Introduction to Machine Learning

5. Support Vector Classification

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10-701

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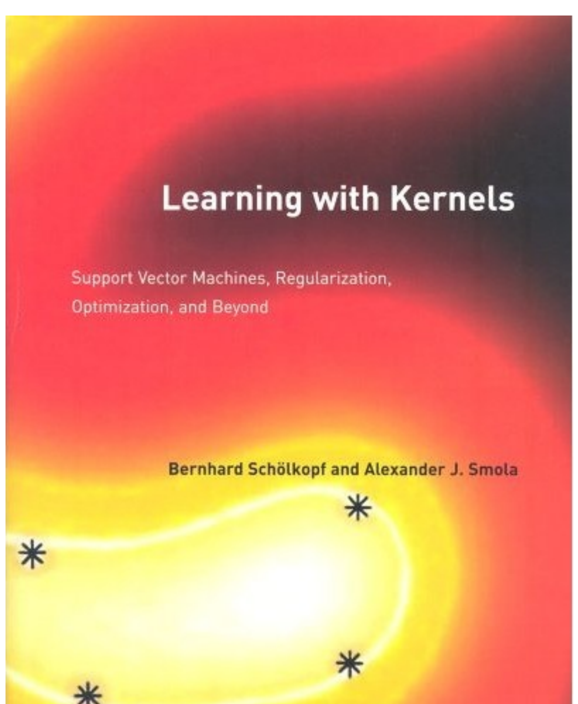
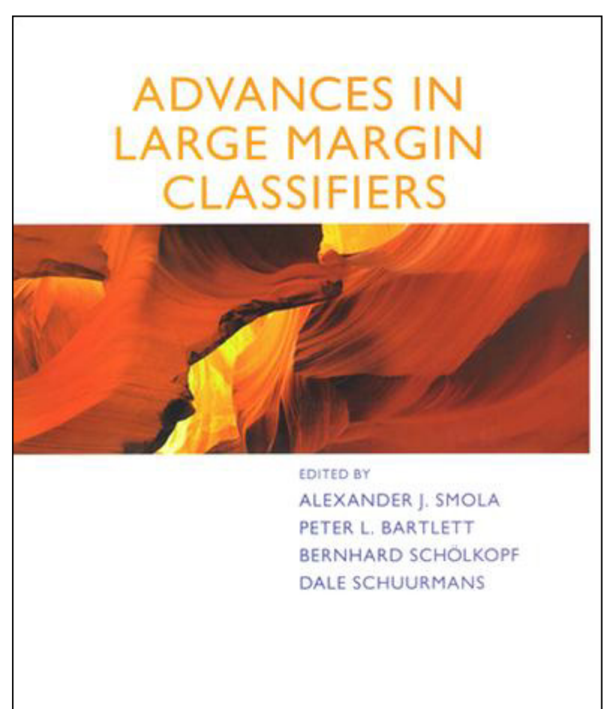
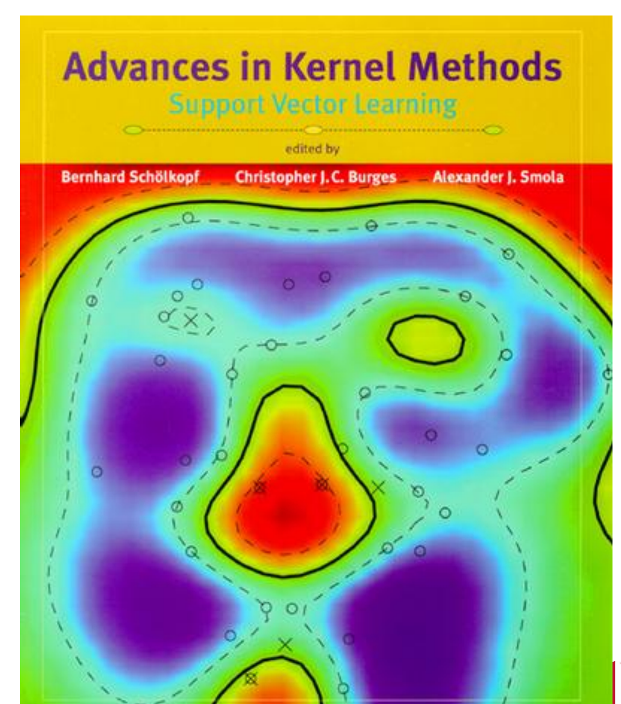
Outline

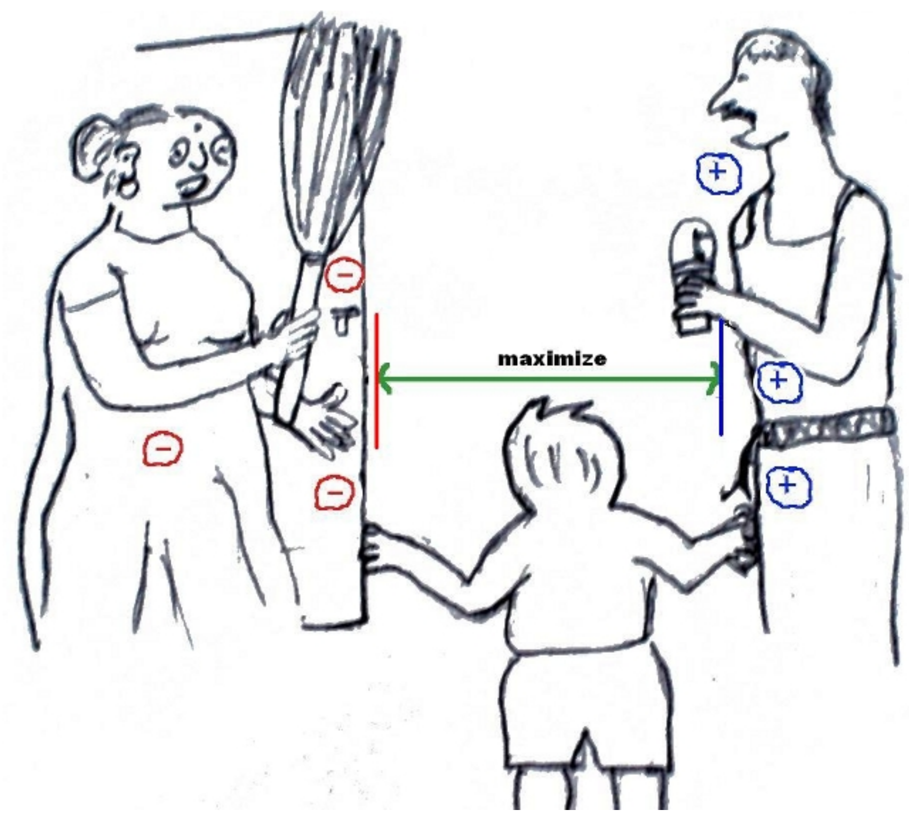
- Support Vector Classification
  Large Margin Separation, optimization problem
- Properties
  Support Vectors, kernel expansion
- Soft margin classifier
  Dual problem, robustness





