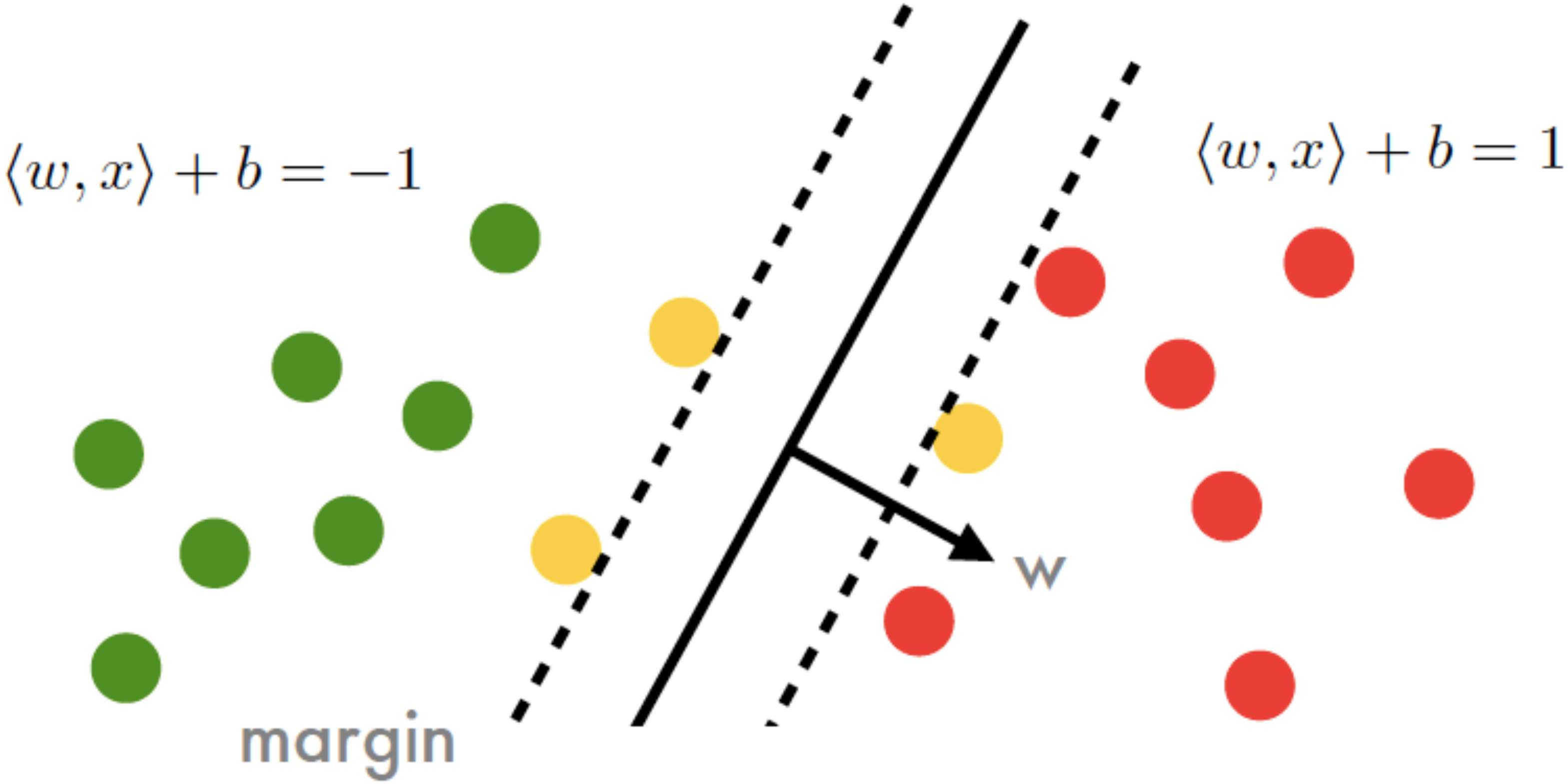
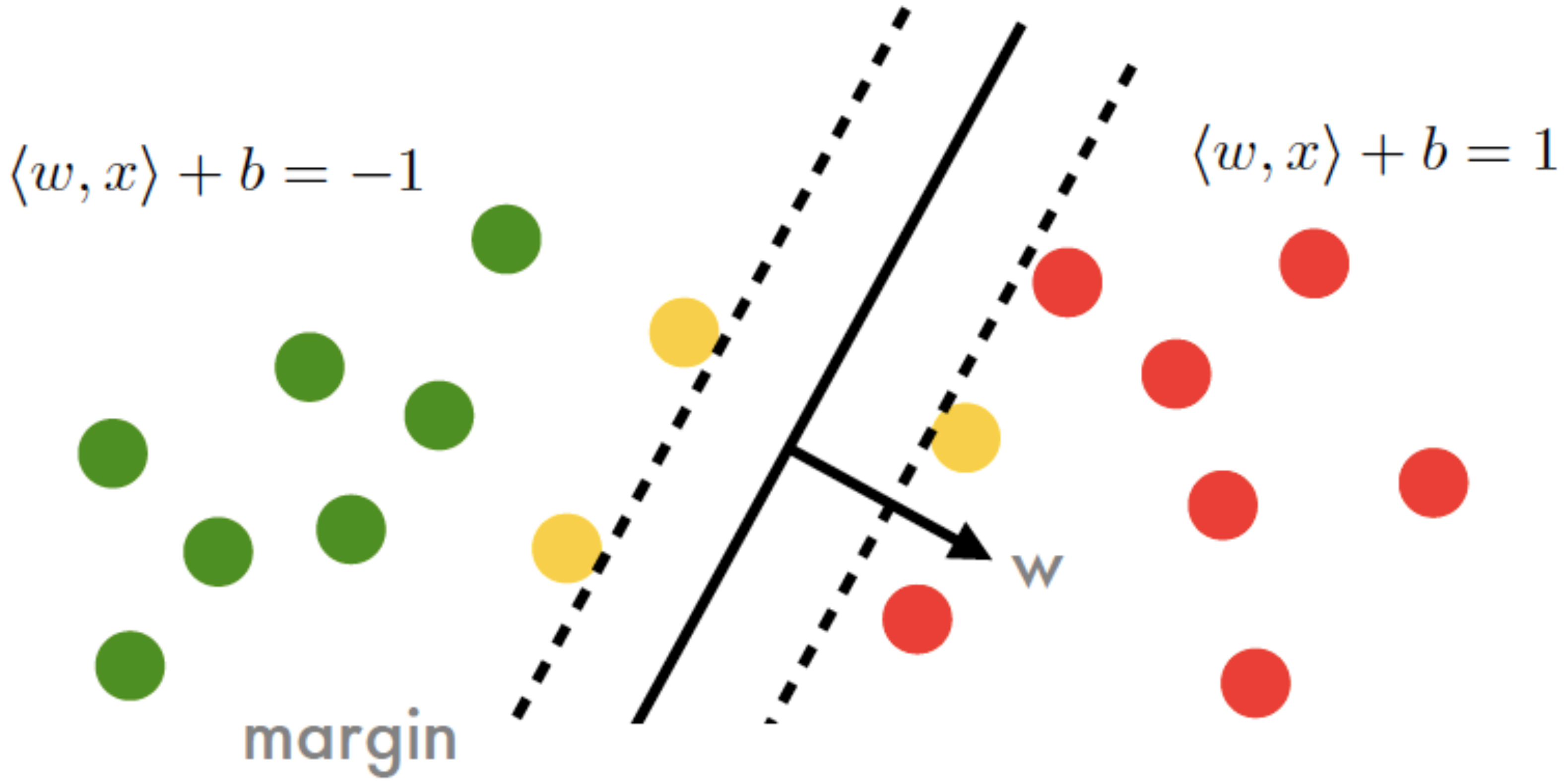


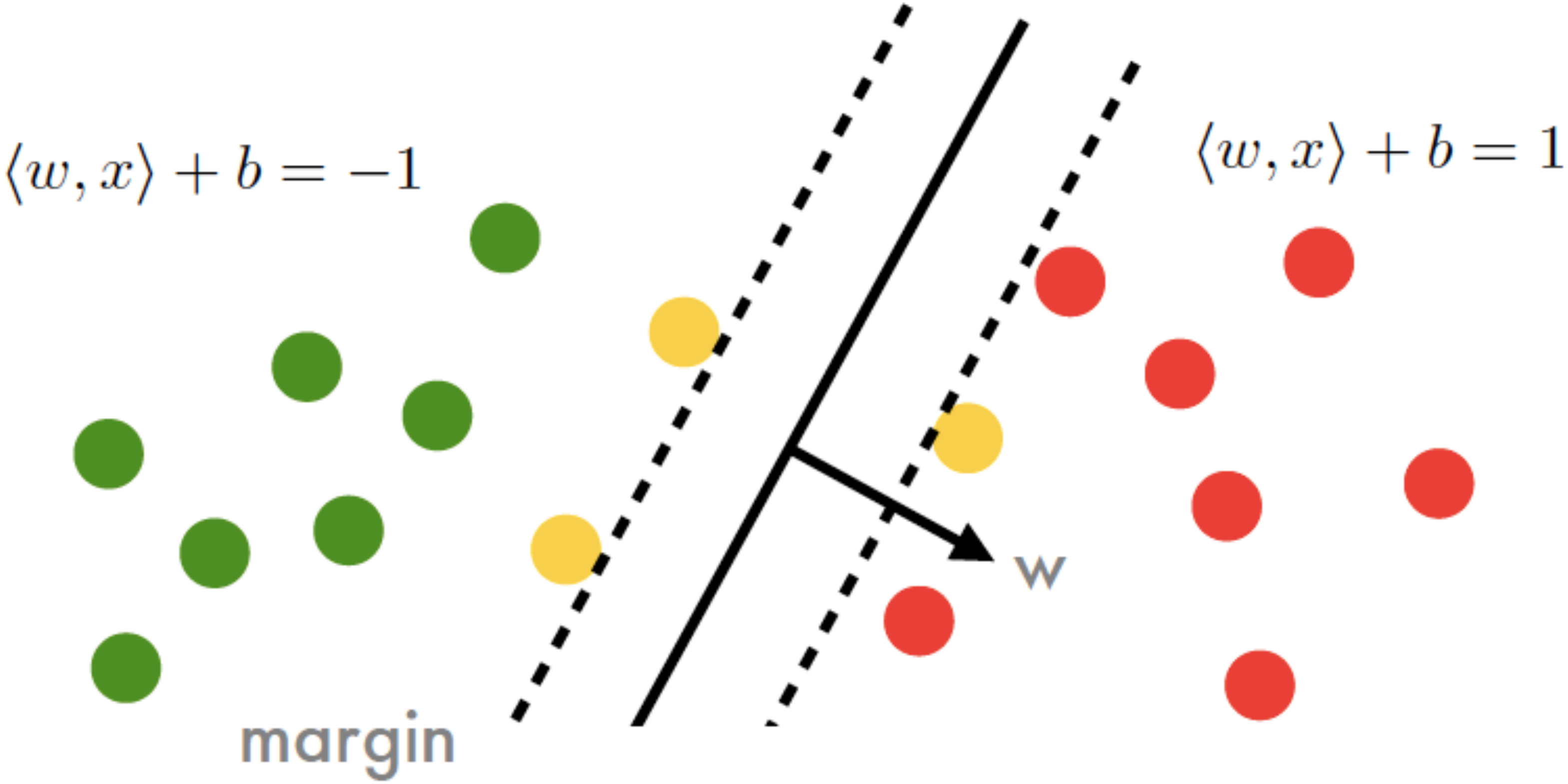
$$\frac{\langle x_+ - x_-, w \rangle}{2\,\|w\|} =$$

Large Margin Classifier



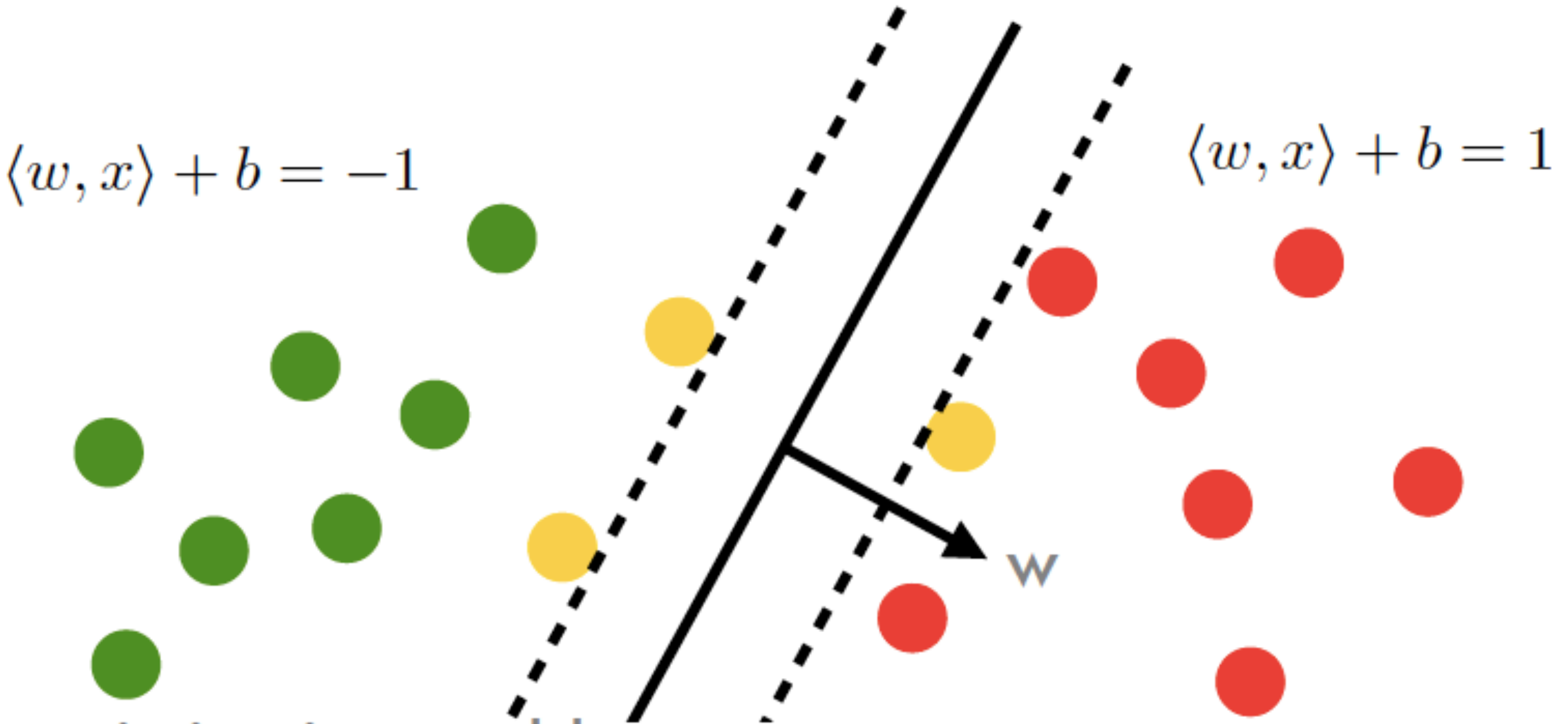
$$\frac{\langle x_+ - x_-, w \rangle}{2\,\|w\|} = \frac{1}{2\,\|w\|}\left[[\langle x_+, w \rangle + b] - [\langle x_-, w \rangle + b]\right] =$$

Large Margin Classifier



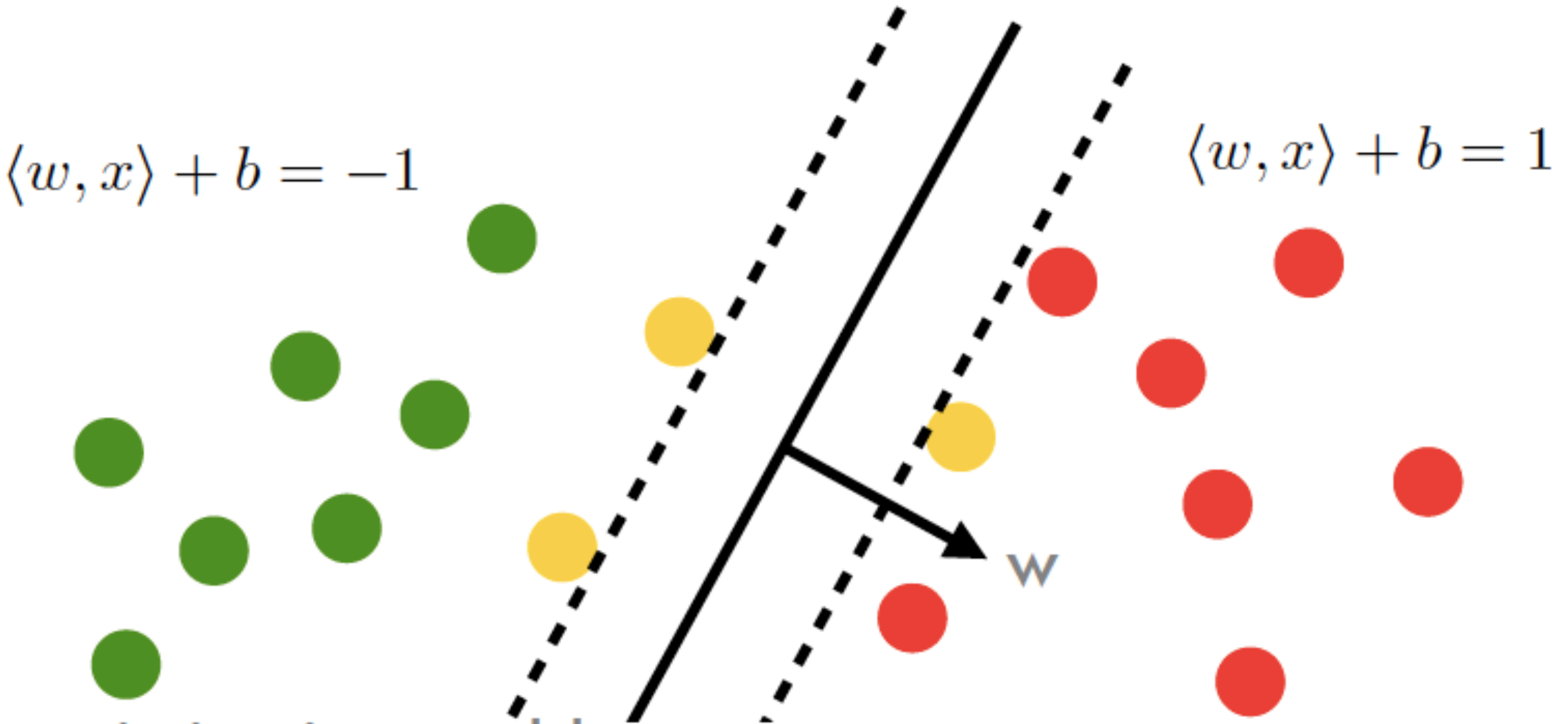
$$\frac{\langle x_+ - x_-, w\rangle}{2\,\|w\|} = \frac{1}{2\,\|w\|}\left[\left[\langle x_+, w\rangle + b\right] - \left[\langle x_-, w\rangle + b\right]\right] = \frac{1}{\|w\|}$$

Large Margin Classifier



optimization problem

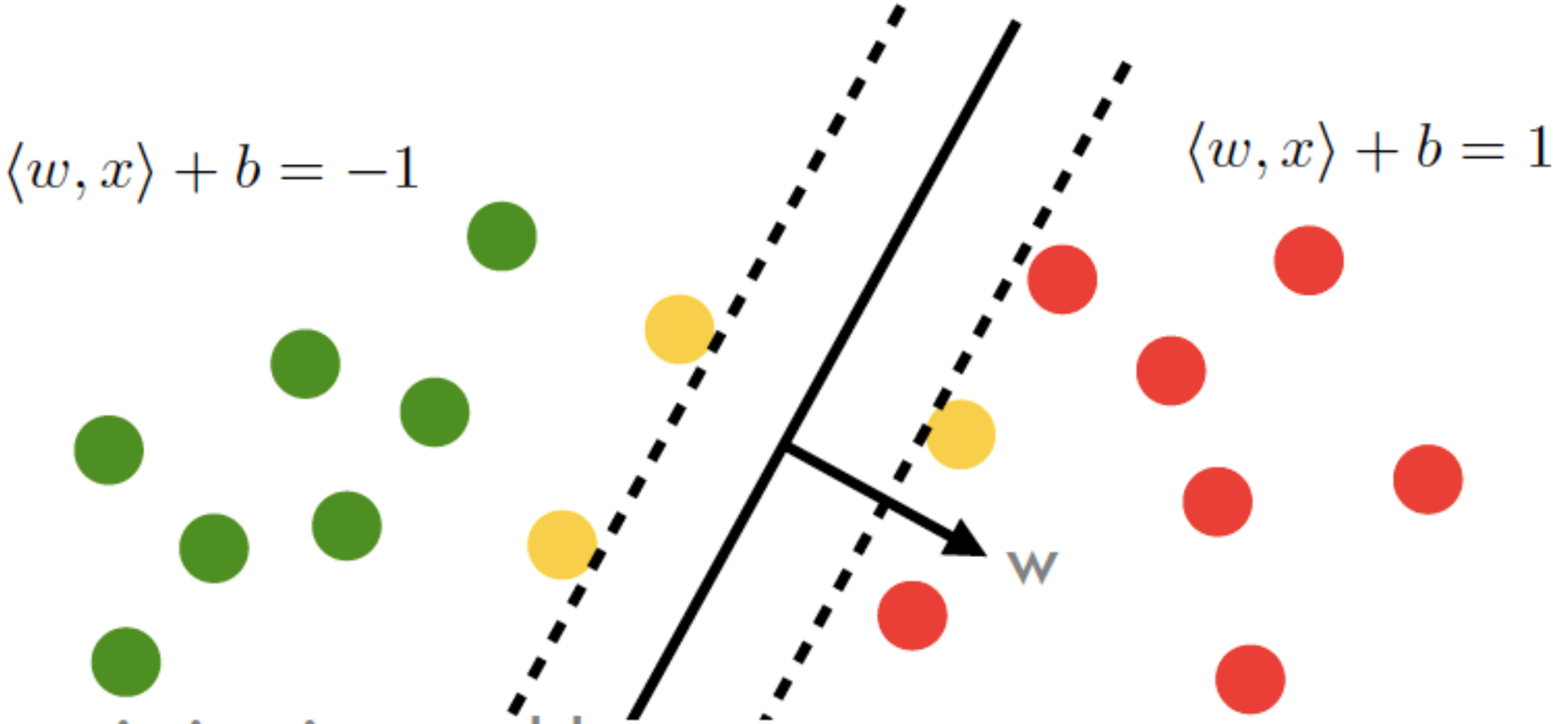
Large Margin Classifier



optimization problem

$$\underset{w,b}{\text{maximize}} \frac{1}{\|w\|} \text{ subject to } y_i \left[\langle x_i, w \rangle + b\right] \geq 1$$

Large Margin Classifier



optimization problem

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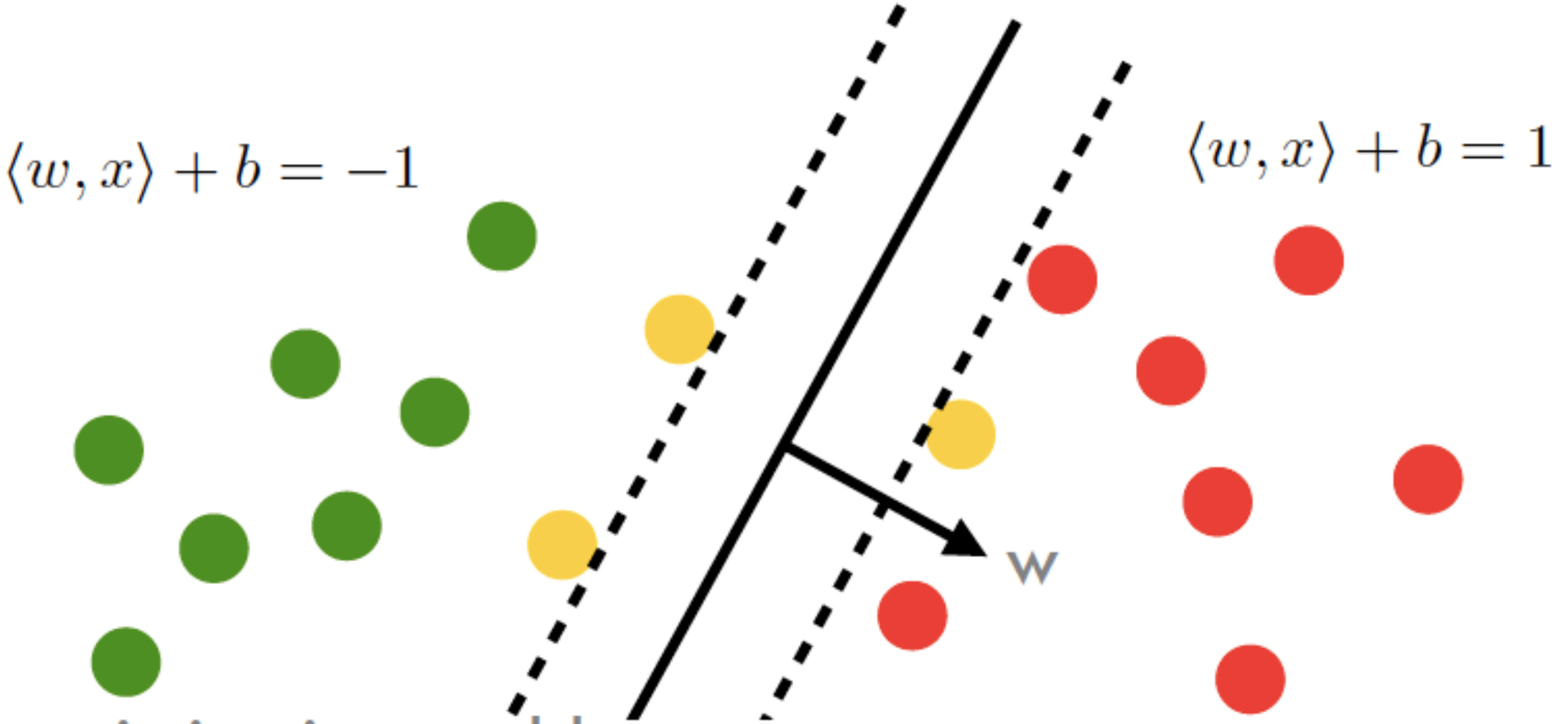

optimization problem

$$\underset{w,b}{\text{minimize}} \frac{1}{2} \|w\|^2 \text{ subject to } y_i \left[\langle x_i, w \rangle + b\right] \geq 1$$

Dual Problem

- Primal optimization problem

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- **Primal optimization problem**

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Dual Problem

- **Primal optimization problem**

$$\underset{w,b}{\text{minimize}} \frac{1}{2}\|w\|^2 \text{ subject to } y_i\left[\langle x_i, w\rangle + b\right] \geq 1$$

- **Lagrange function**

constraint

$$L(w,b,\alpha) = \frac{1}{2}\|w\|^2 - \sum_i \alpha_i \left[y_i\left[\langle x_i, w\rangle + b\right] - 1\right]$$

Dual Problem

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$$\underset{w,b}{\text{minimize}} \frac{1}{2}\|w\|^2 \text{ subject to } y_i\left[\langle x_i, w\rangle + b\right] \geq 1$$

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Optimality in w, b is at saddle point with α

- Derivatives in w, b need to vanish

Dual Problem

- **Lagrange function**

$$L(w, b, \alpha) = \frac{1}{2} \|w\|^2 - \sum_i \alpha_i \left[y_i \left[\langle x_i, w \rangle + b \right] - 1 \right]$$

Dual Problem

- Lagrange function

$$L(w, b, \alpha) = \frac{1}{2} \|w\|^2 - \sum_i \alpha_i \left[y_i \left[\langle x_i, w \rangle + b \right] - 1 \right]$$

- Derivatives in w, b need to vanish

$$\partial_w L(w, b, a) = w - \sum_i \alpha_i y_i x_i = 0$$

Dual Problem

- Lagrange function

$$L(w, b, \alpha) = \frac{1}{2}\|w\|^2 - \sum_i \alpha_i \left[y_i \left[\langle x_i, w\rangle + b\right] - 1\right]$$

- Derivatives in w, b need to vanish

$$\partial_w L(w, b, a) = w - \sum_i \alpha_i y_i x_i = 0$$

$$\partial_b L(w, b, a) = \sum_i \alpha_i y_i = 0$$

Dual Problem

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$$L(w, b, \alpha) = \frac{1}{2}\|w\|^2 - \sum_i \alpha_i \left[y_i \left[\langle x_i, w \rangle + b\right] - 1\right]$$

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Dual Problem

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$$L(w, b, \alpha) = \frac{1}{2}\|w\|^2 - \sum_i \alpha_i \left[y_i \left[\langle x_i, w\rangle + b\right] - 1\right]$$

- Derivatives in w, b need to vanish

$$\partial_w L(w, b, a) = w - \sum_i \alpha_i y_i x_i = 0$$

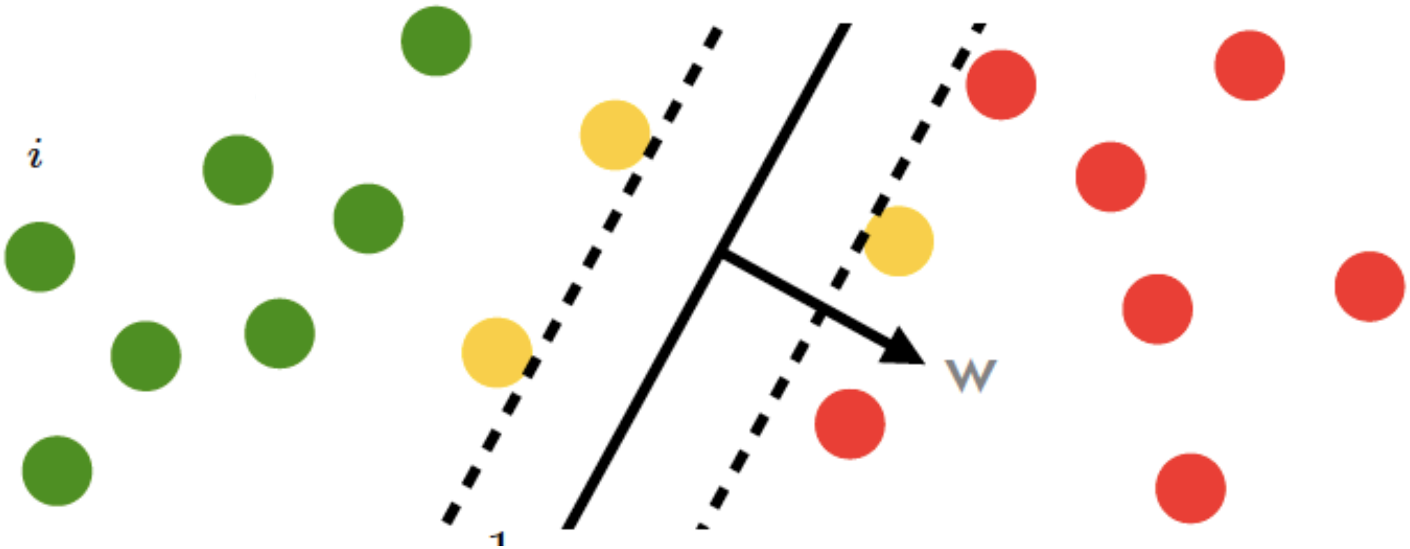
$$\partial_b L(w, b, a) = \sum_i \alpha_i y_i = 0$$

- Plugging terms back into L yields

$$\underset{\alpha}{\text{maximize}} - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j \langle x_i, x_j\rangle + \sum_i \alpha_i$$

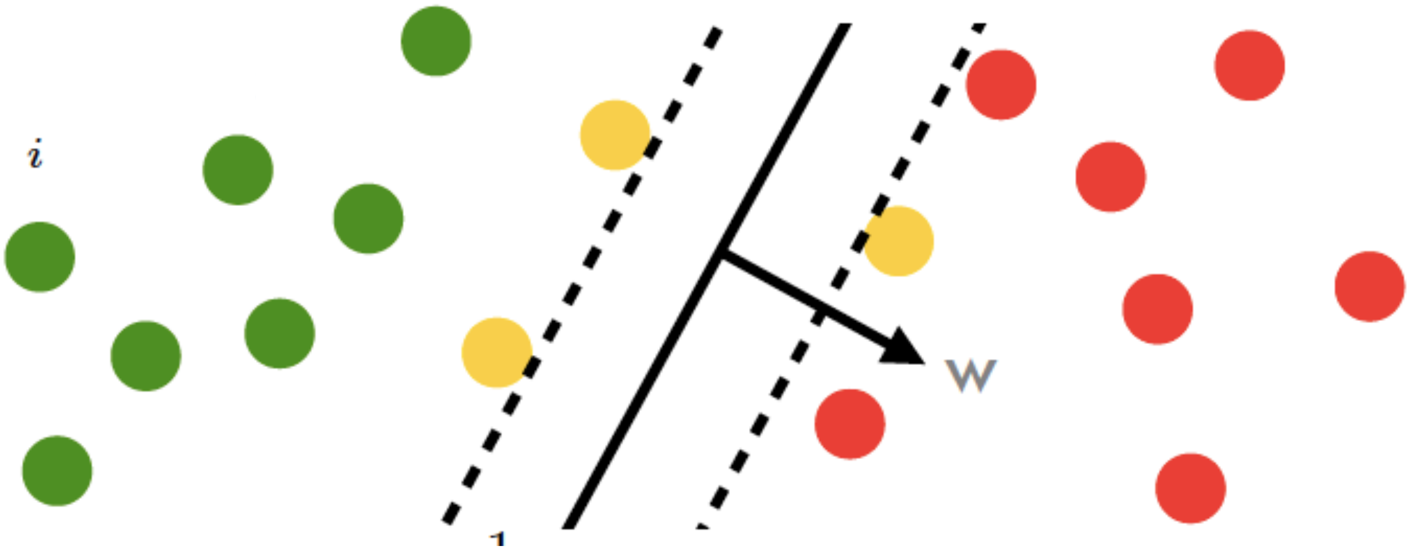
$$\text{subject to } \sum \alpha_i y_i = 0 \text{ and } \alpha_i \geq 0$$