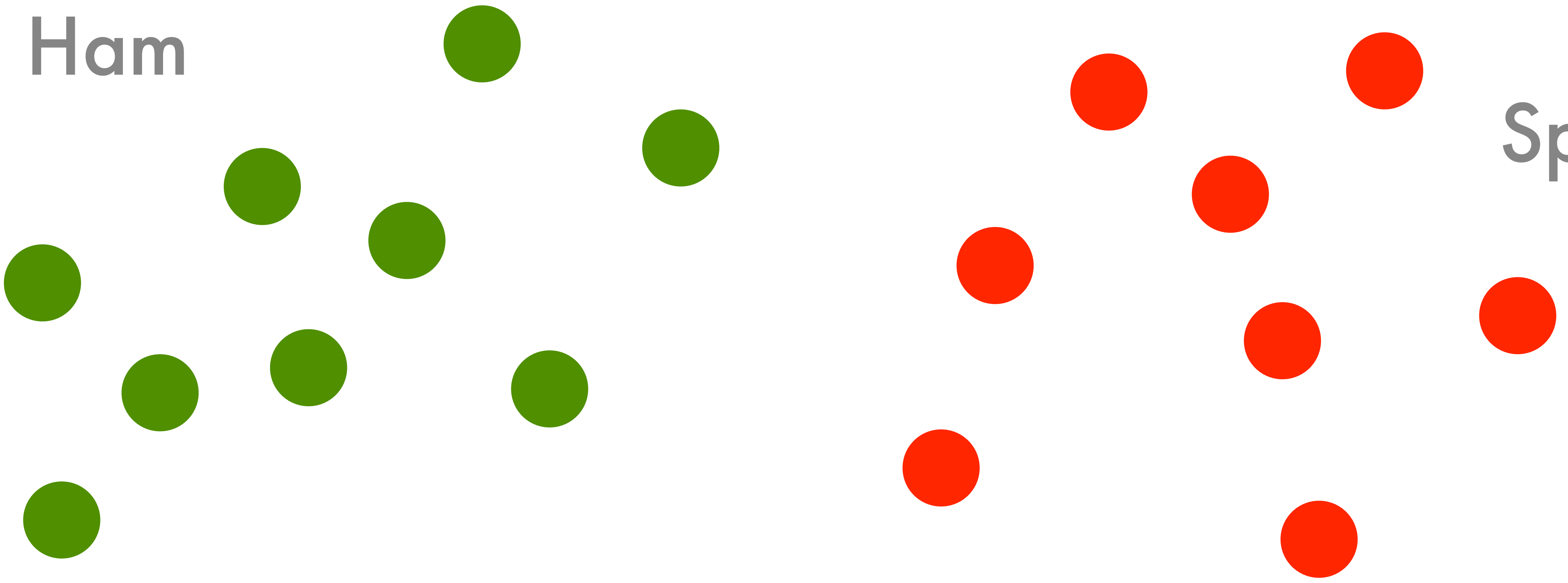


Support Vector Machines

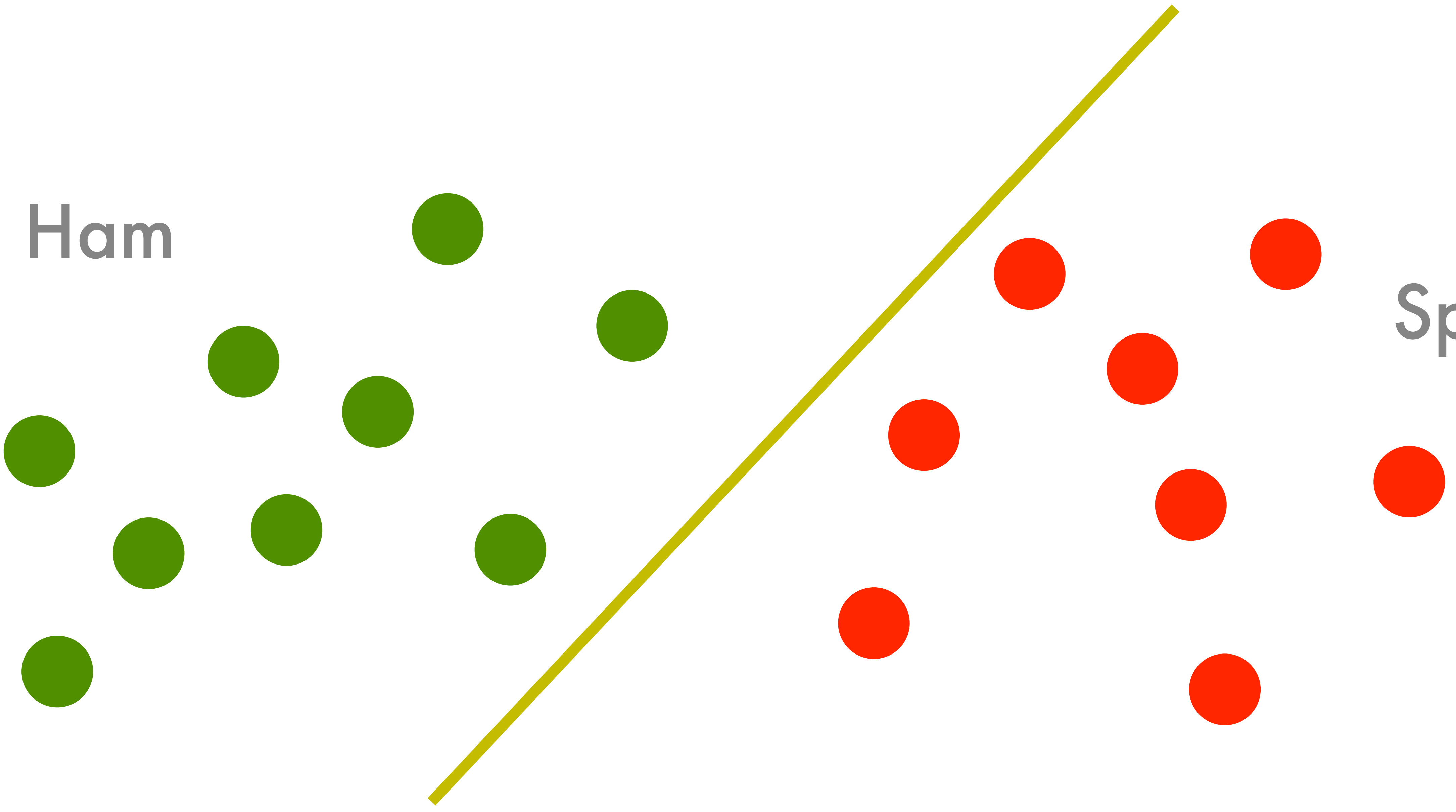


http://maktoons.blogspot.com/2009/03/support-vector-machine.html

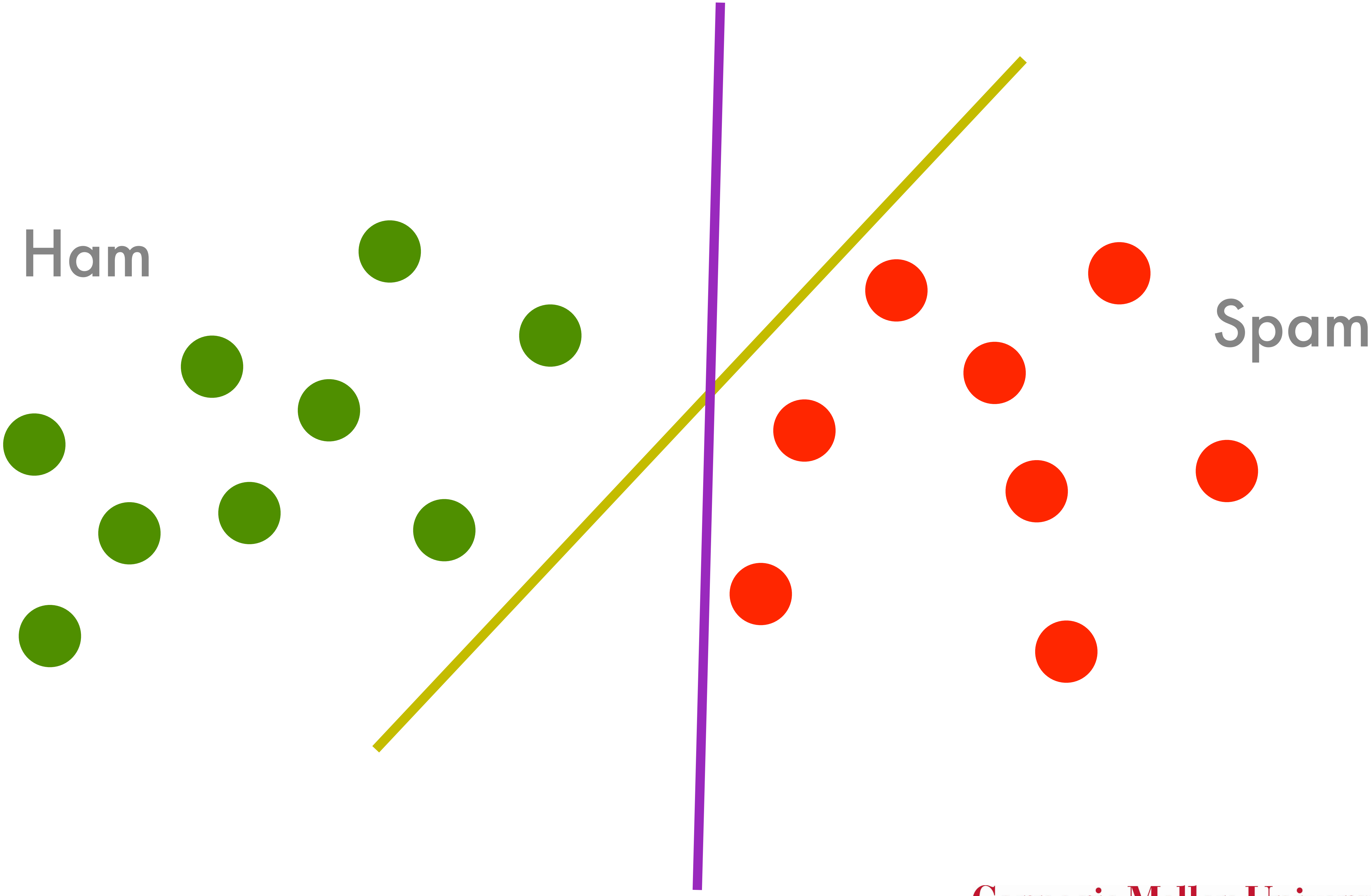
Linear Separator



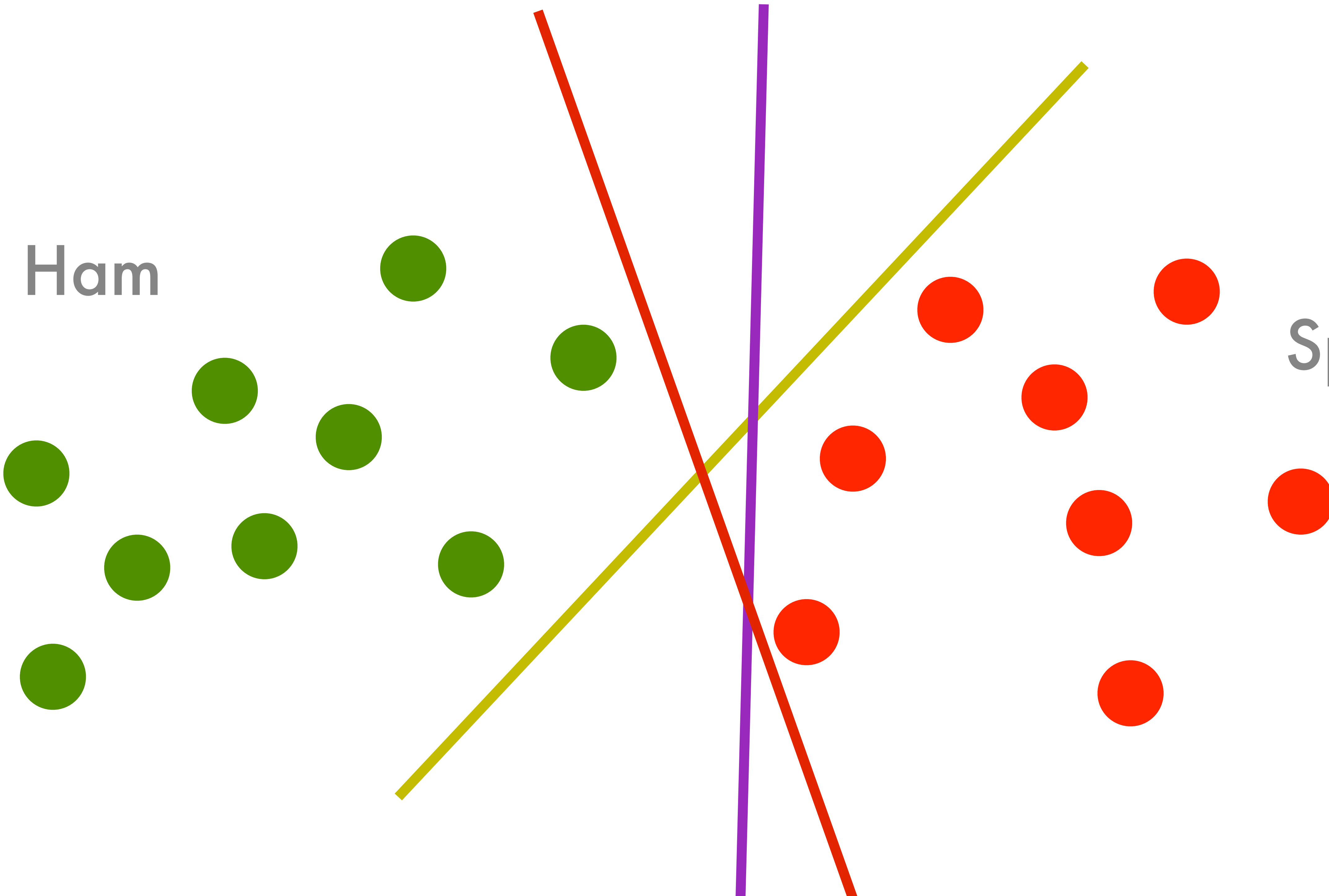
Linear Separator



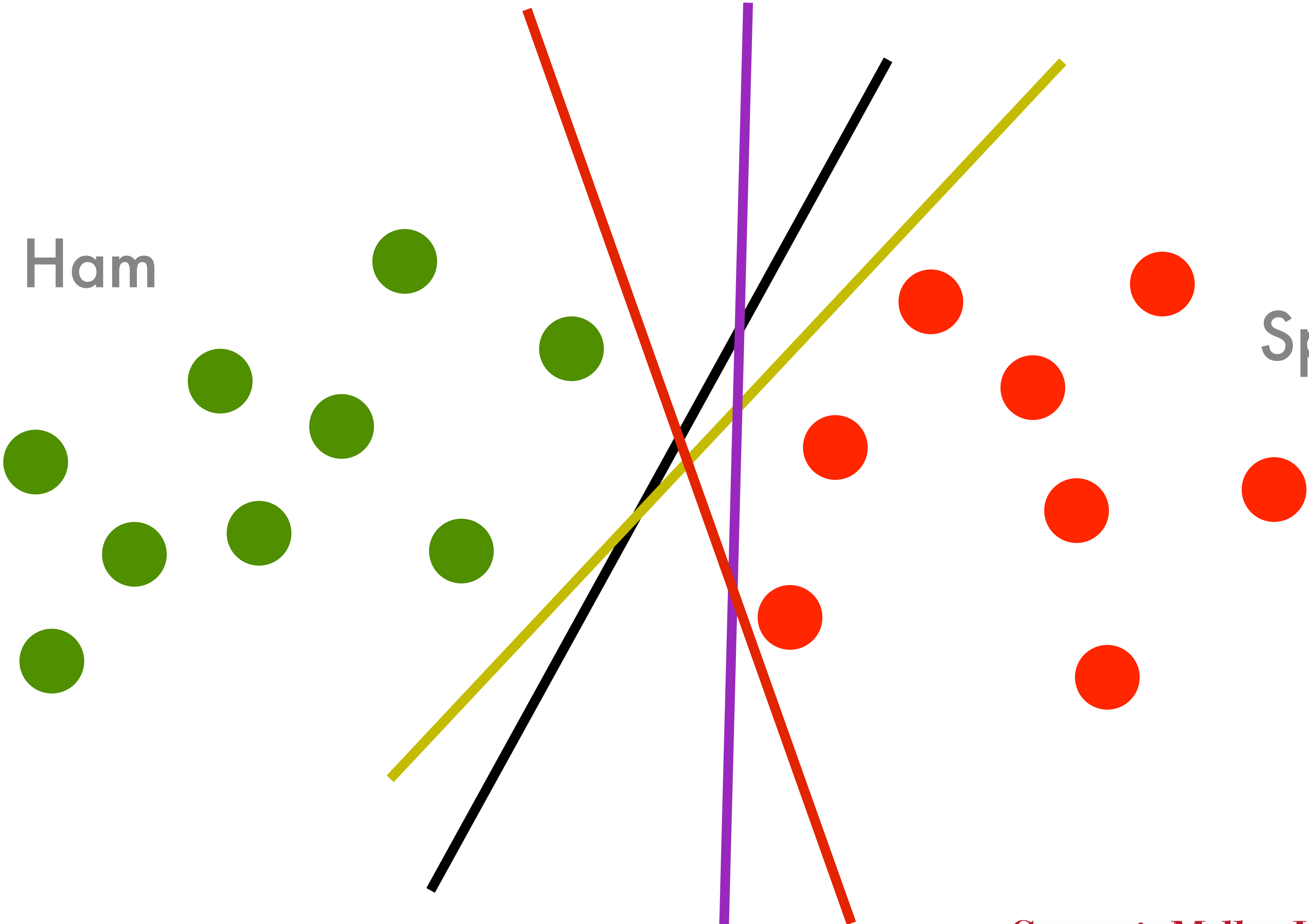
Linear Separator



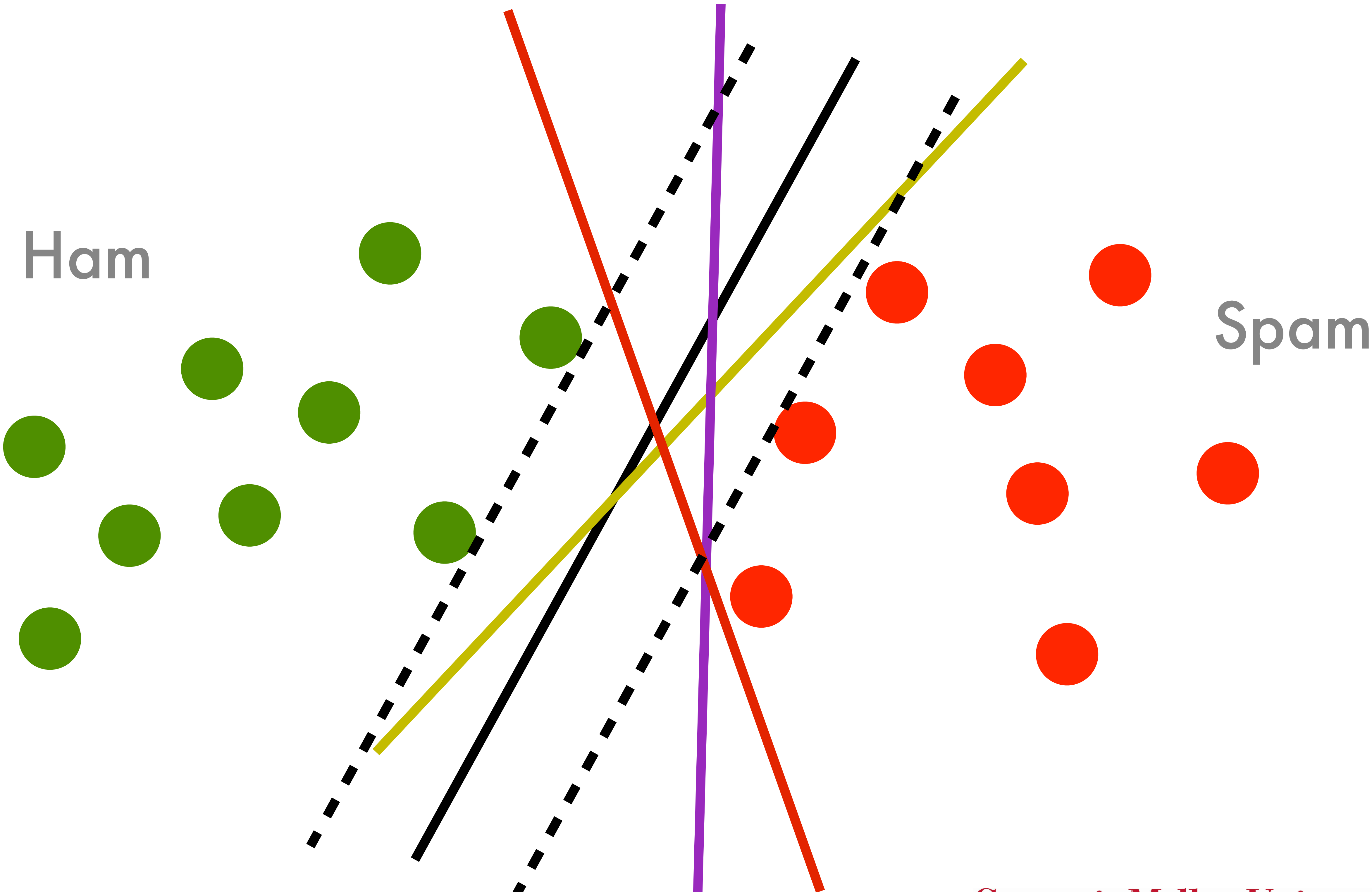
Linear Separator



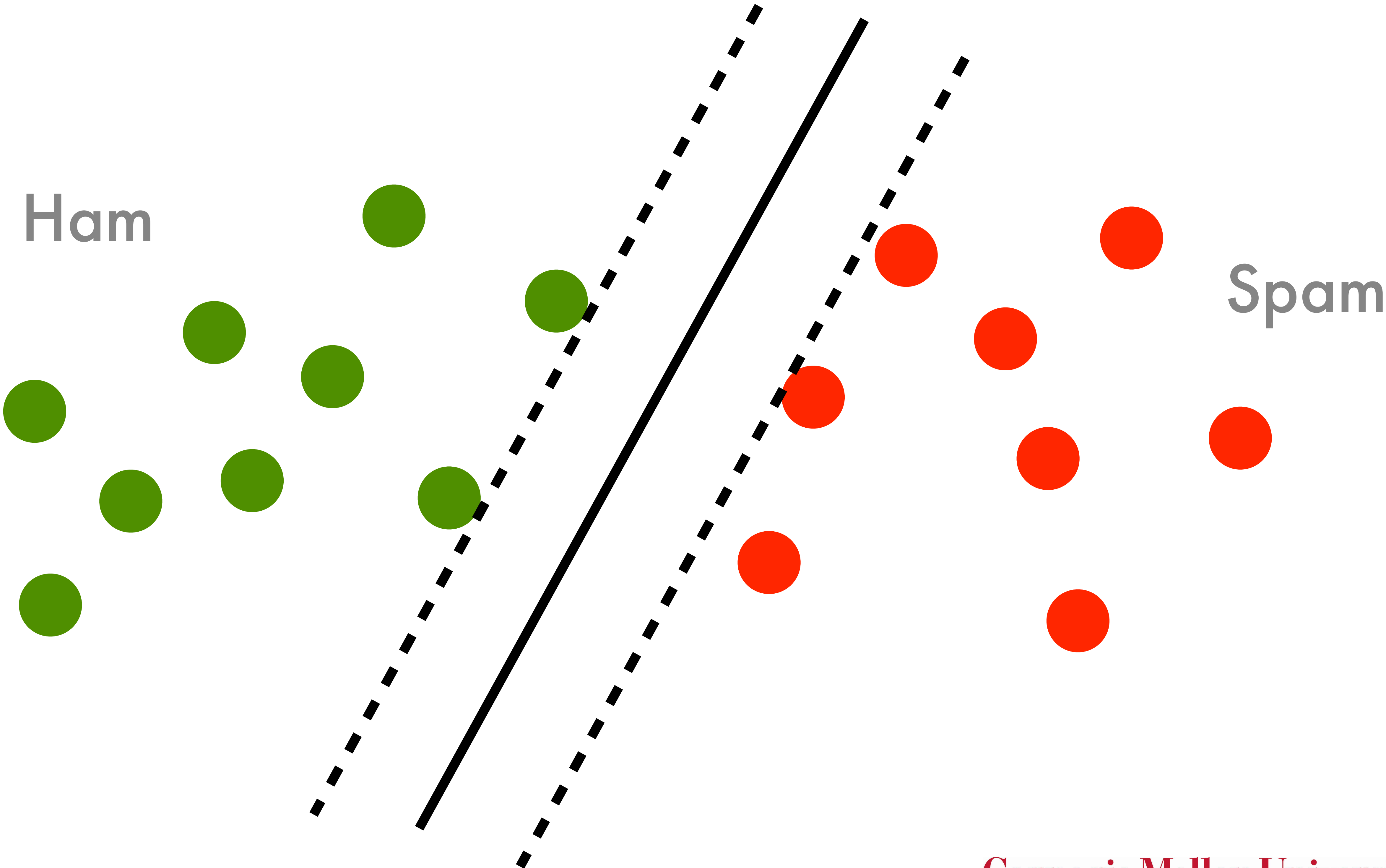
Linear Separator



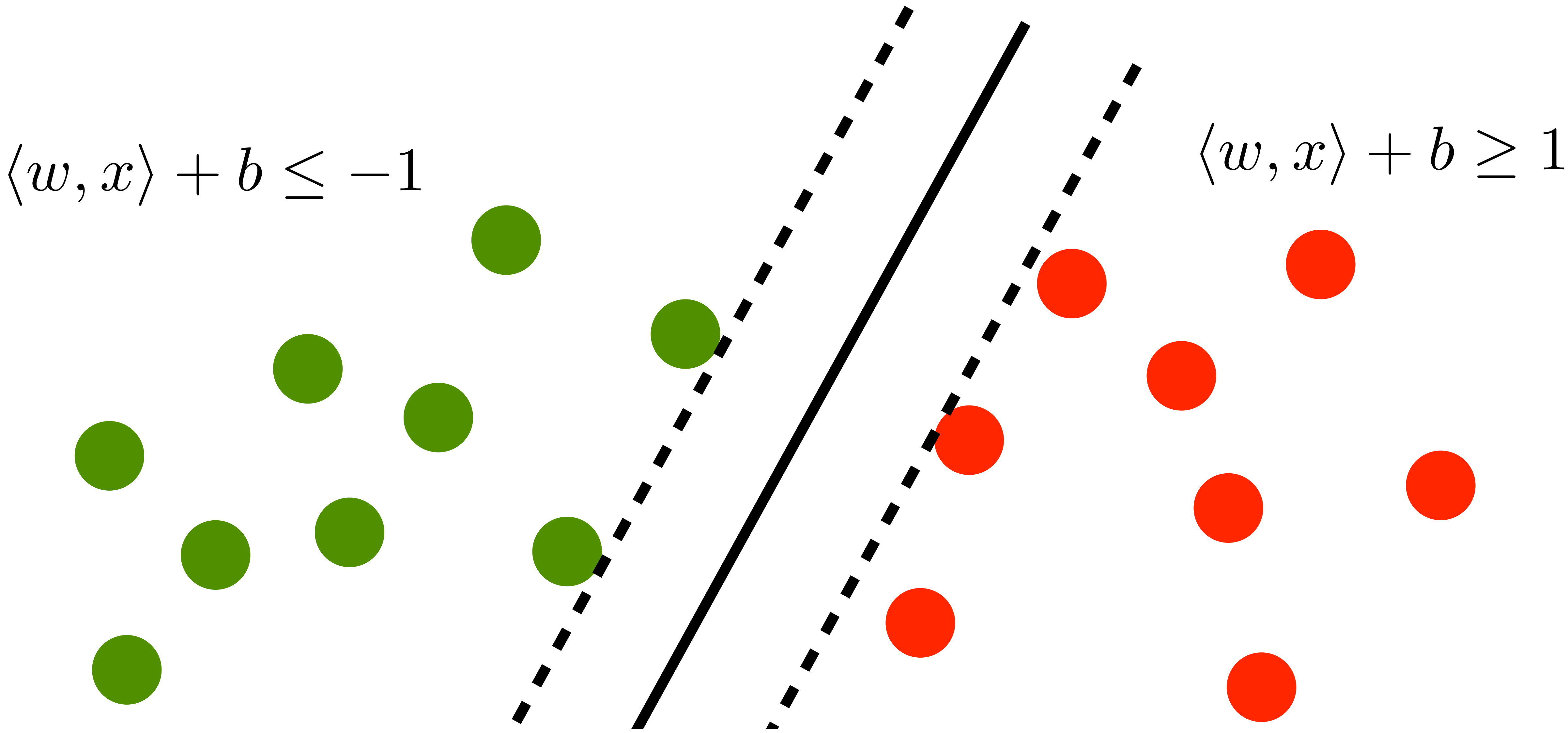
Linear Separator



Linear Separator