Support Vector Machines



Support Vector Machines

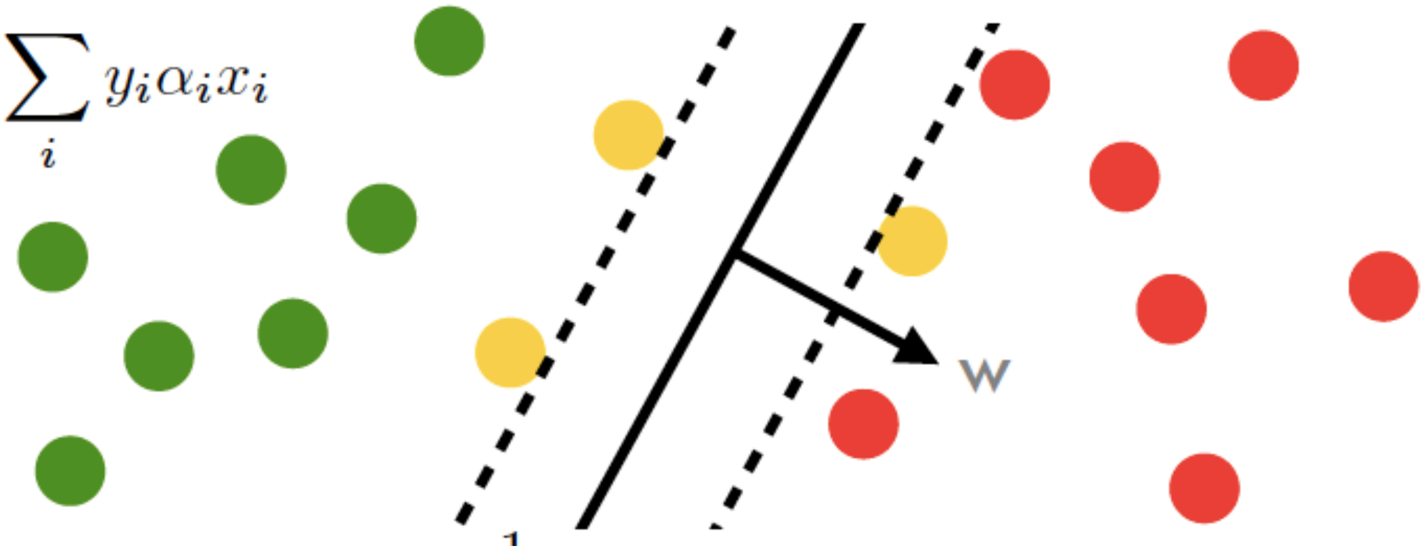
$$\underset{w,b}{\text{minimize}}\ \frac{1}{2}\|w\|^2 \text{ subject to } y_i\left[\langle x_i, w\rangle + b\right] \geq 1$$



Support Vector Machines

$$\underset{w,b}{\text{minimize}}\ \frac{1}{2}\|w\|^2 \ \text{ subject to } y_i\left[\langle x_i, w\rangle + b\right] \geq 1$$

$$w = \sum_i y_i \alpha_i x_i$$



Support Vector Machines

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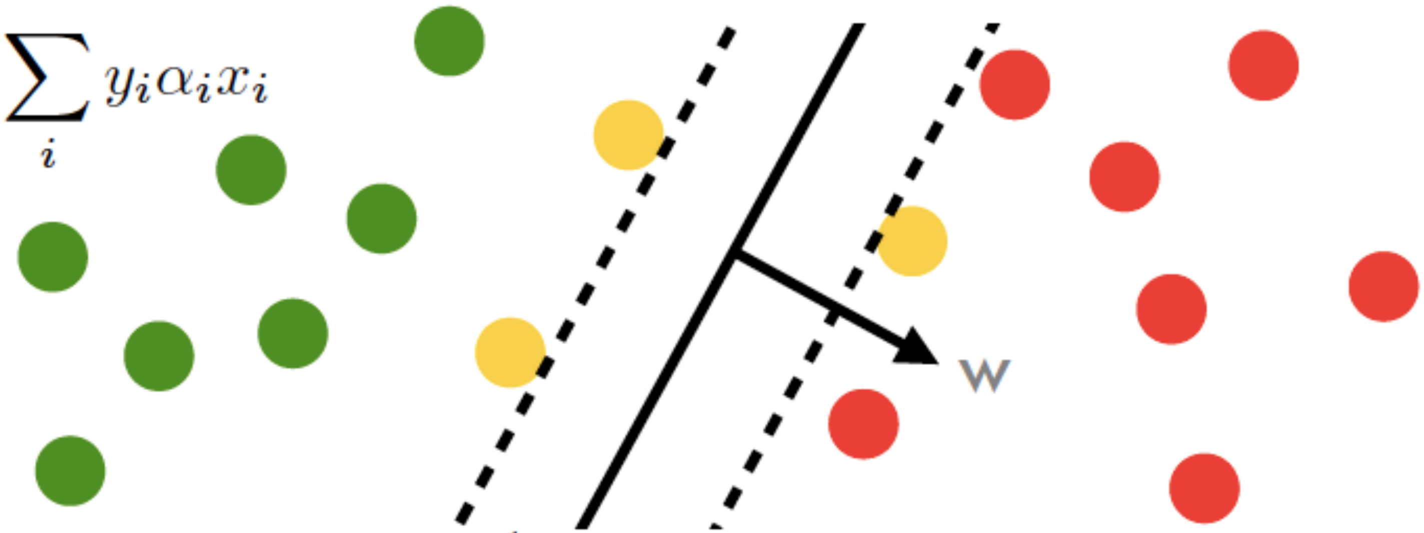
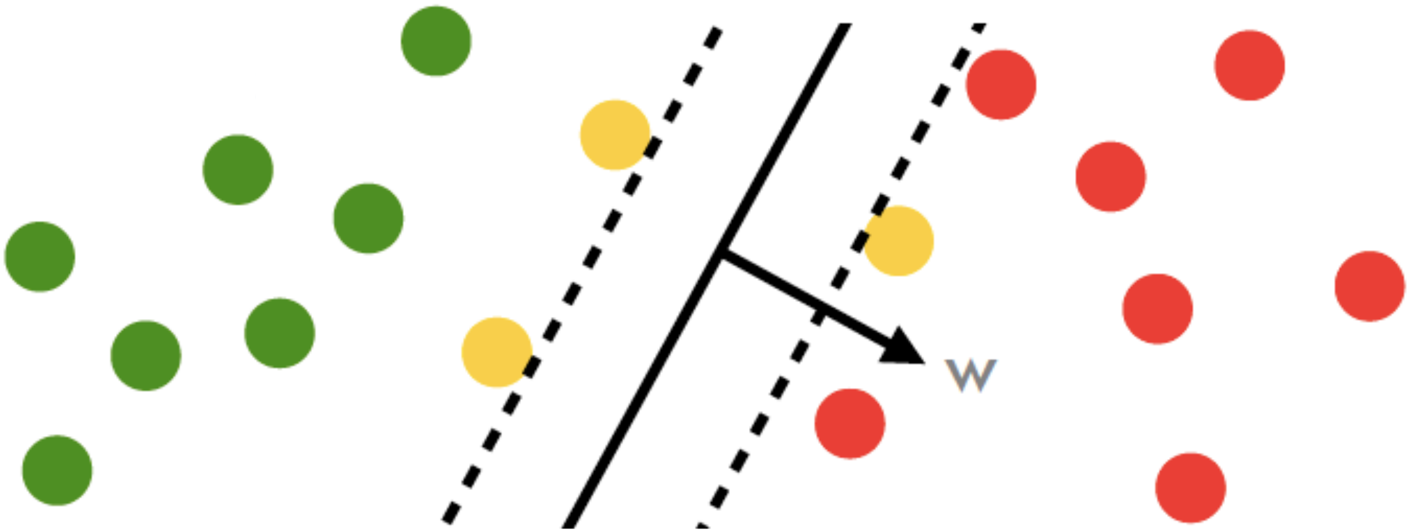


$$\underset{\alpha}{\text{maximize}} - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j \langle x_i, x_j\rangle + \sum_i \alpha_i$$

$$\text{subject to } \sum \alpha_i y_i = 0 \text{ and } \alpha_i \geq 0$$

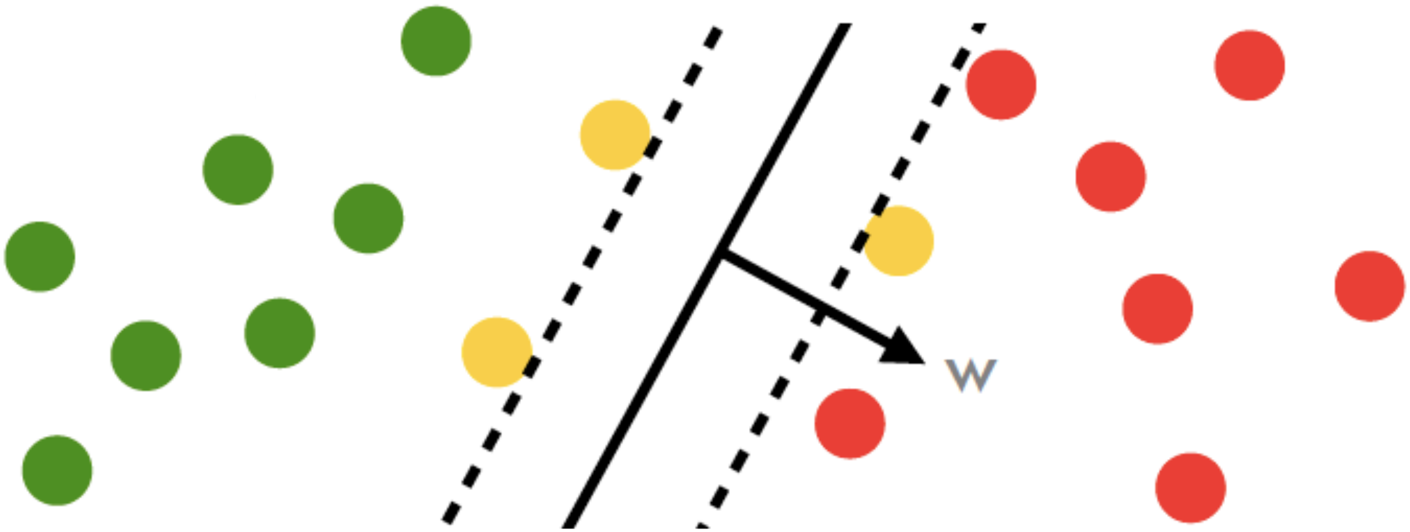
Five minutes break

Support Vector Machines



Support Vector Machines

$$\underset{w.b}{\text{minimize}} \frac{1}{2} \|w\|^2 \text{ subject to } y_i \left[\langle x_i, w \rangle + b\right] \geq 1$$



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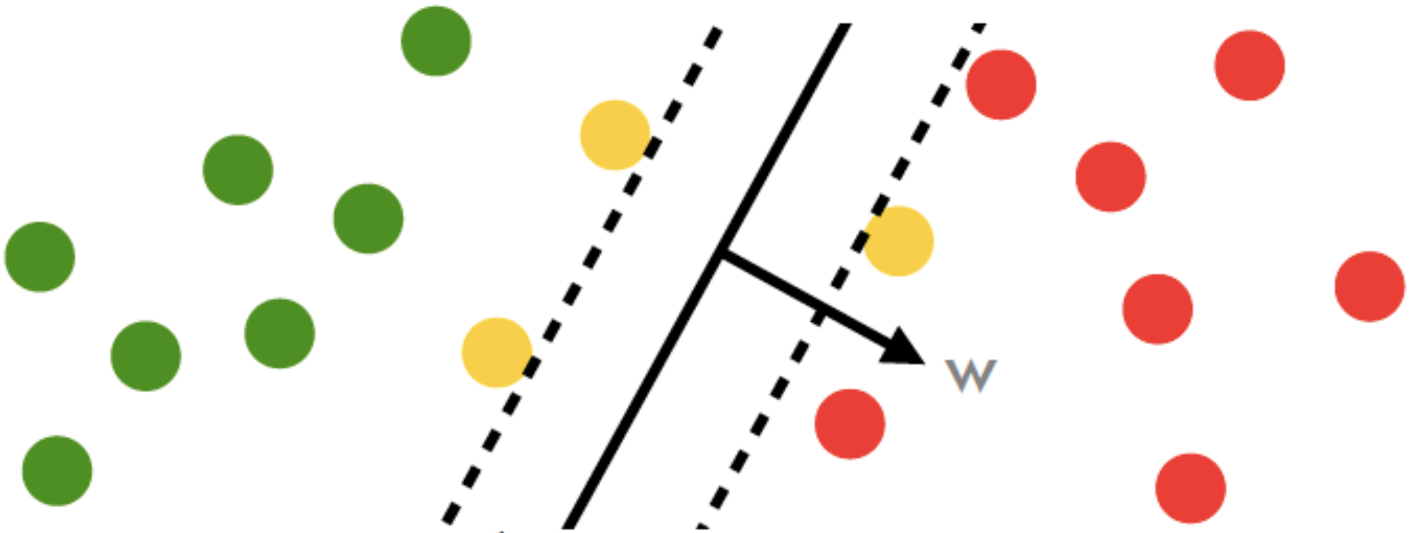

$$\underset{\alpha}{\text{maximize}} - \frac{1}{2}\sum_{i,j}\alpha_i\alpha_j y_i y_j \left\langle x_i, x_j\right\rangle + \sum_i \alpha_i$$

$$\text{subject to } \sum \alpha_i y_i = 0 \text{ and } \alpha_i \geq 0$$

Support Vector Machines

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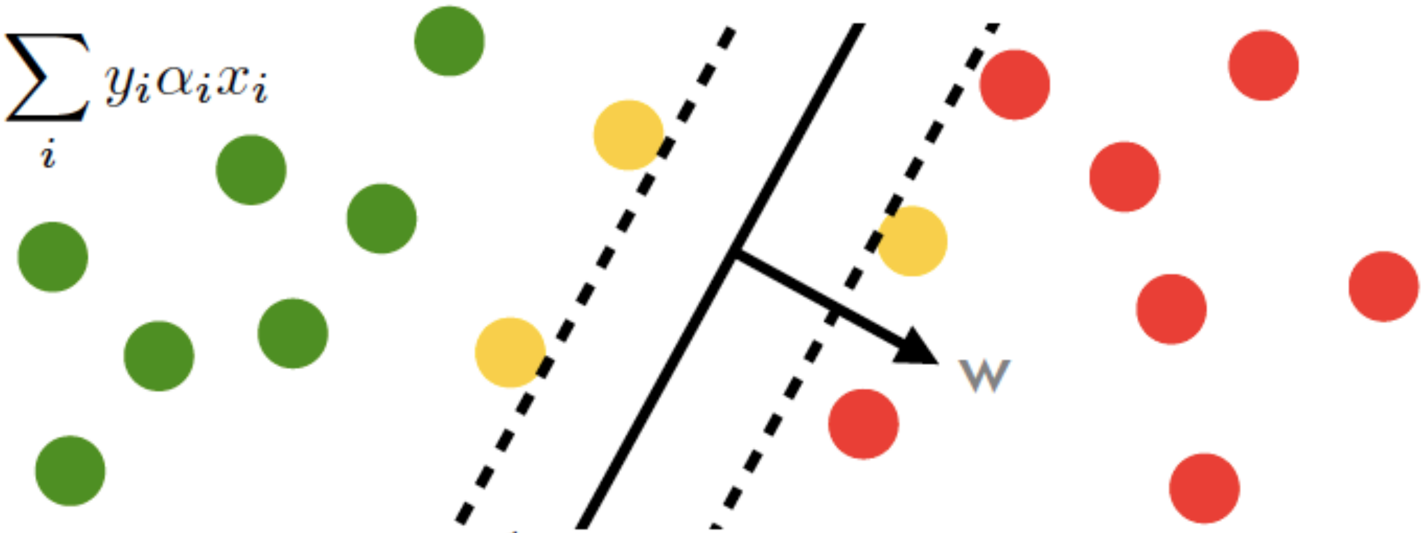


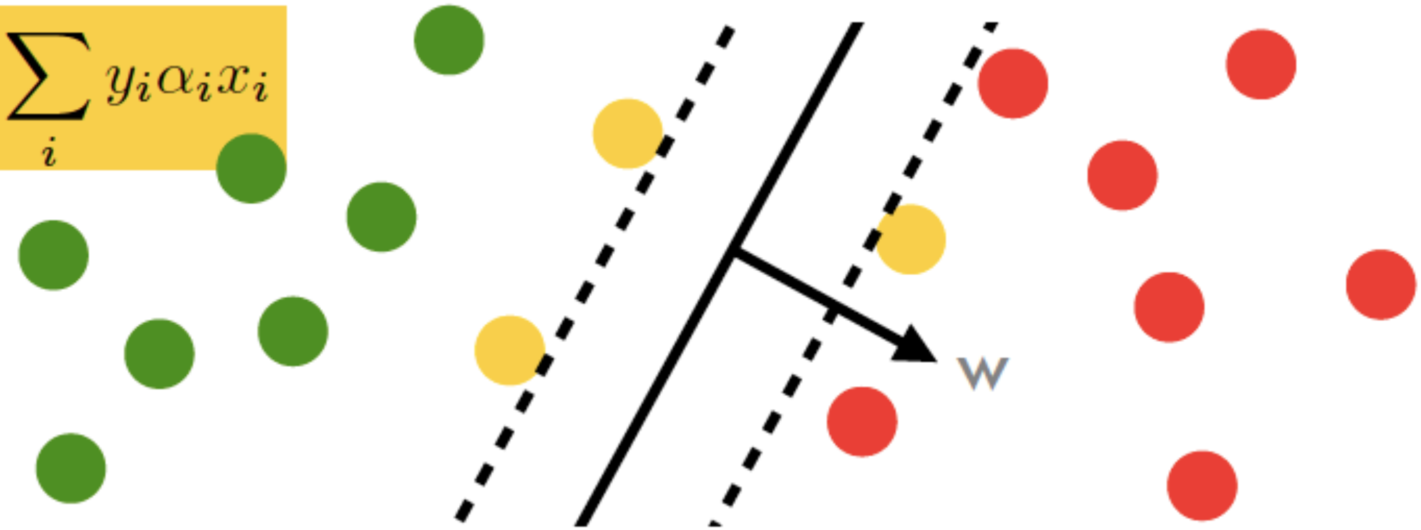
$$\underset{\alpha}{\text{maximize}} - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle + \sum_i \alpha_i$$

$$\text{subject to } \sum \alpha_i y_i = 0 \text{ and } \alpha_i \geq 0$$

Support Vectors

$$\underset{w,b}{\text{minimize}}\ \frac{1}{2}\|w\|^2 \ \text{ subject to } y_i\left[\langle x_i, w\rangle + b\right] \geq 1$$

$$w = \sum_i y_i \alpha_i x_i$$



Karush Kuhn Tucker
Optimality condition

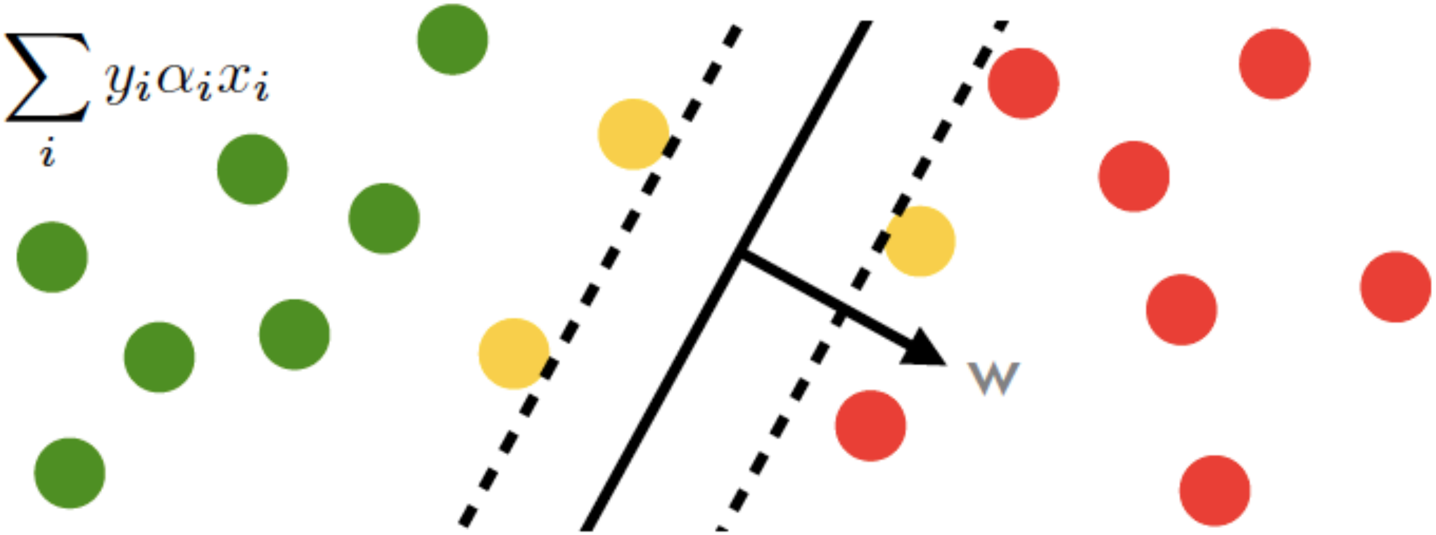
$$\alpha_i\left[y_i\left[\langle w, x_i\rangle + b\right] - 1\right] = 0$$

$$\alpha_i = 0$$

$$\alpha_i > 0 \Longrightarrow y_i\left[\langle w, x_i\rangle + b\right] = 1$$

Properties

$$w = \sum_i y_i \alpha_i x_i$$



Properties

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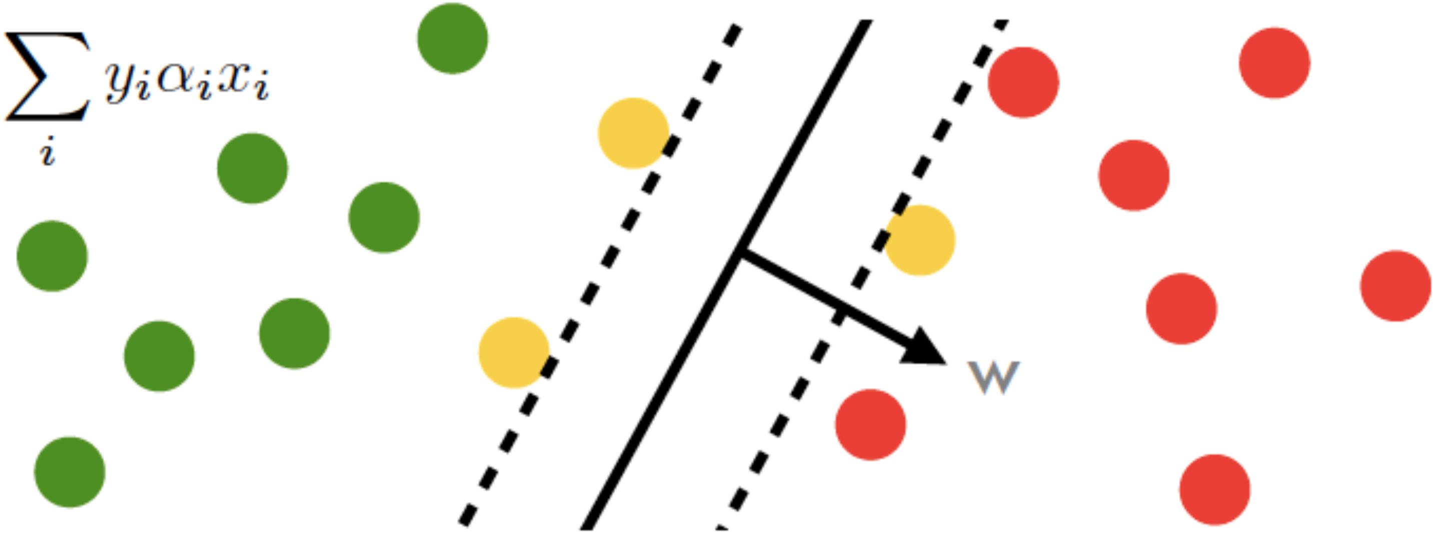
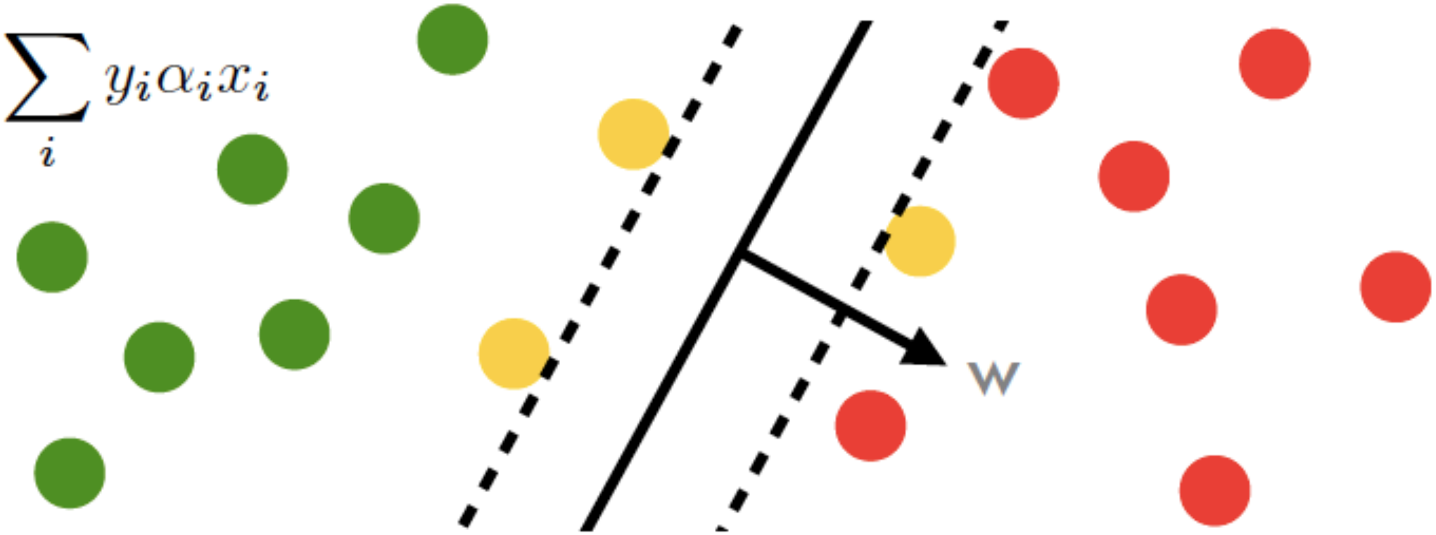


- Weight vector w as weighted linear combination of instances

Properties

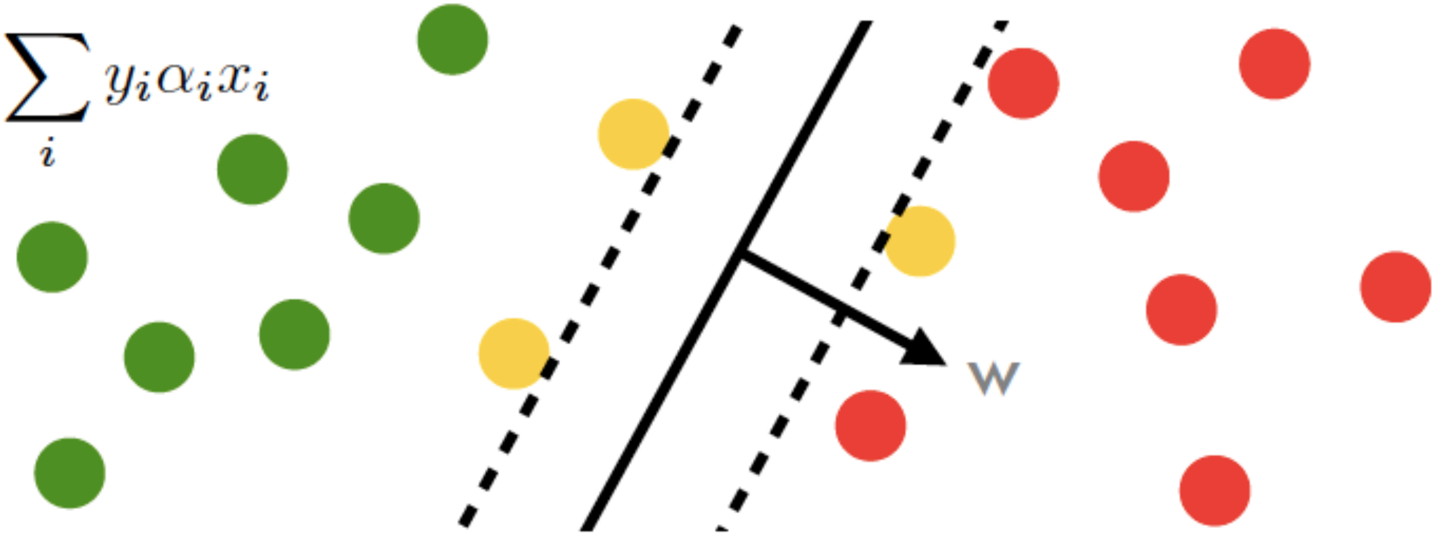
$$w = \sum_i y_i \alpha_i x_i$$



- Weight vector w as weighted linear combination of instances
- Only points on margin matter (ignore the rest and get same solution)

Properties

$$w = \sum_i y_i \alpha_i x_i$$



- Weight vector w as weighted linear combination of instances
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Properties

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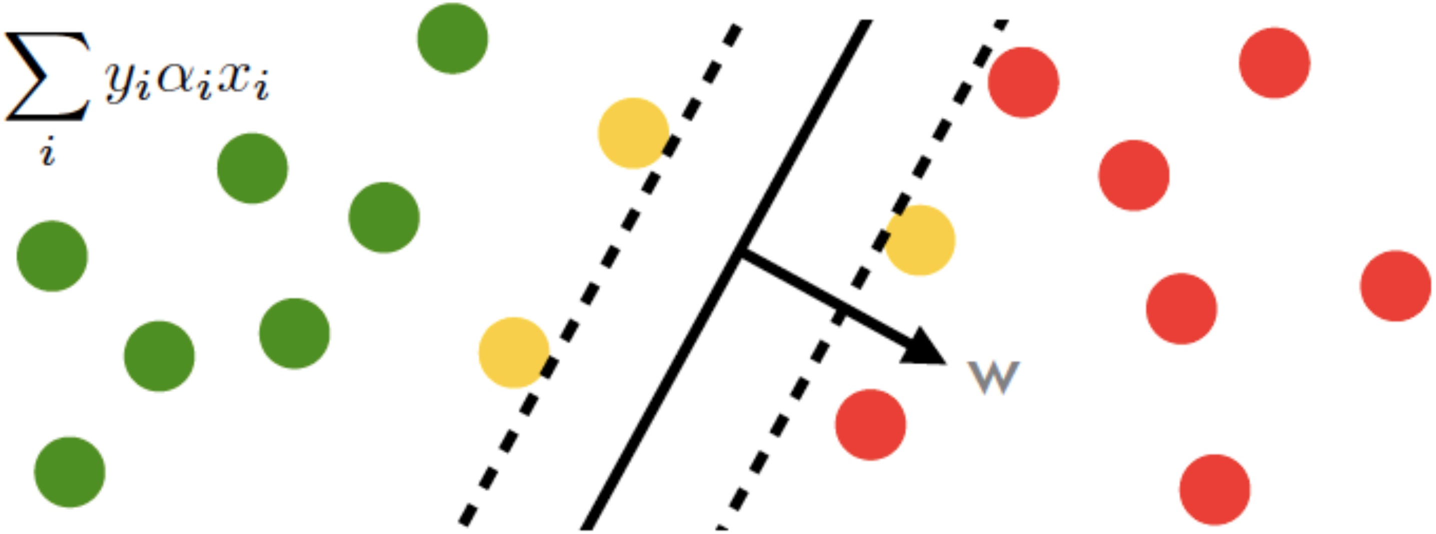
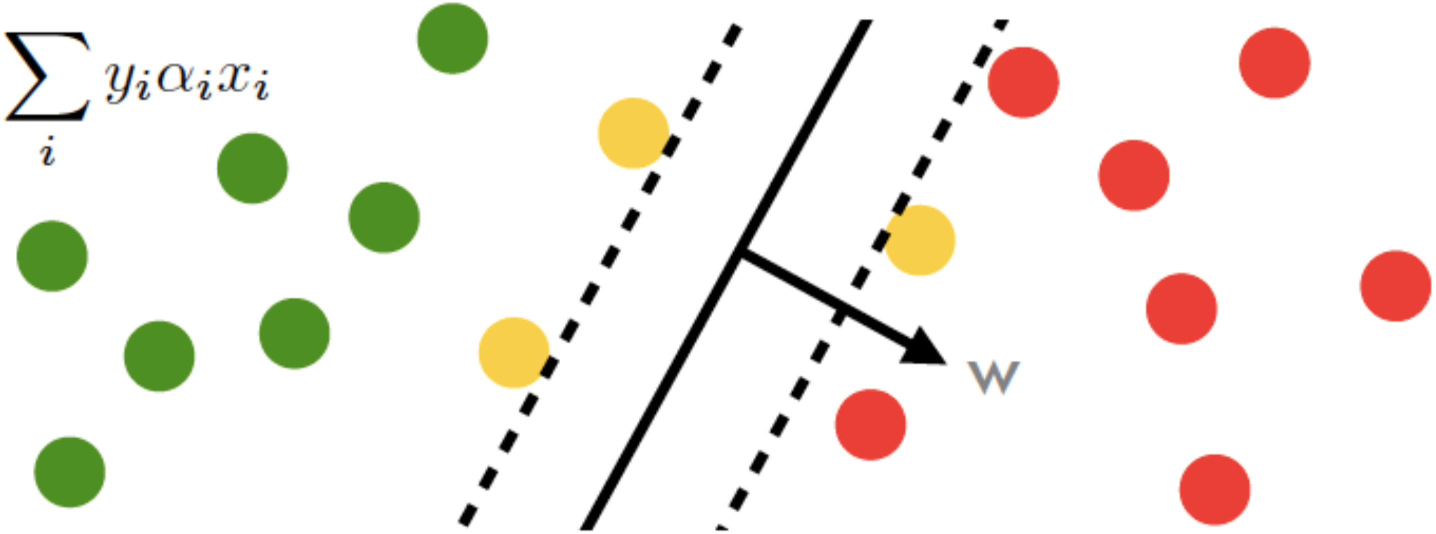