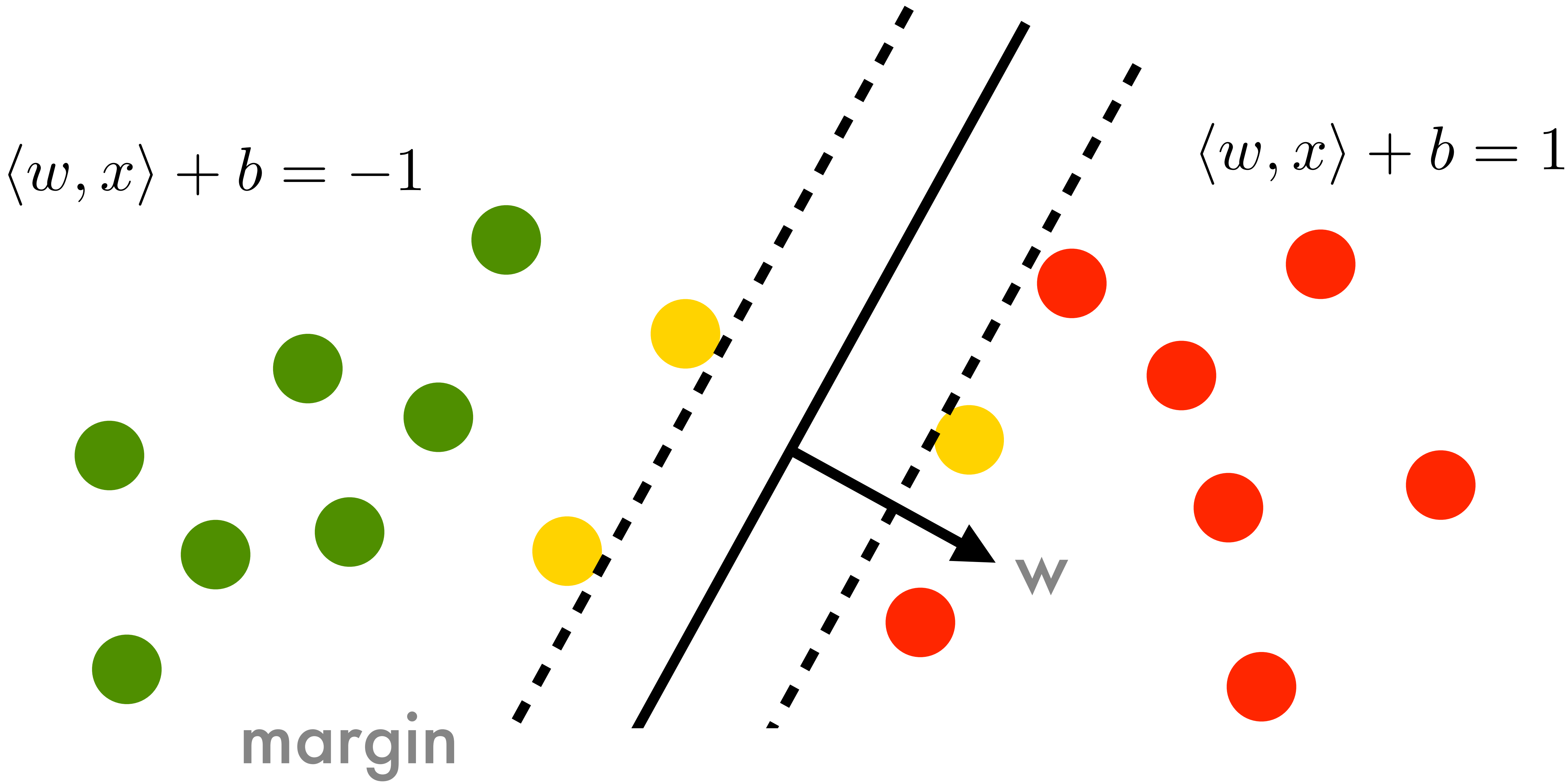
Large Margin Classifier



linear function

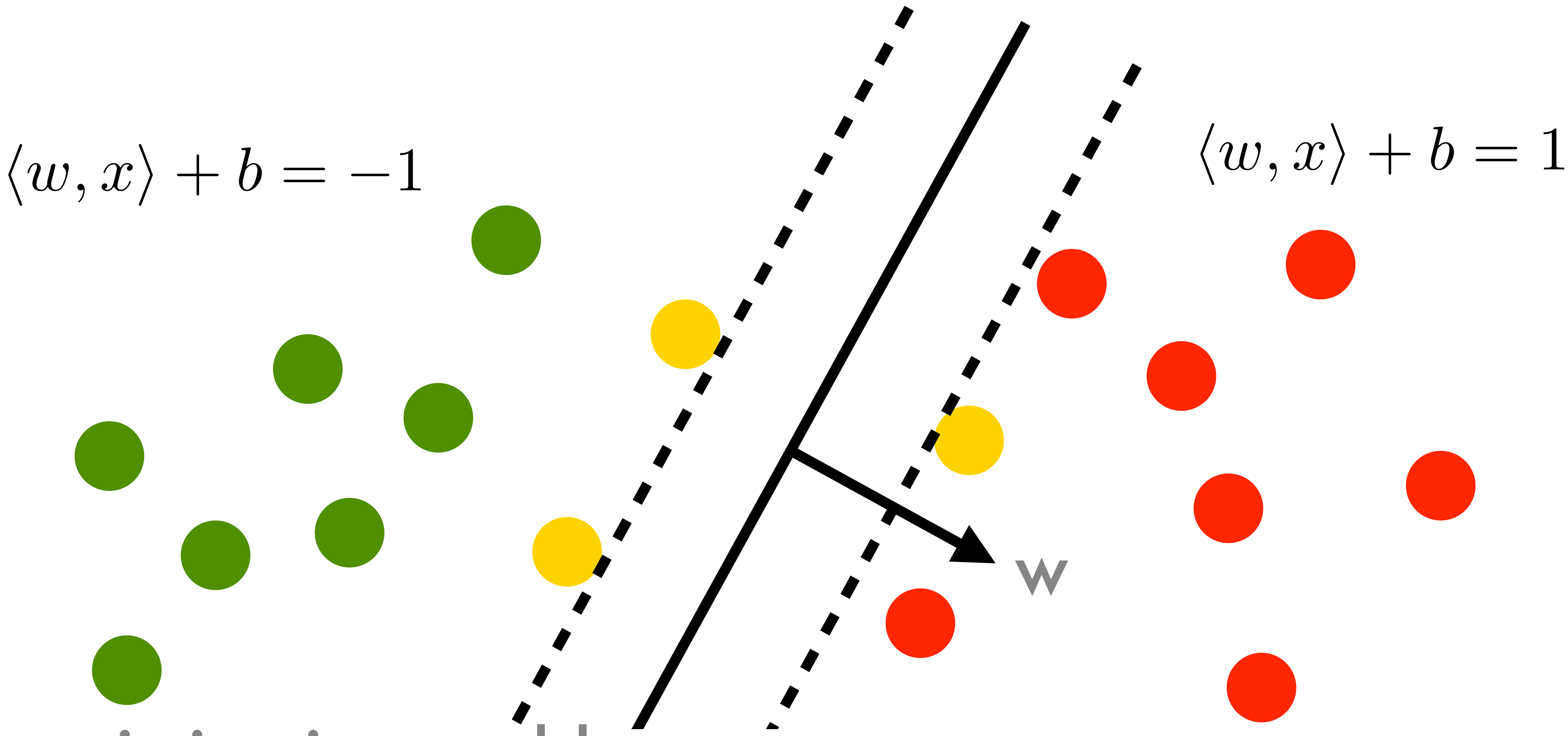
$$f(x) = \langle w, x \rangle + b$$

Large Margin Classifier



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

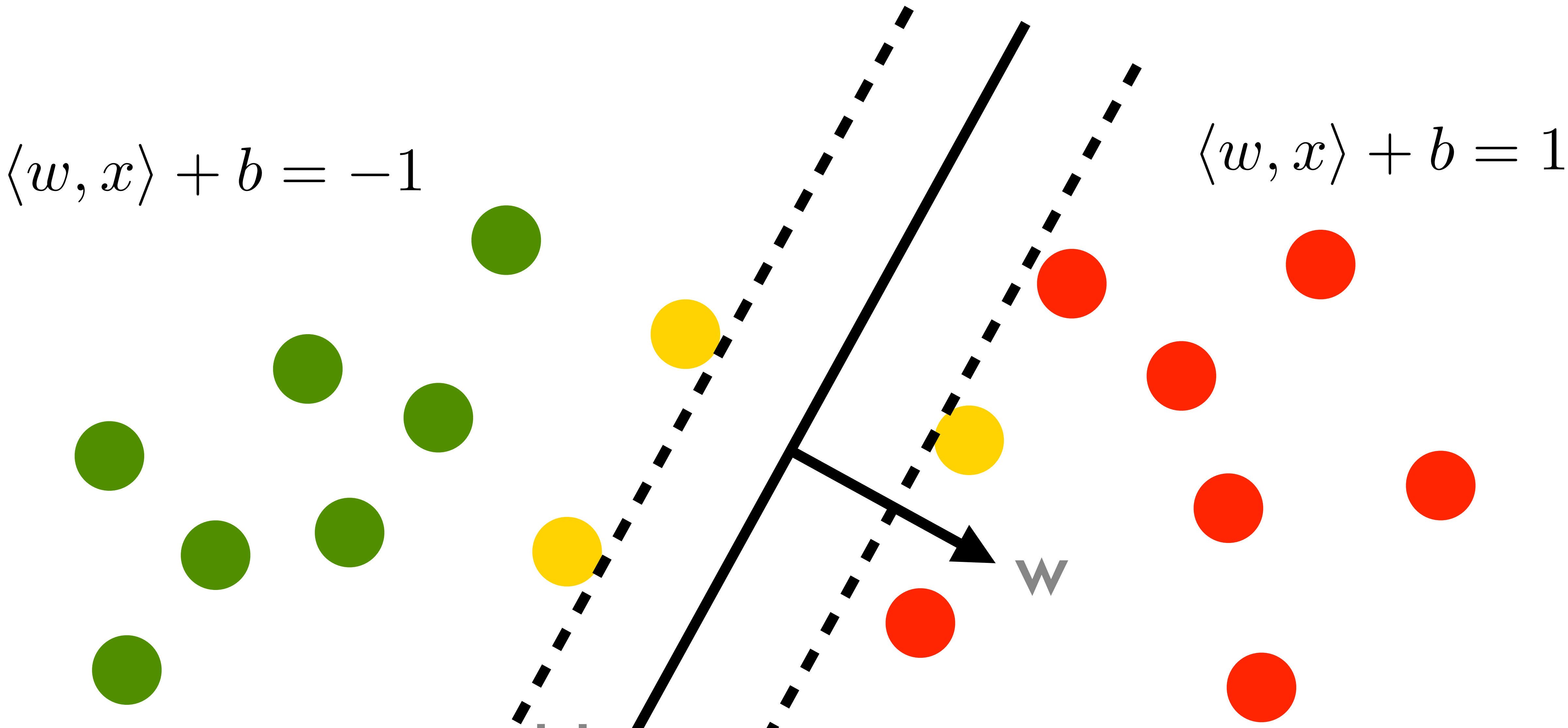
Large Margin Classifier



optimization problem

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

Large Margin Classifier



optimization problem

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

Dual Problem

- Primal optimization problem

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