- Weight vector w as weighted linear combination of instances
- Only points on margin matter (ignore the rest and get same solution)
- Only inner products matter
  - Quadratic program

Properties

$$w = \sum_i y_i \alpha_i x_i$$



- Weight vector w as weighted linear combination of instances
- Only points on margin matter (ignore the rest and get same solution)
- Only inner products matter
  - Quadratic program
  - We can replace the inner product by a kernel

Properties

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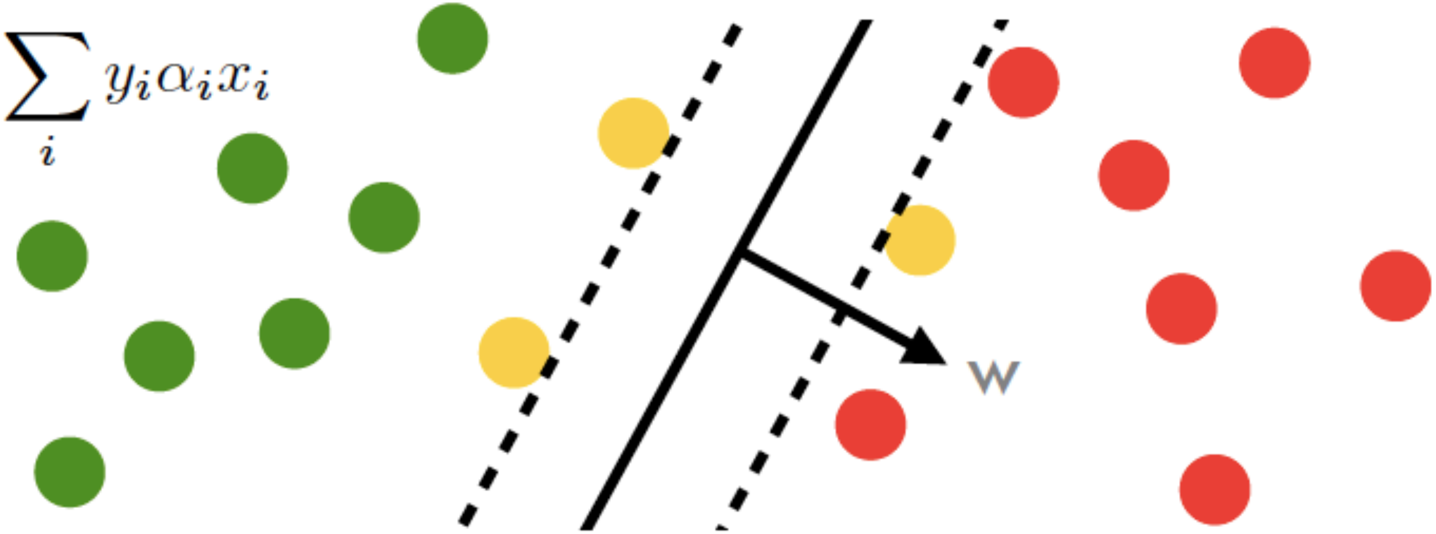
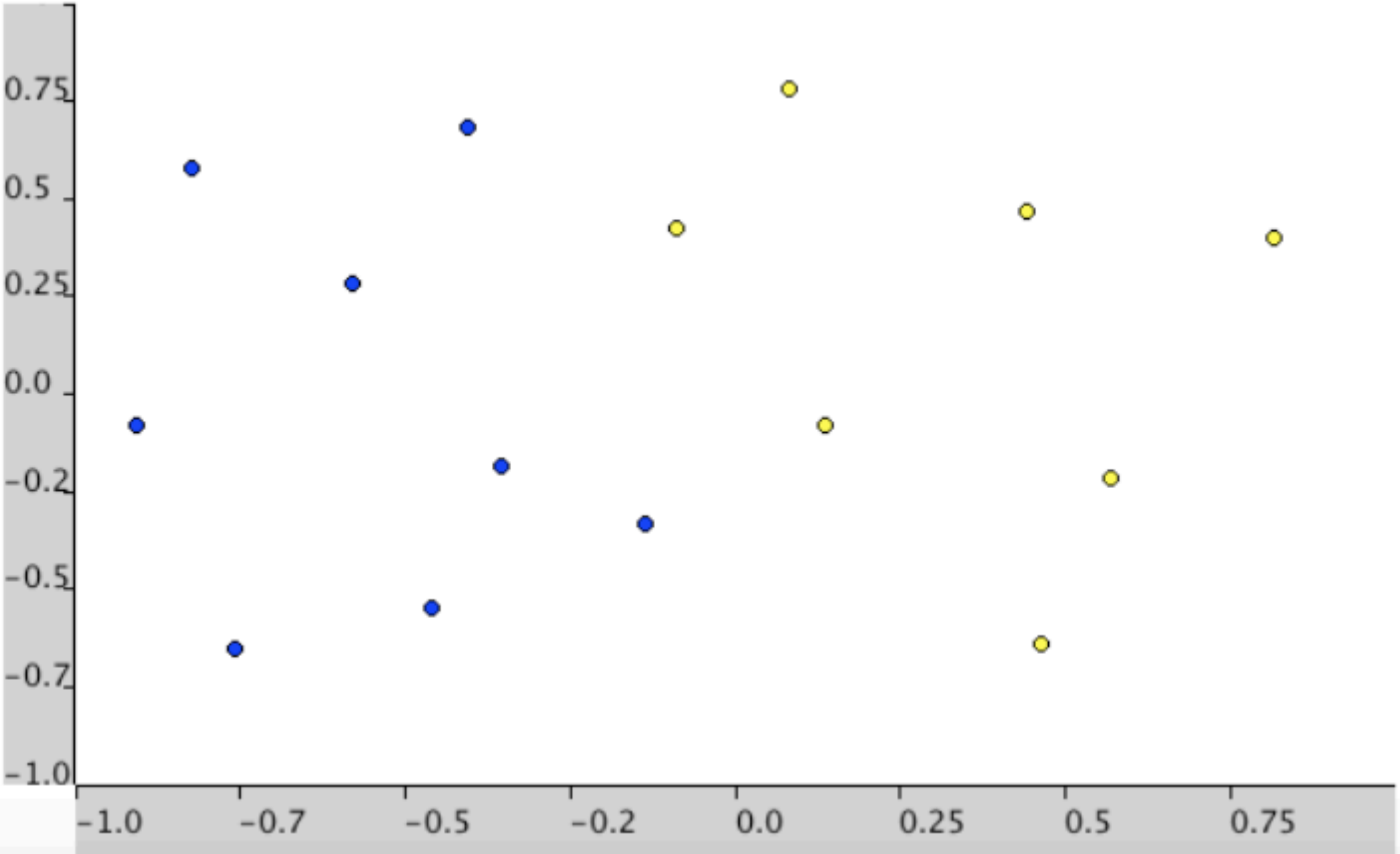


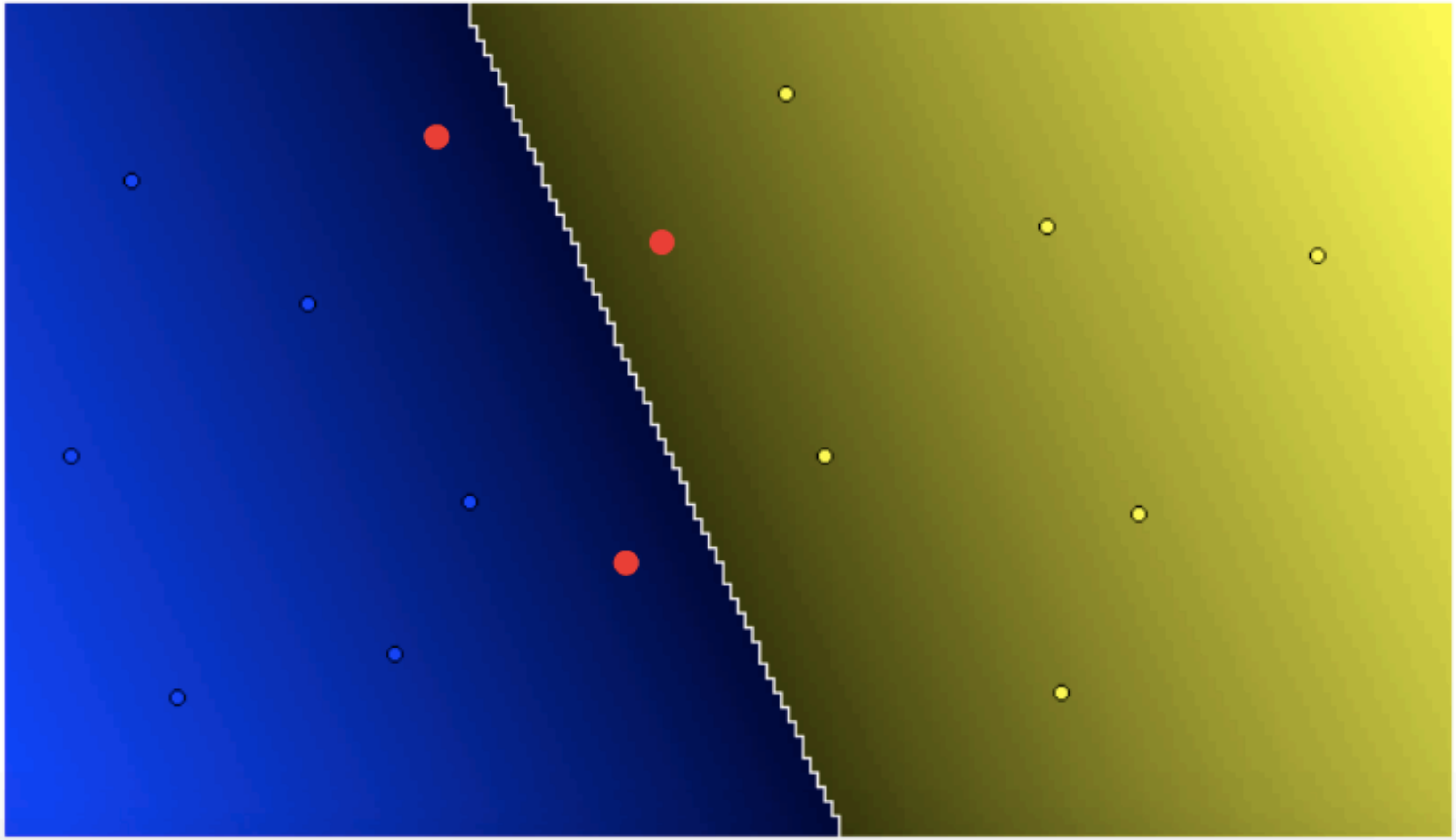
- Weight vector w as weighted linear combination of instances
- Only points on margin matter (ignore the rest and get same solution)
- Only inner products matter
  - Quadratic program
  - We can replace the inner product by a kernel
- Keeps instances away from the margin

Example

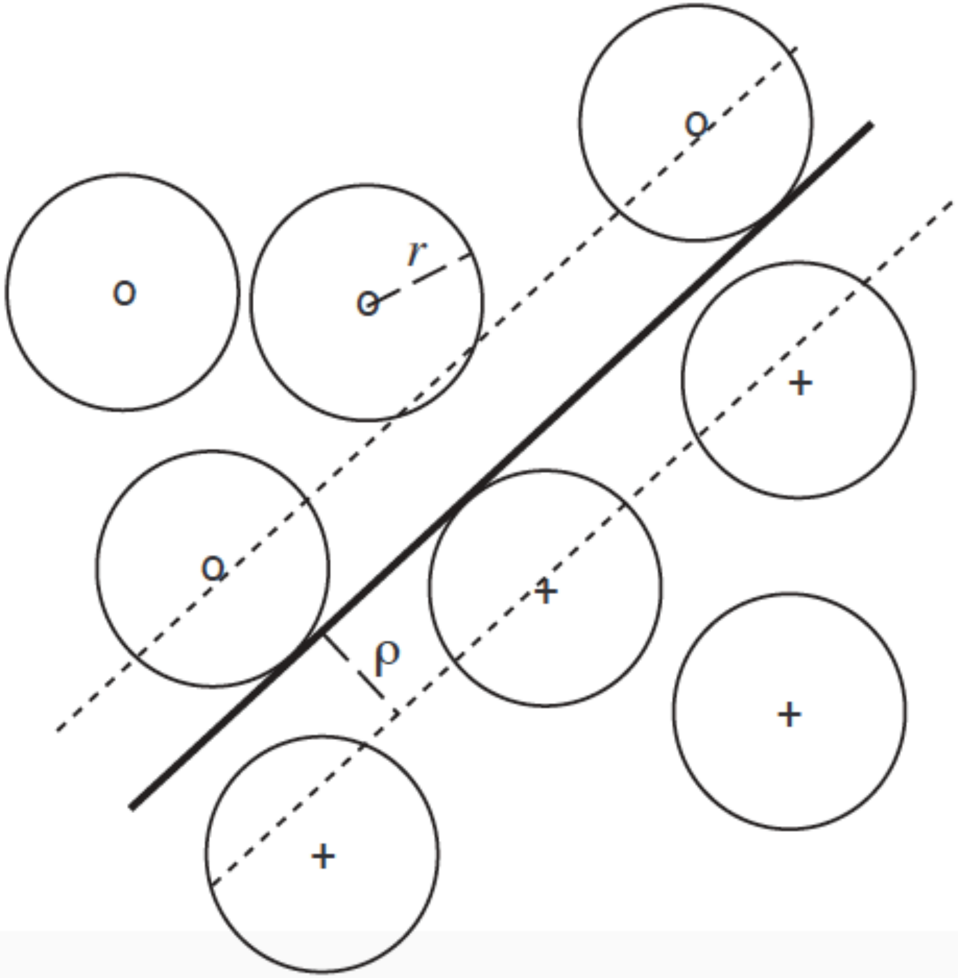


Example

Number of Support Vectors: **3** (-ve: 2, +ve: 1) Total number of points: 15



Why large margins?