- Lagrange function

constraint

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

Optimality in w, b is at saddle point with α

- Derivatives in w, b need to vanish

Dual Problem

- **Lagrange function**

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

- **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**

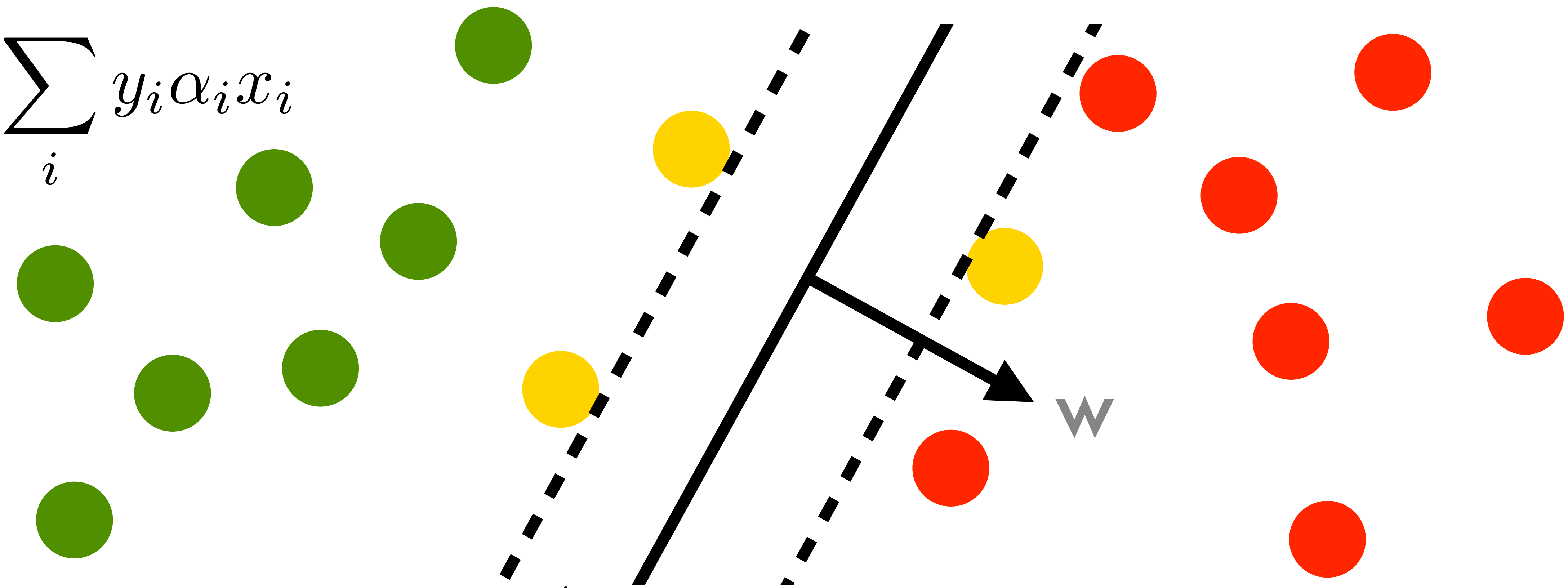
$$\underset{\alpha}{\text{maximize}} - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle + \sum_i \alpha_i$$

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

Support Vector Machines