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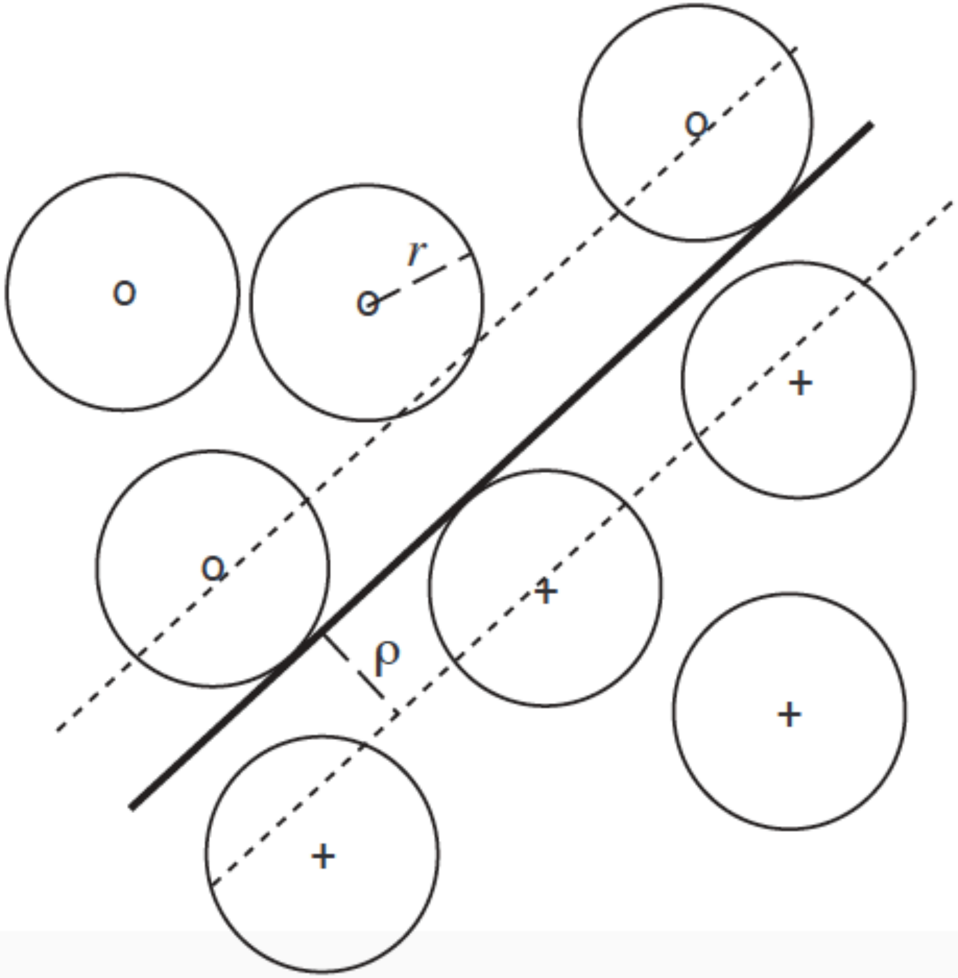
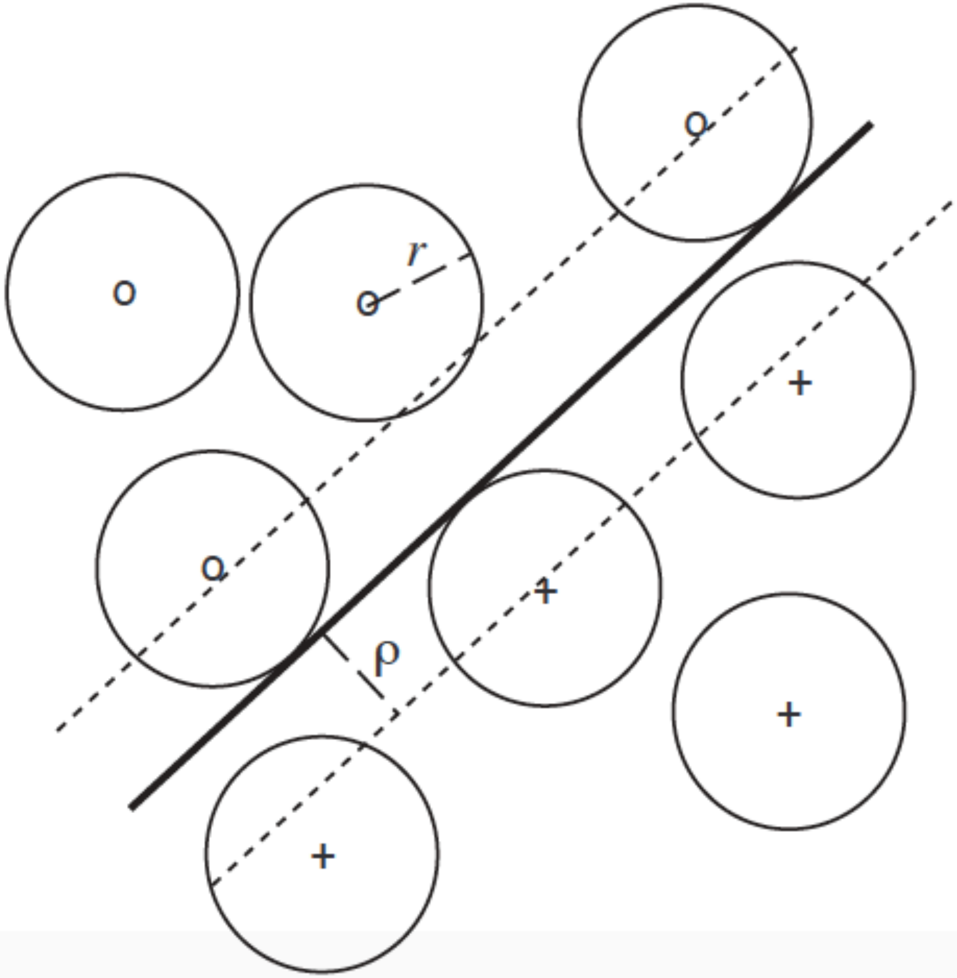


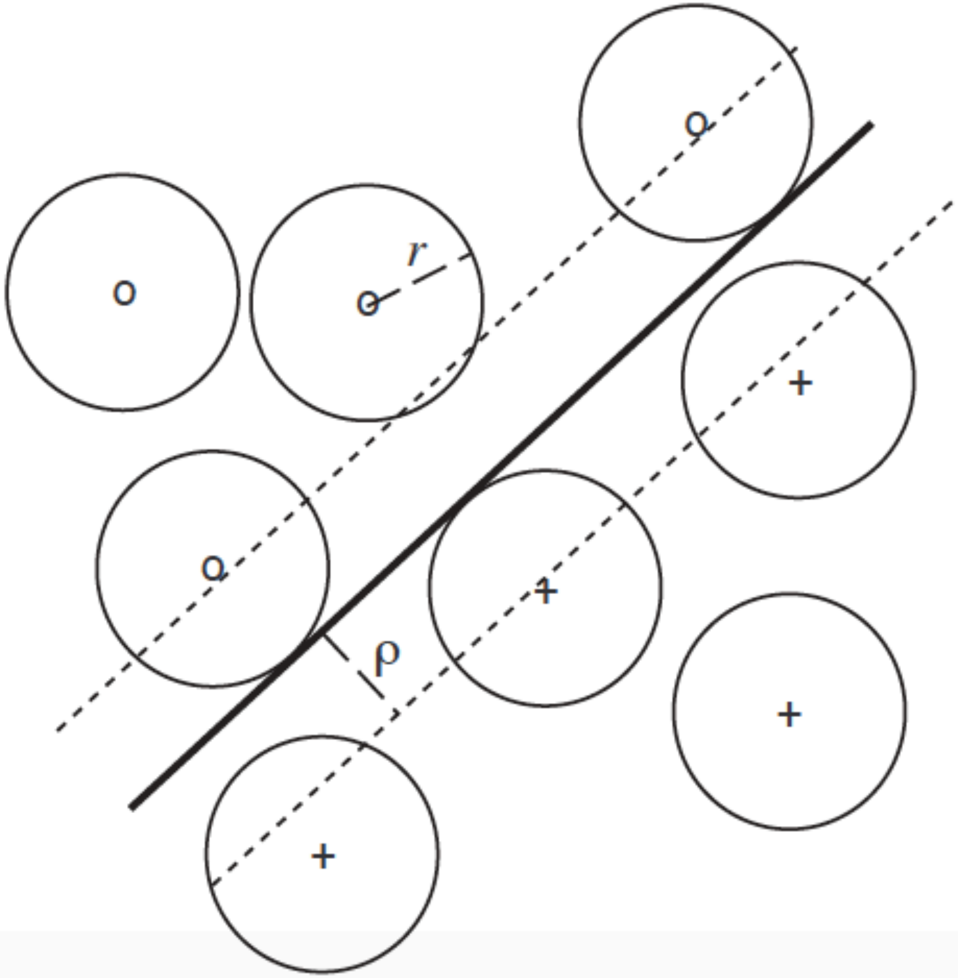
- Maximum robustness relative to uncertainty

Why large margins?



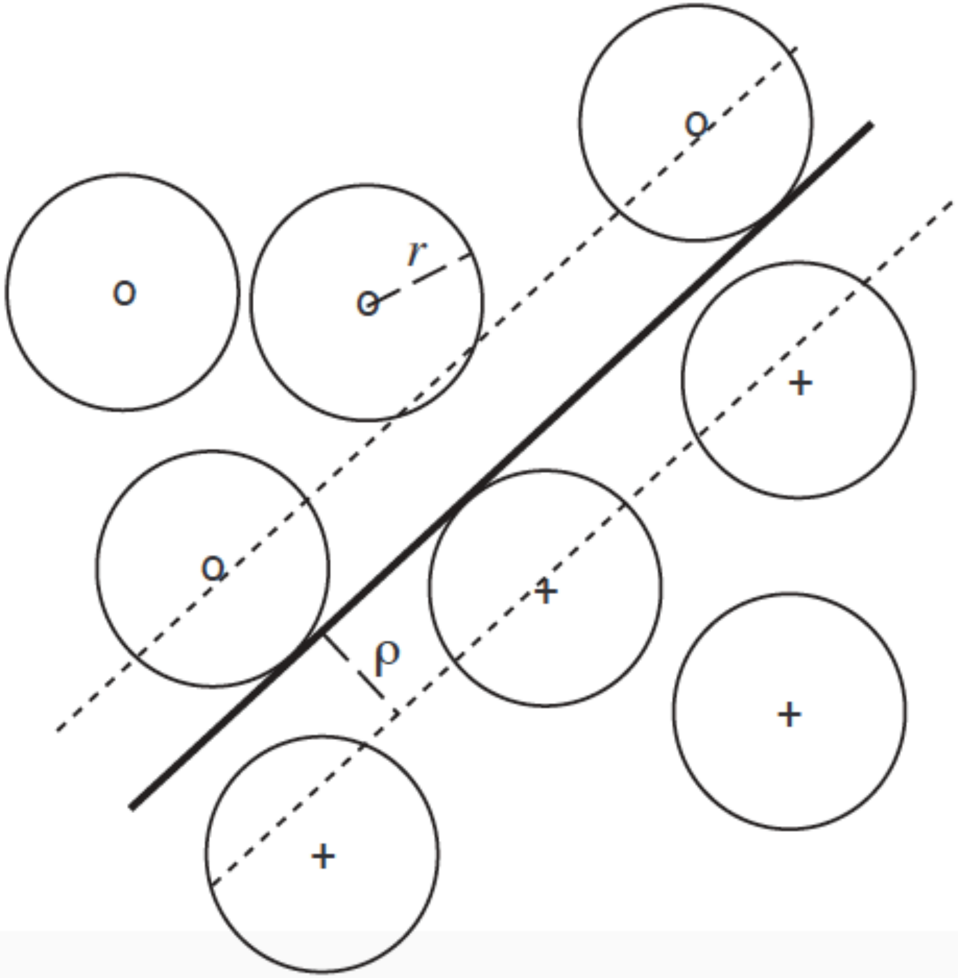
- Maximum robustness relative to uncertainty
- Symmetry breaking

Why large margins?



- Maximum robustness relative to uncertainty
- Symmetry breaking
- Independent of correctly classified instances

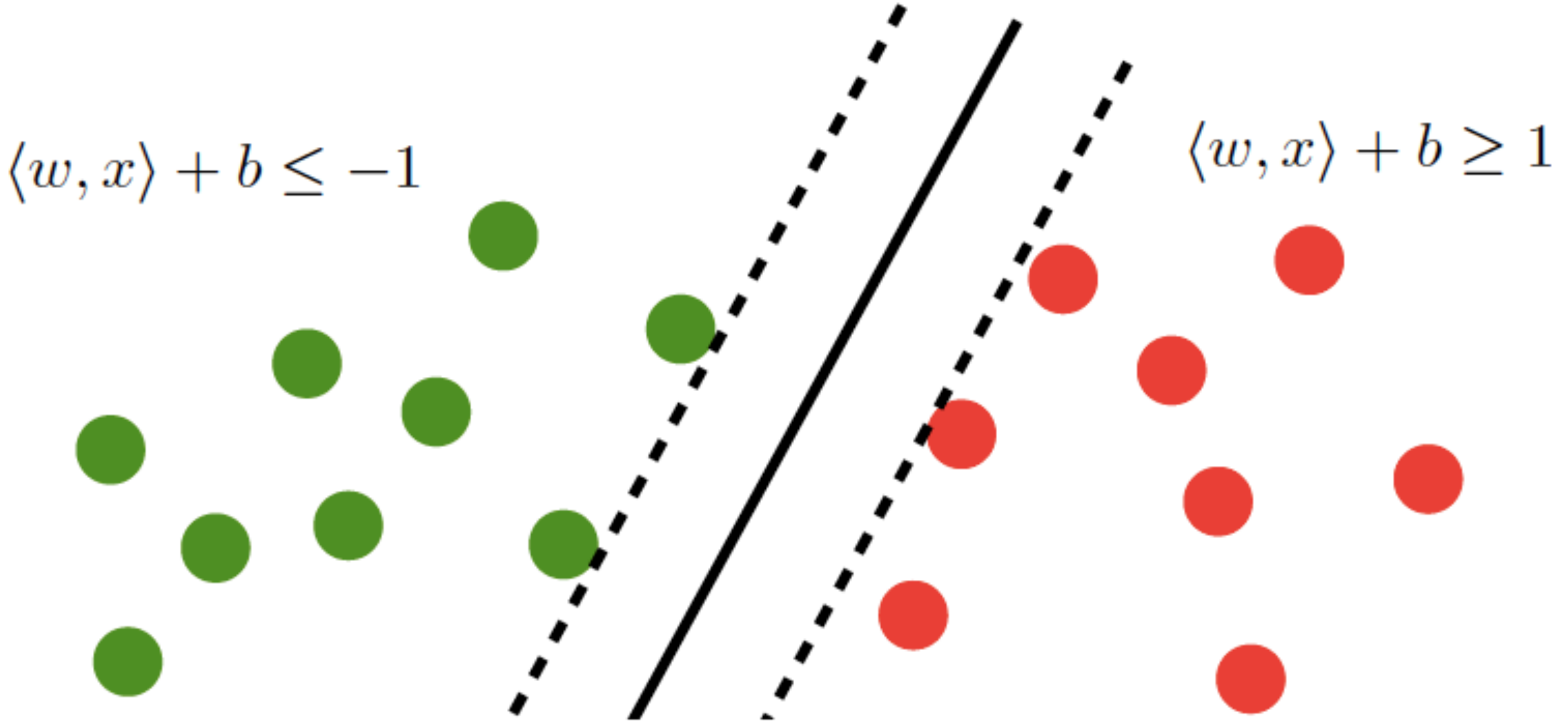
Why large margins?



- Maximum robustness relative to uncertainty
- Symmetry breaking
- Independent of correctly classified instances
- Easy to find for easy problems