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

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



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

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

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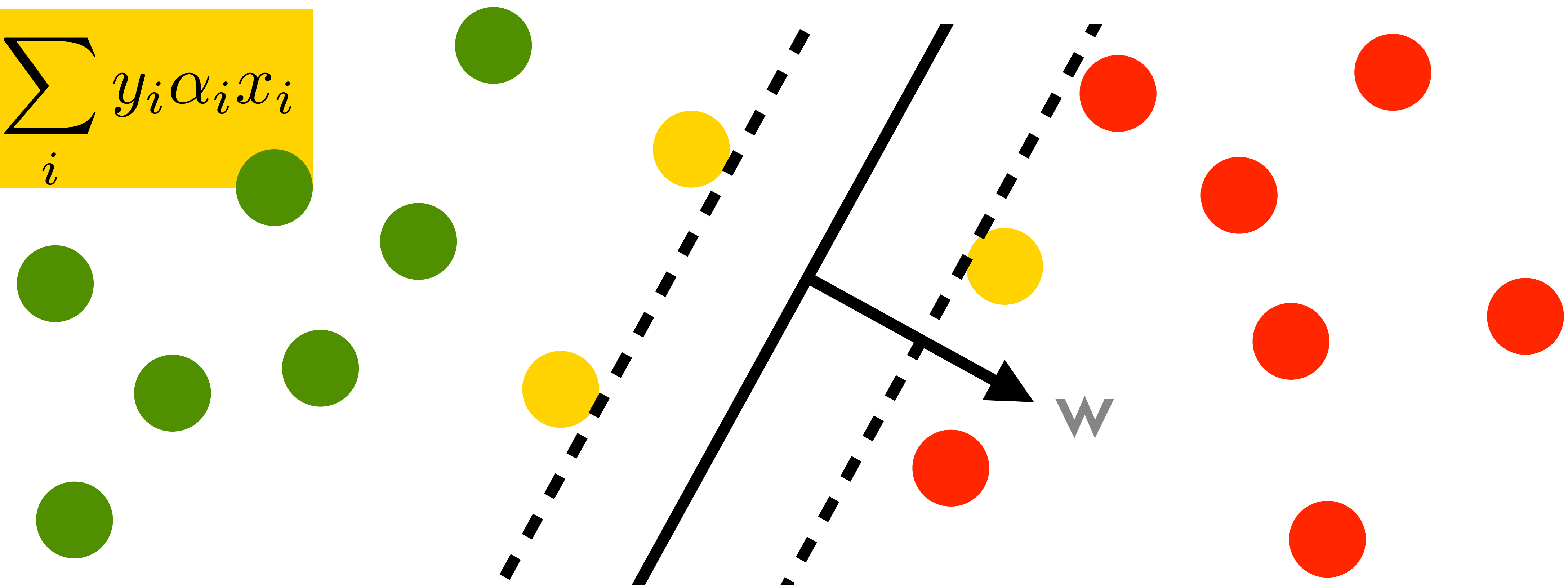
Support Vectors

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

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



Karush Kuhn Tucker
Optimality condition

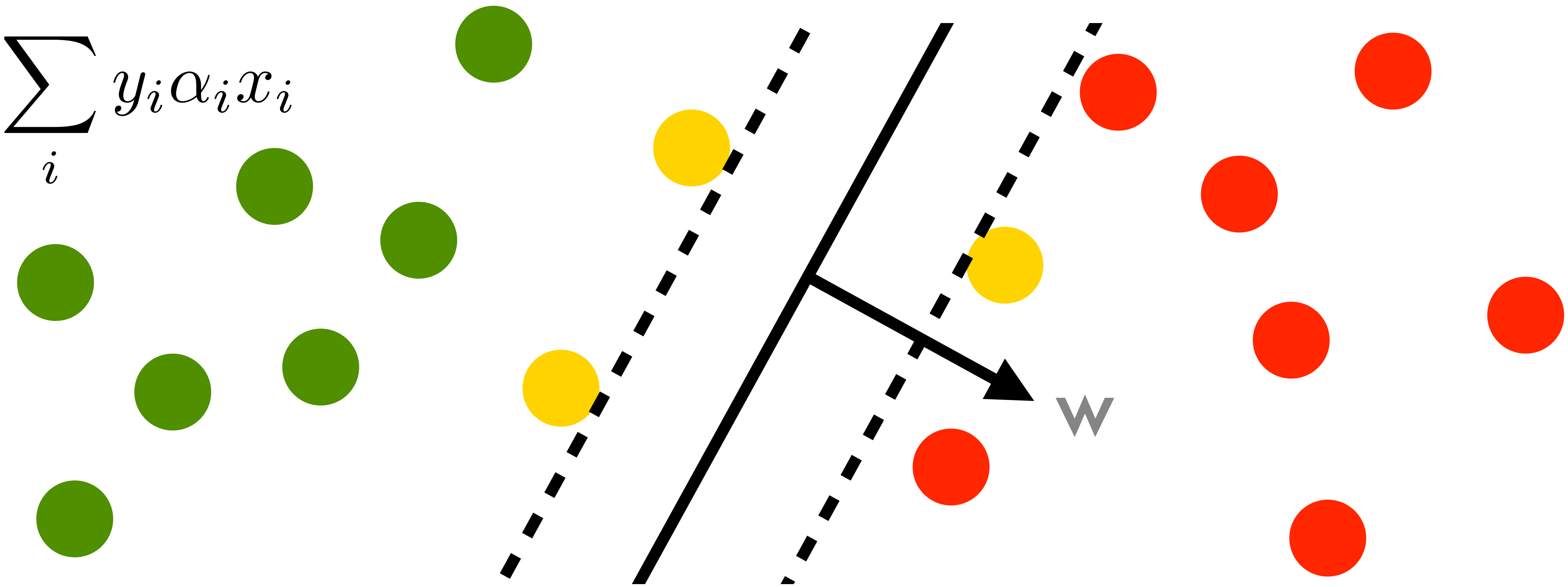
$$\alpha_i \left[y_i \left[\langle w, x_i \rangle + b\right] - 1\right] = 0$$

$$\alpha_i = 0$$

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

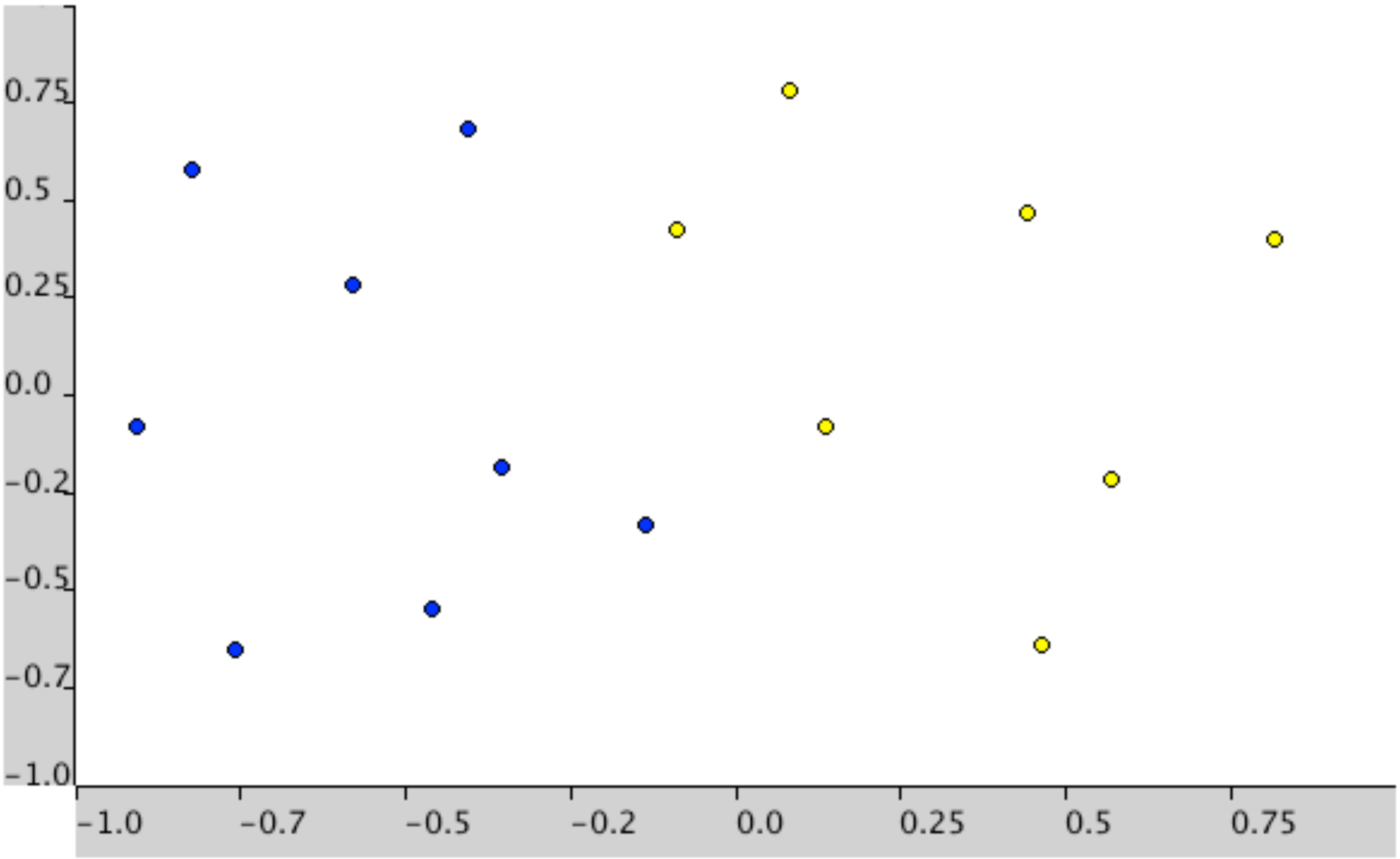
Properties

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



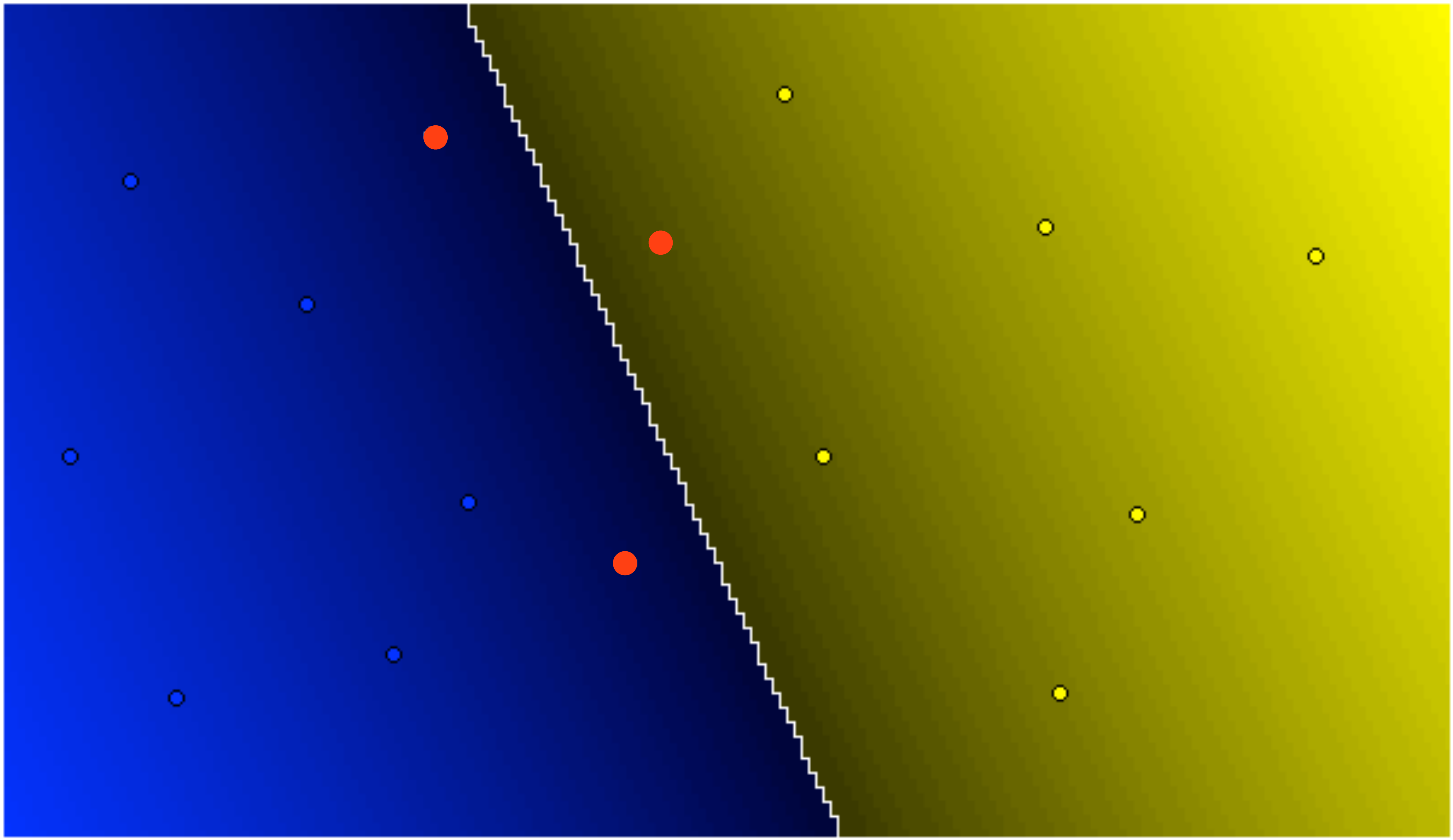
- Weight vector w as weighted linear combination of instances
- Only points on margin matter (ignore the rest and get same solution)
- Only inner products matter
  - Quadratic program
  - We can replace the inner product by a kernel
- Keeps instances away from the margin