Soft Margin Classifiers

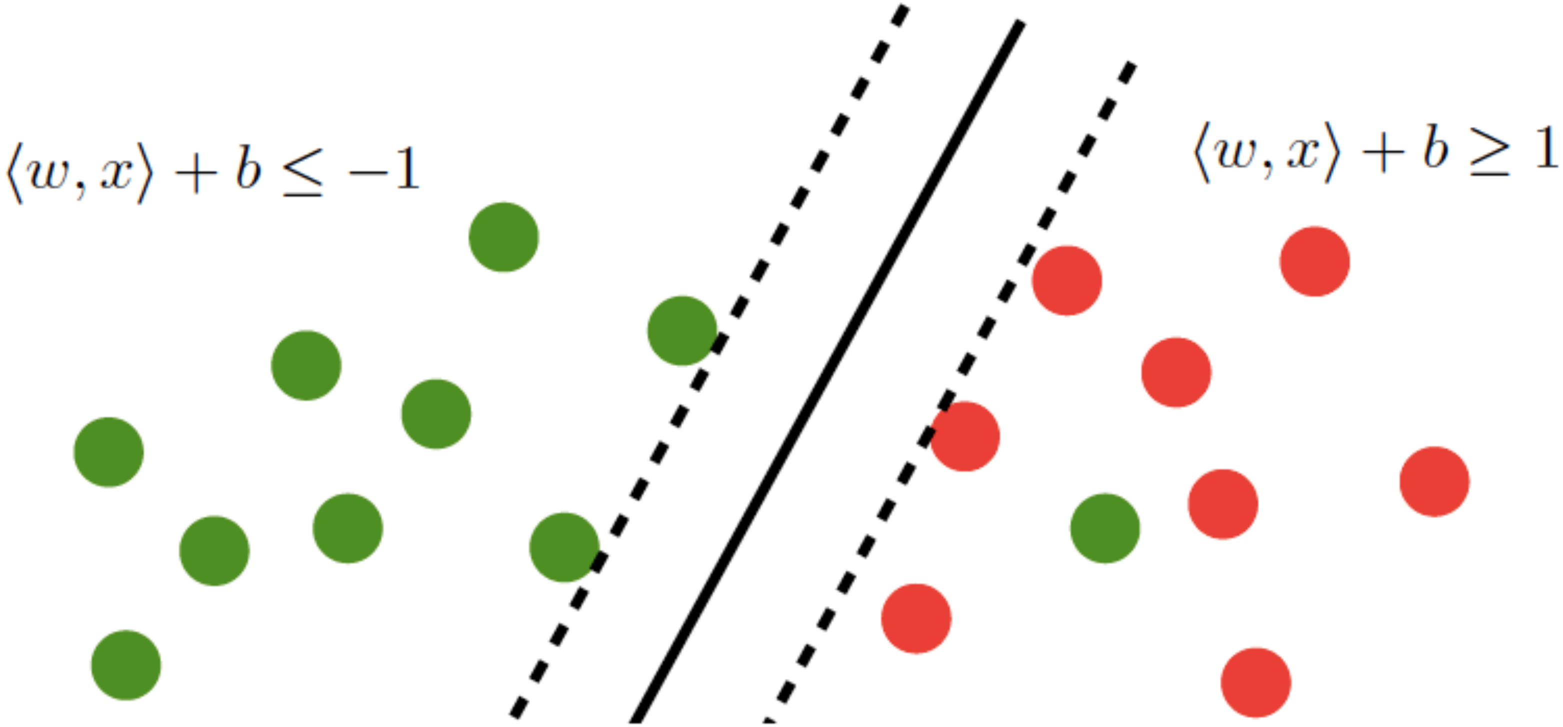
Large Margin Classifier



linear function

$$f(x) = \langle w, x\rangle + b$$

Large Margin Classifier



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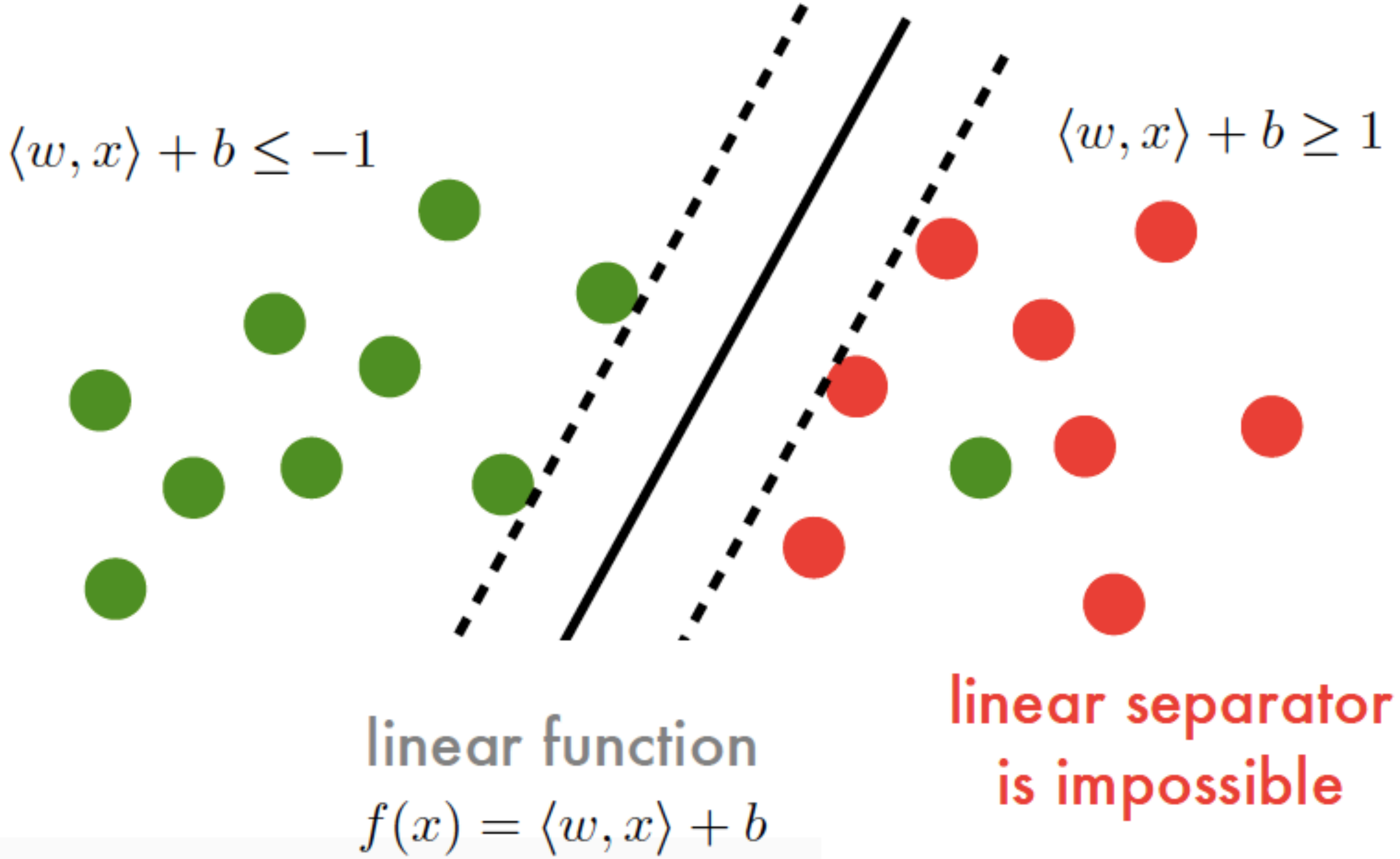
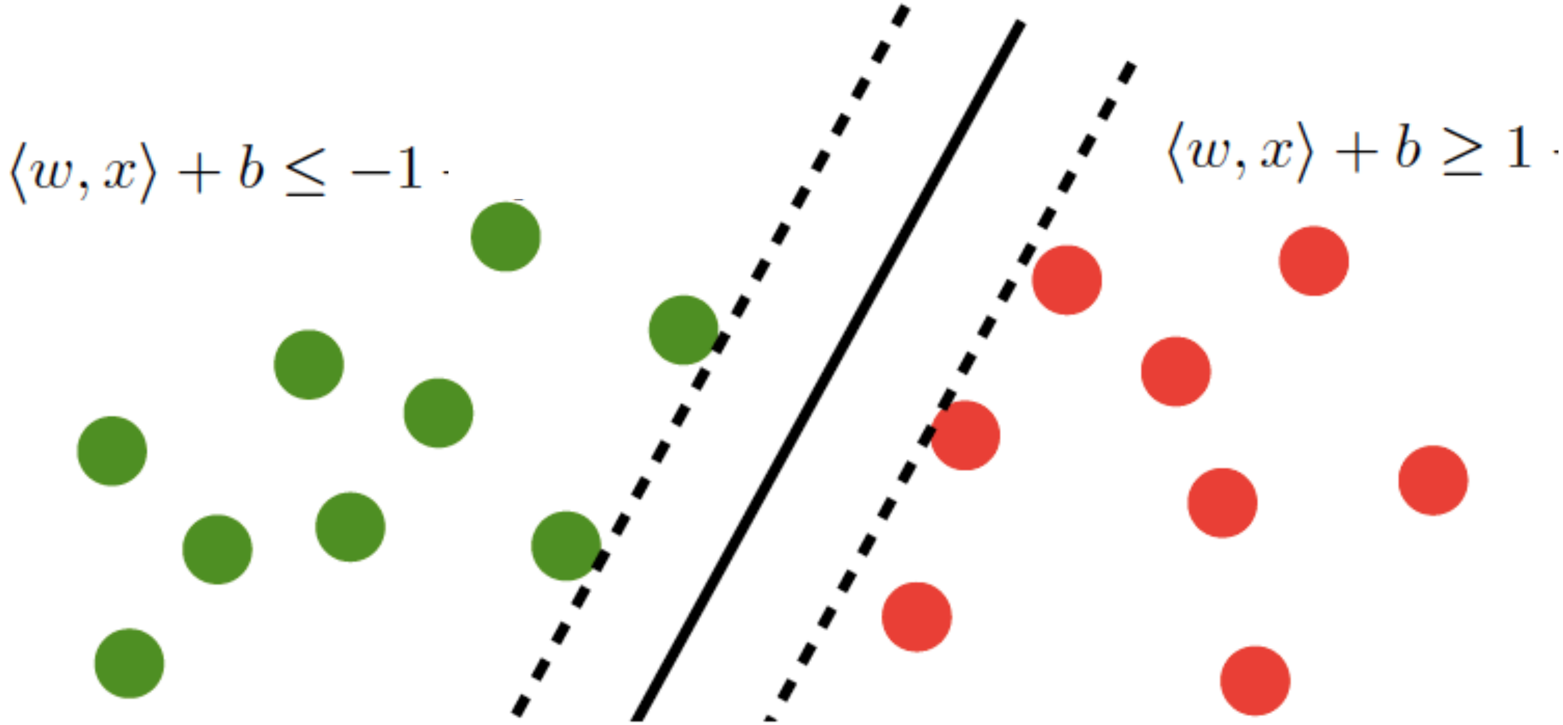
Large Margin Classifier



Adding slack variables



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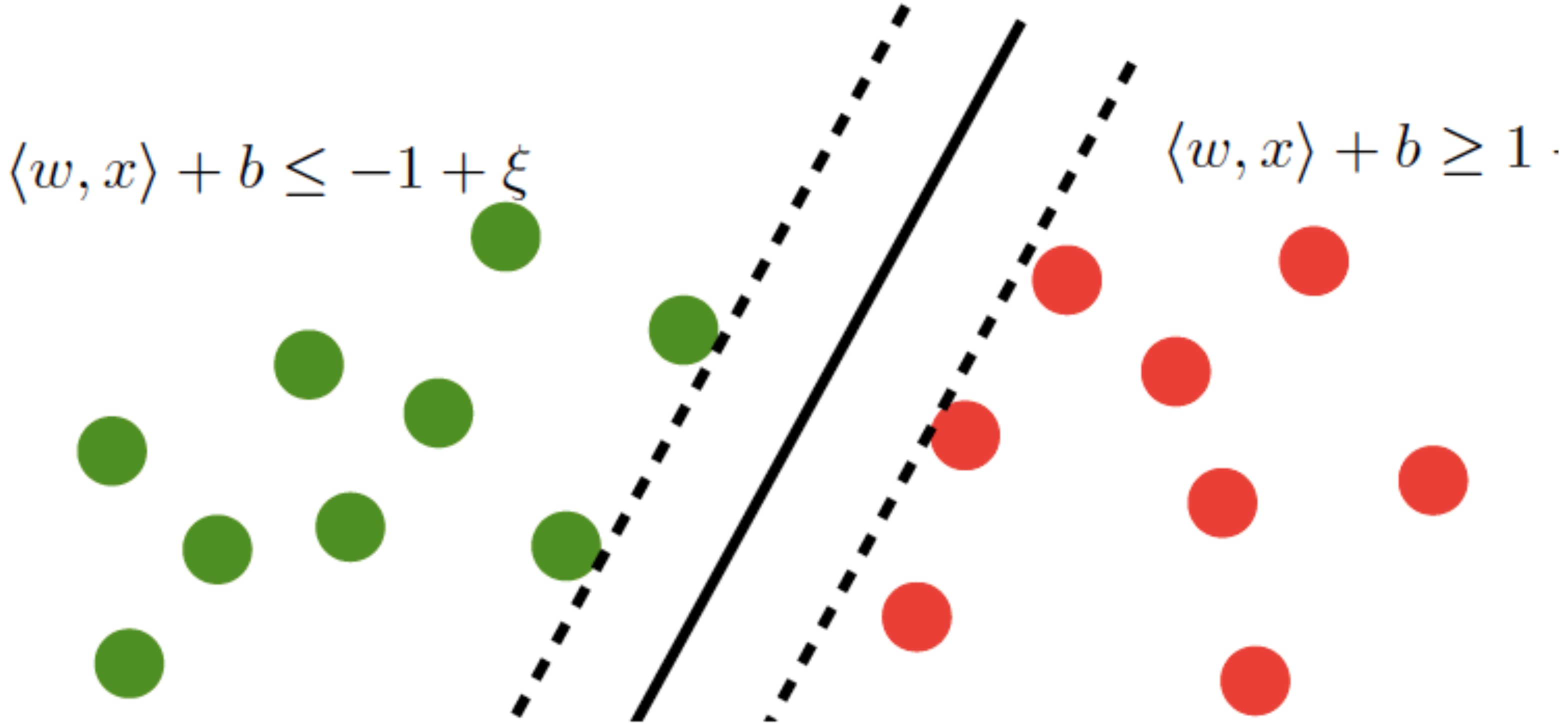

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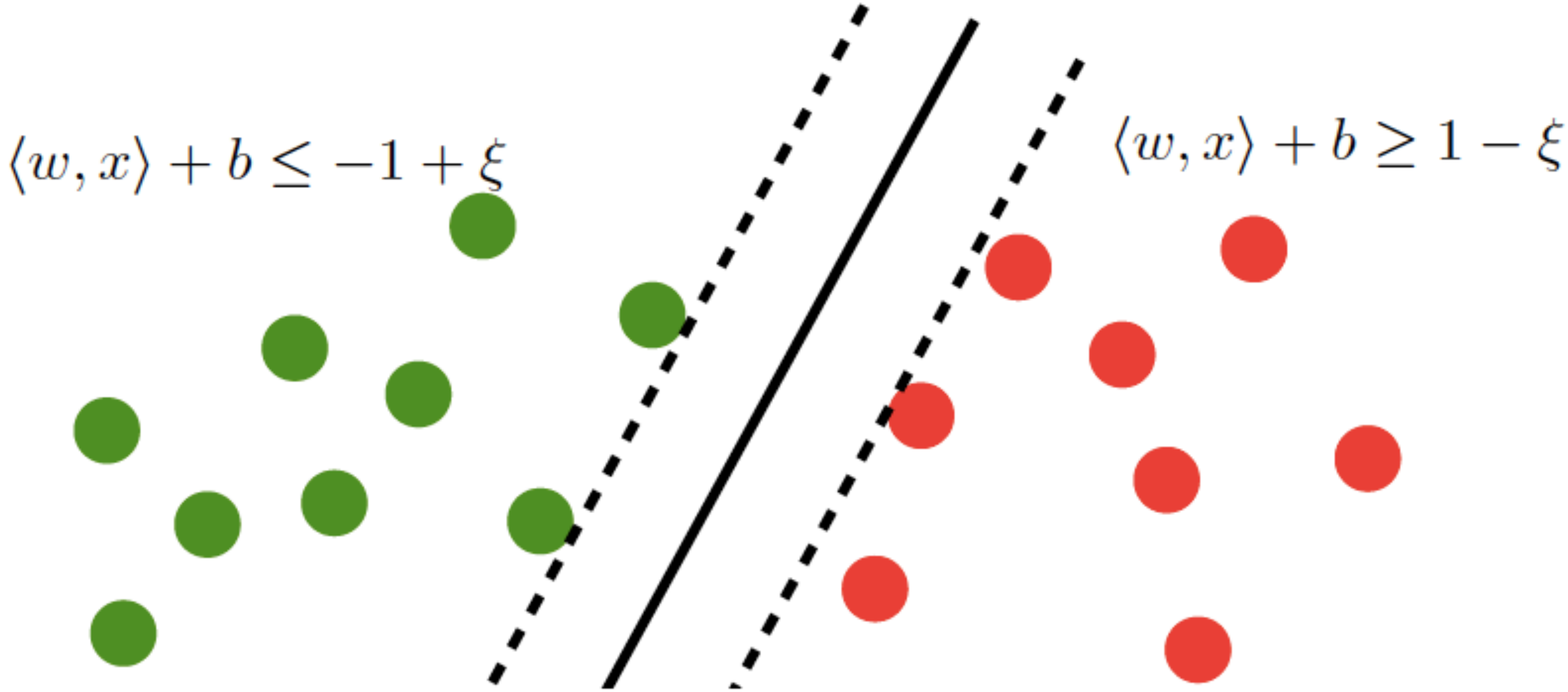