Example

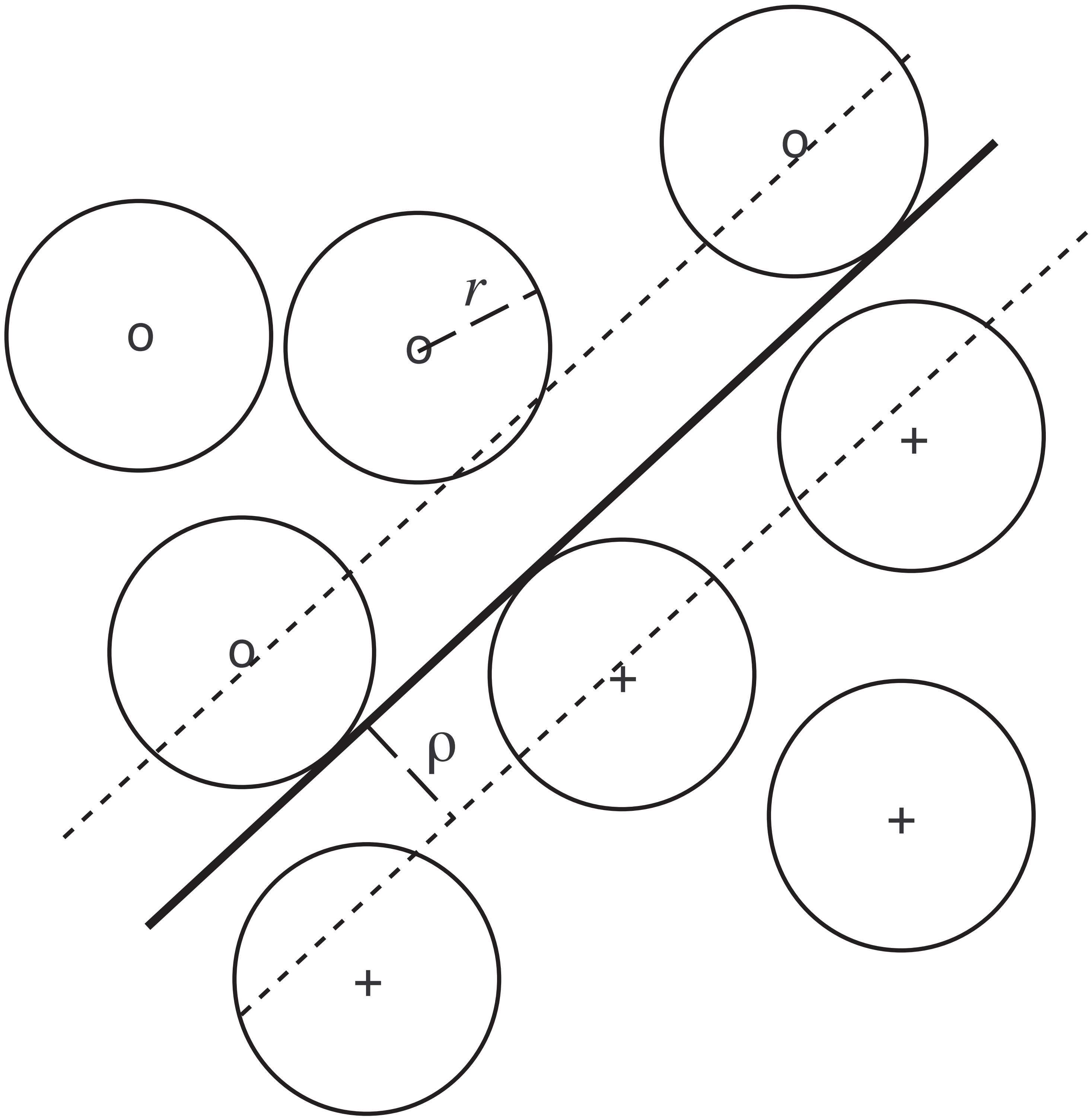


Example

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



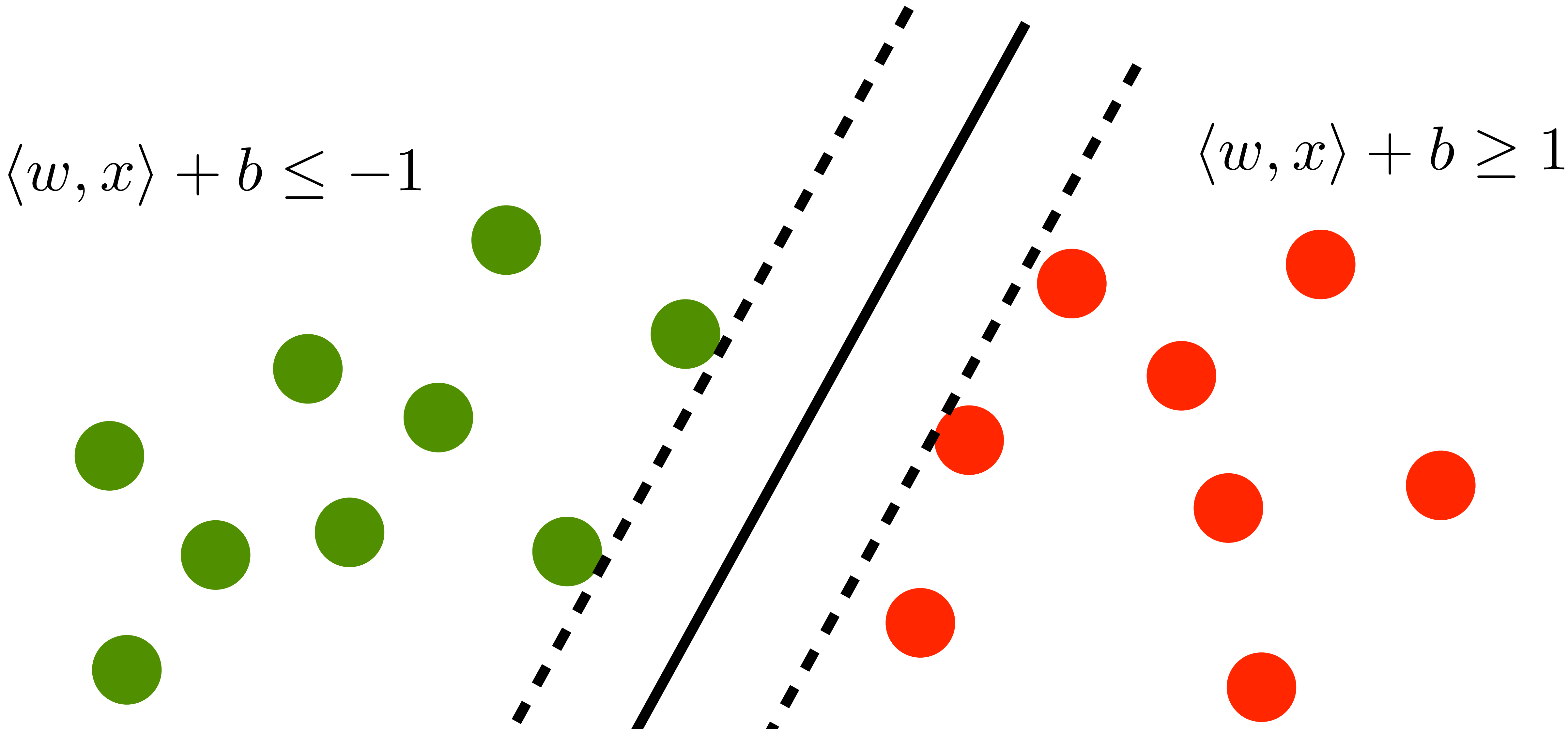
Why large margins?