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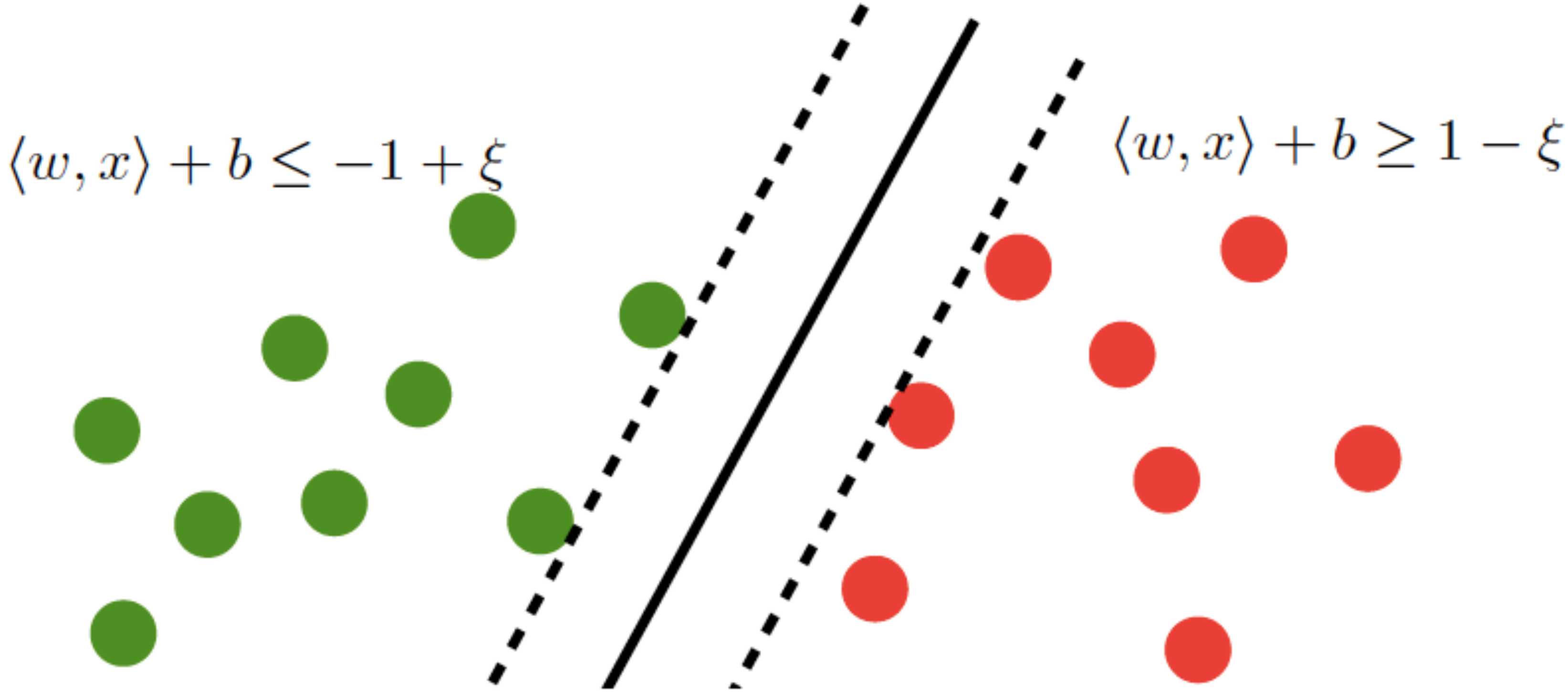
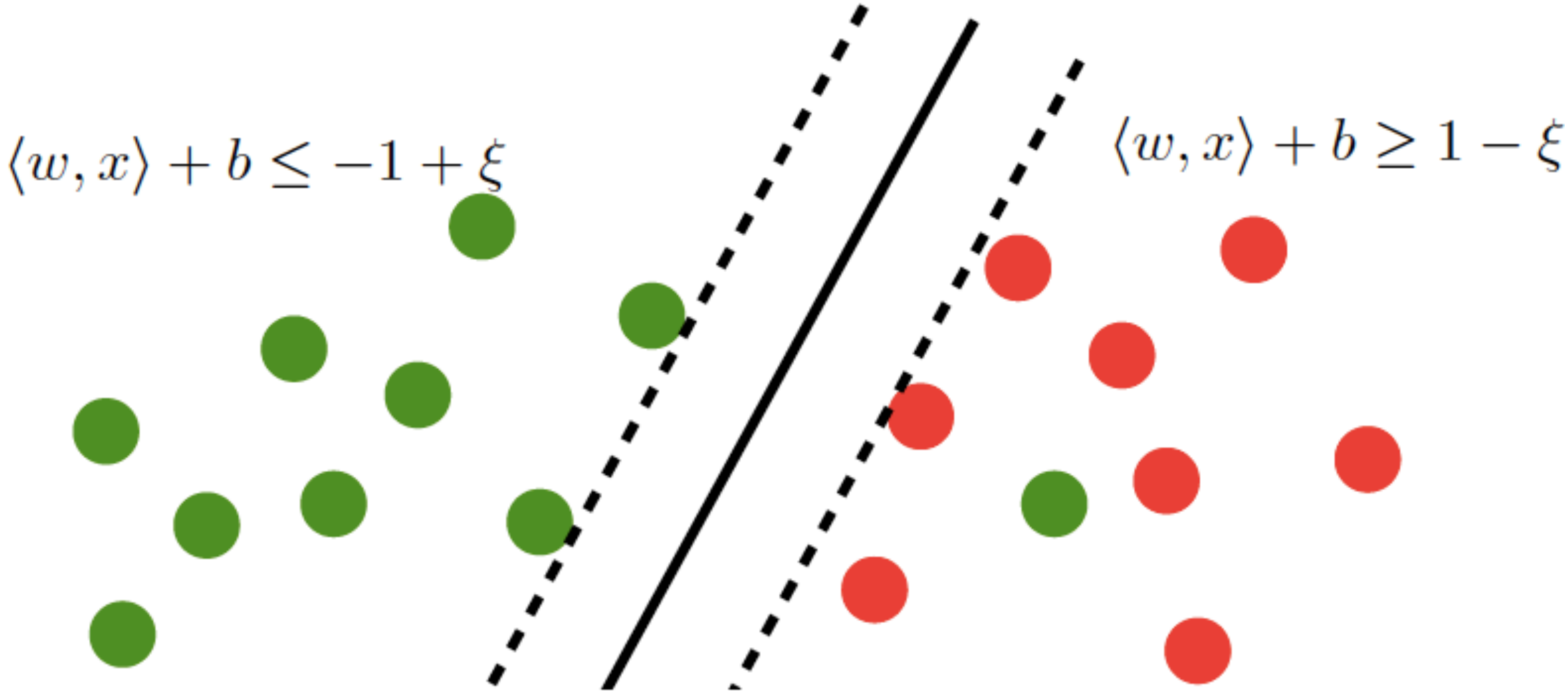


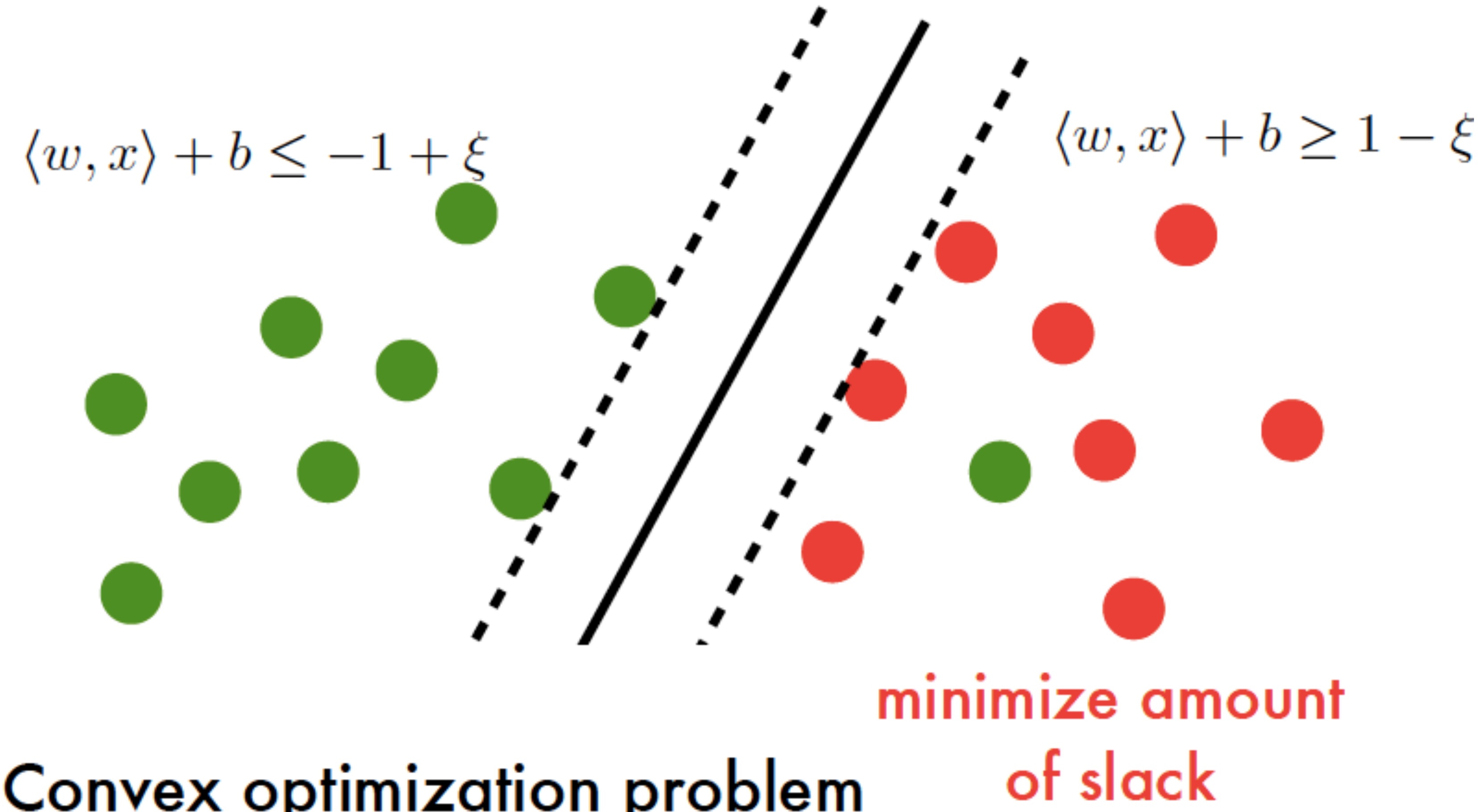
Convex optimization problem

Adding slack variables



Convex optimization problem

Adding slack variables



Convex optimization problem

Adding slack variables

Adding slack variables

- **Hard margin problem**

$$\underset{w,b}{\text{minimize}}\ \frac{1}{2}\|w\|^2 \ \text{ subject to } y_i\left[\langle w, x_i\rangle + b\right] \geq 1$$

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- With slack variables

$$\underset{w,b}{\text{minimize}}\ \frac{1}{2}\|w\|^2 + C\sum_i \xi_i$$

$$\text{subject to } y_i\left[\langle w, x_i\rangle + b\right] \geq 1 - \xi_i \text{ and } \xi_i \geq 0$$

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Problem is always feasible.

Dual Problem

Dual Problem

- Primal optimization problem

$$\underset{w,b}{\text{minimize}} \ \frac{1}{2}\|w\|^2 + C\sum_i \xi_i$$

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Dual Problem

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$$\text{subject to } y_i\left[\langle w, x_i\rangle + b\right] \geq 1 - \xi_i \text{ and } \xi_i \geq 0$$

- **Lagrange function**

$$L(w,b,\alpha) = \frac{1}{2}\|w\|^2 + C\sum_i \xi_i - \sum_i \alpha_i\left[y_i\left[\langle x_i, w\rangle + b\right] + \xi_i - 1\right] - \sum_i \eta_i\xi_i$$

Dual Problem

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Optimality in w,b,ξ is at saddle point with α,η

- Derivatives in w,b,ξ need to vanish

Dual Problem

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$$L(w, b, \alpha) = \frac{1}{2}\|w\|^2 + C\sum_i \xi_i - \sum_i \alpha_i \left[y_i \left[\langle x_i, w\rangle + b\right] + \xi_i - 1\right] - \sum_i \eta_i \xi_i$$

Dual Problem

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- **Derivatives in w, b need to vanish**

$$\partial_w L(w,b,\xi,\alpha,\eta) = w - \sum_i \alpha_i y_i x_i = 0$$

$$\partial_b L(w,b,\xi,\alpha,\eta) = \sum_i \alpha_i y_i = 0$$

$$\partial_{\xi_i} L(w,b,\xi,\alpha,\eta) = C - \alpha_i - \eta_i = 0$$

Dual Problem

- Lagrange function

$$L(w, b, \alpha) = \frac{1}{2}\|w\|^2 + C\sum_i \xi_i - \sum_i \alpha_i \left[y_i \left[\langle x_i, w\rangle + b\right] + \xi_i - 1\right] - \sum_i \eta_i \xi_i$$

- Derivatives in w, b need to vanish

$$\partial_w L(w, b, \xi, \alpha, \eta) = w - \sum_i \alpha_i y_i x_i = 0$$

$$\partial_b L(w, b, \xi, \alpha, \eta) = \sum_i \alpha_i y_i = 0$$

$$\partial_{\xi_i} L(w, b, \xi, \alpha, \eta) = C - \alpha_i - \eta_i = 0$$

- Plugging terms back into L yields

$$\underset{\alpha}{\text{maximize}} - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j \langle x_i, x_j\rangle + \sum_i \alpha_i$$

$$\text{subject to } \sum_i \alpha_i y_i = 0 \text{ and } \alpha_i \in [0, C]$$

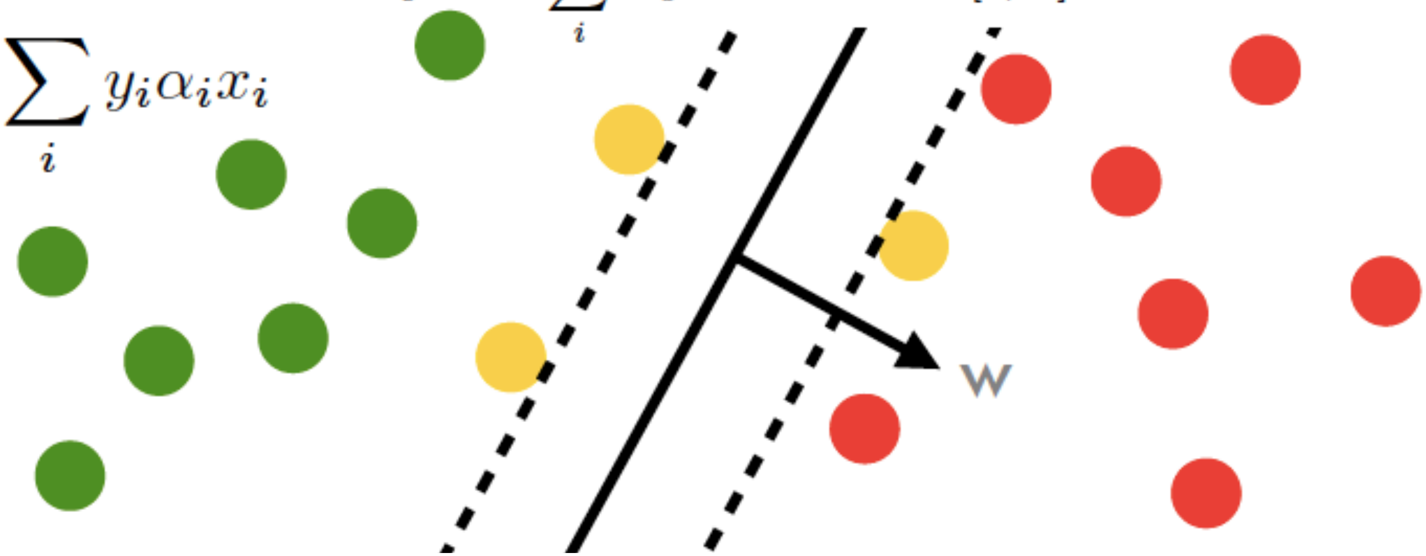
bound influence

Karush Kuhn Tucker Conditions

$$\underset{\alpha}{\text{maximize}} - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle + \sum_i \alpha_i$$

$$\text{subject to } \sum_i \alpha_i y_i = 0 \text{ and } \alpha_i \in [0, C]$$

$$w = \sum_i y_i \alpha_i x_i$$



Karush Kuhn Tucker Conditions

$$\underset{\alpha}{\text{maximize}} - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle + \sum_i \alpha_i$$

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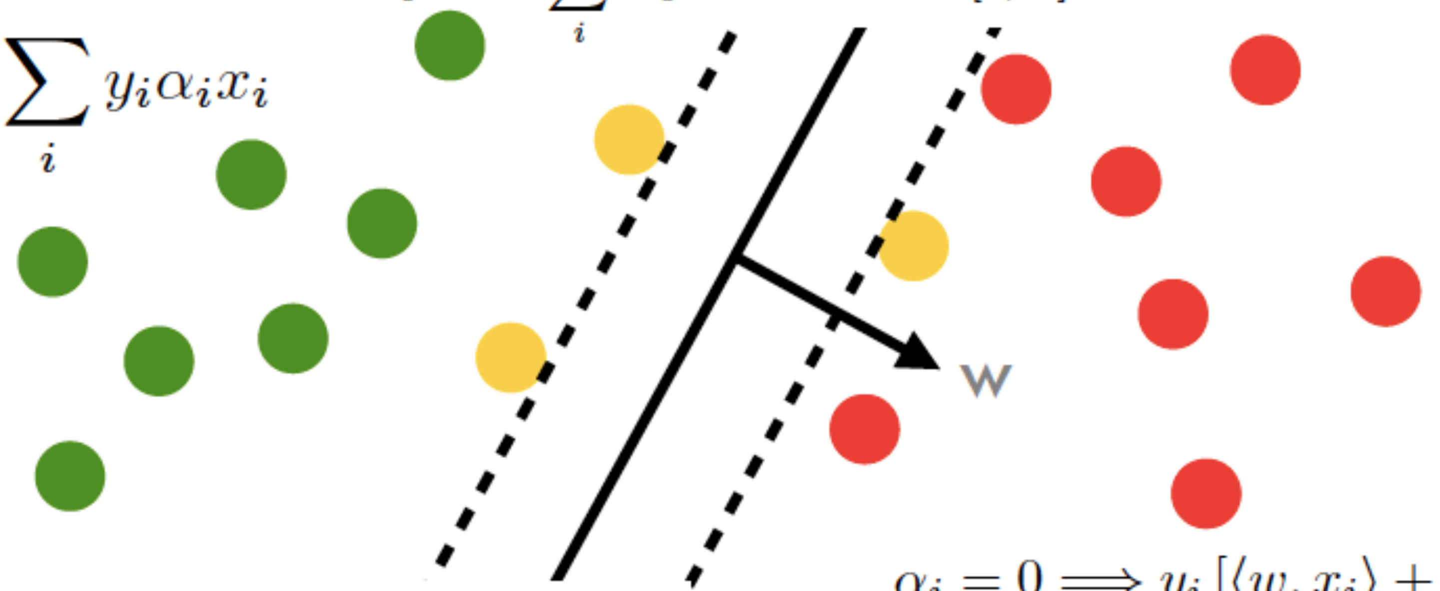

$$\alpha_i = 0 \implies y_i [\langle w, x_i \rangle + b] \geq 1$$

$$\alpha_i [y_i [\langle w, x_i \rangle + b] + \xi_i - 1] = 0$$

$$\eta_i \xi_i = 0$$

$$0 < \alpha_i < C \implies y_i [\langle w, x_i \rangle + b] = 1$$

$$\alpha_i = C \implies y_i [\langle w, x_i \rangle + b] \leq 1$$

That’s all!