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


MAGIC Etch A Sketch® SCREEN
SOFT
CLASSIFIERS

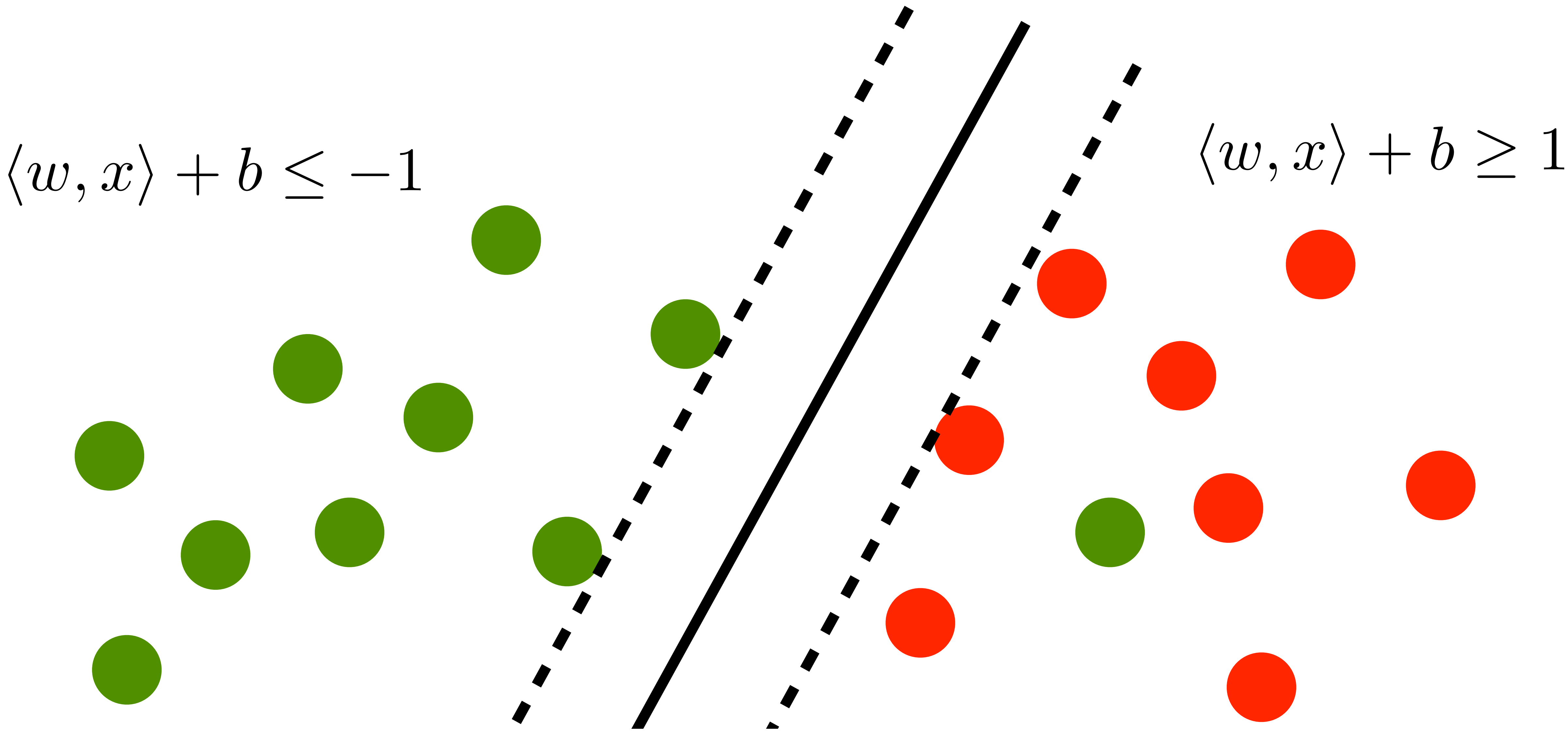
Large Margin Classifier



linear function

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

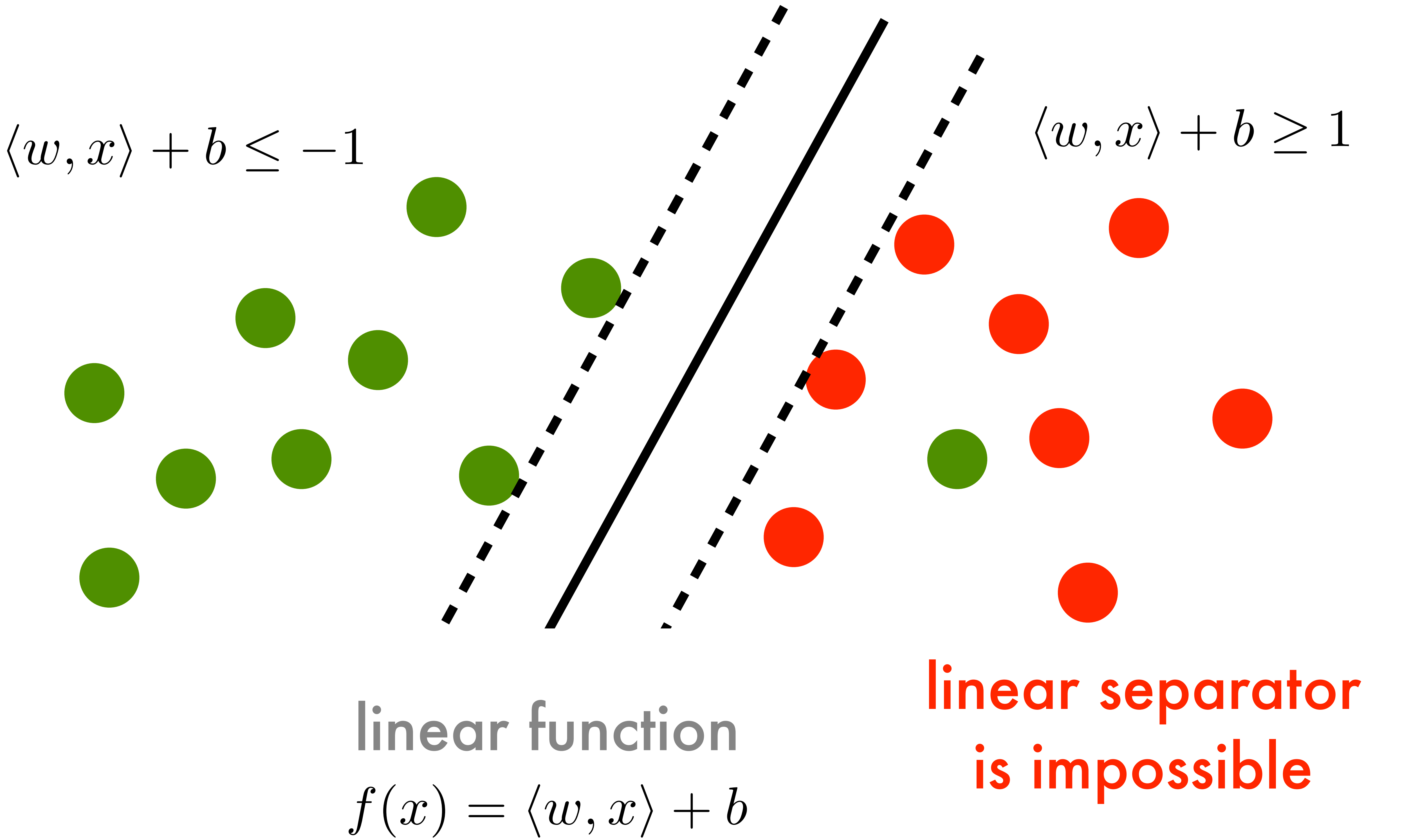
Large Margin Classifier



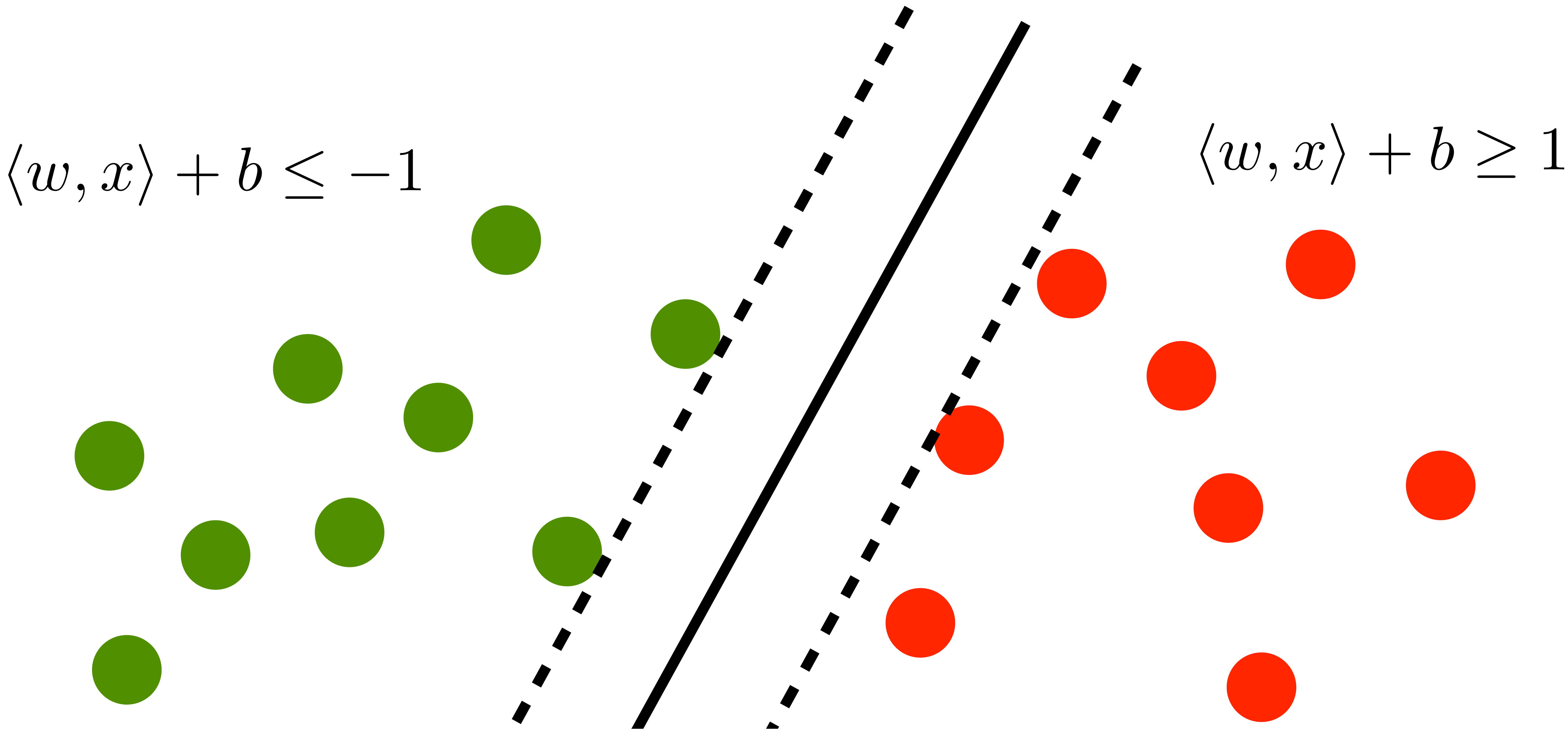
linear function

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

Large Margin Classifier

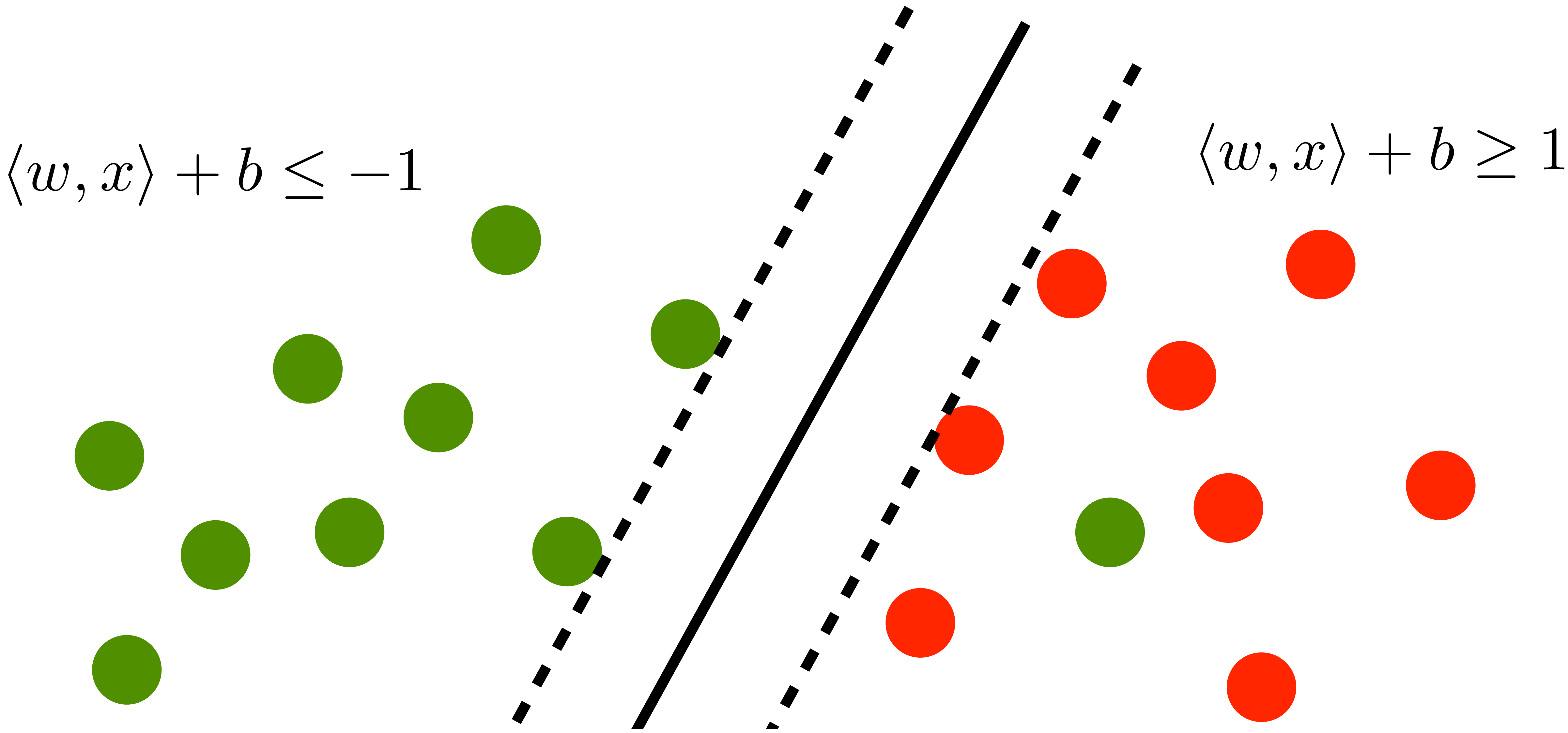


Large Margin Classifier



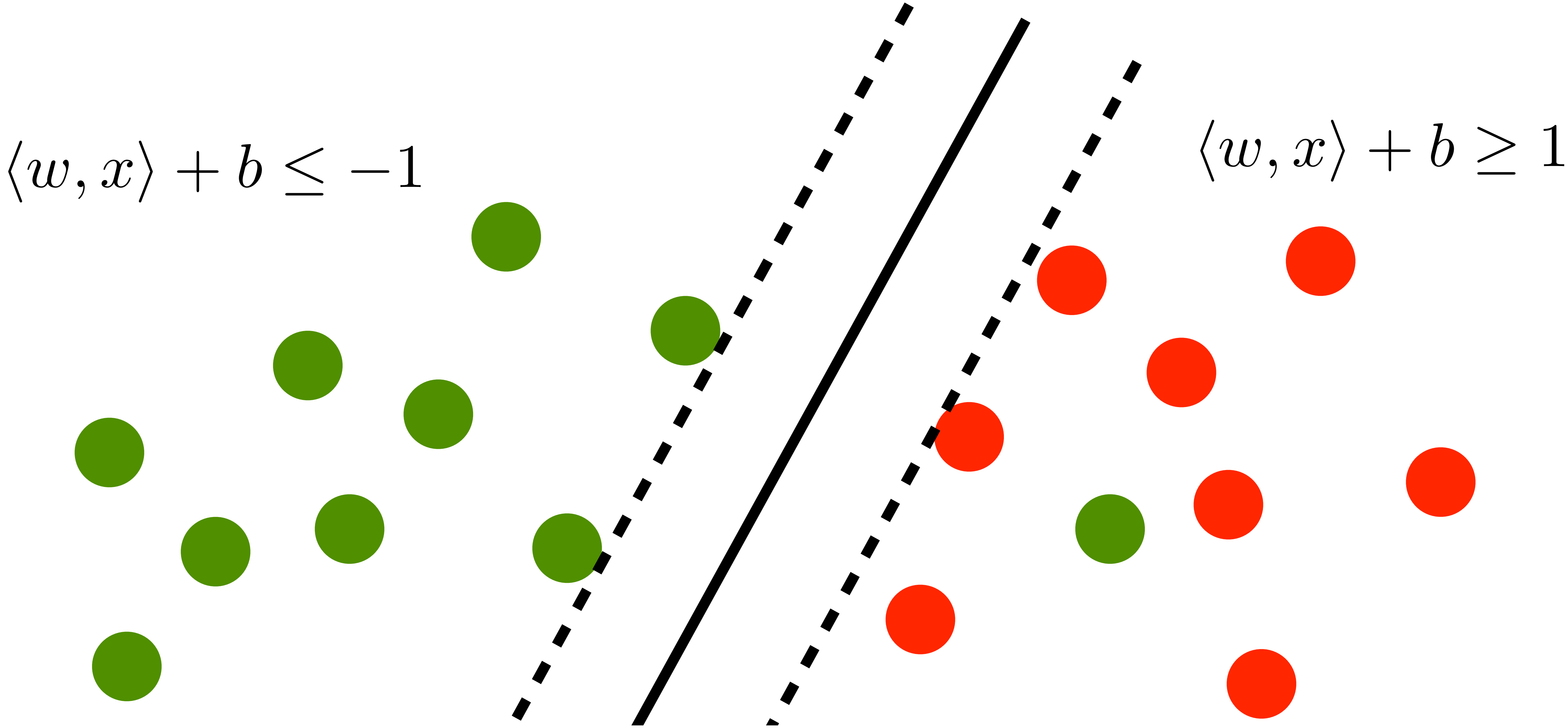
Theorem (Minsky & Papert)
Finding the minimum error separating hyperplane is NP hard

Large Margin Classifier



Theorem (Minsky & Papert)
Finding the minimum error separating hyperplane is NP hard

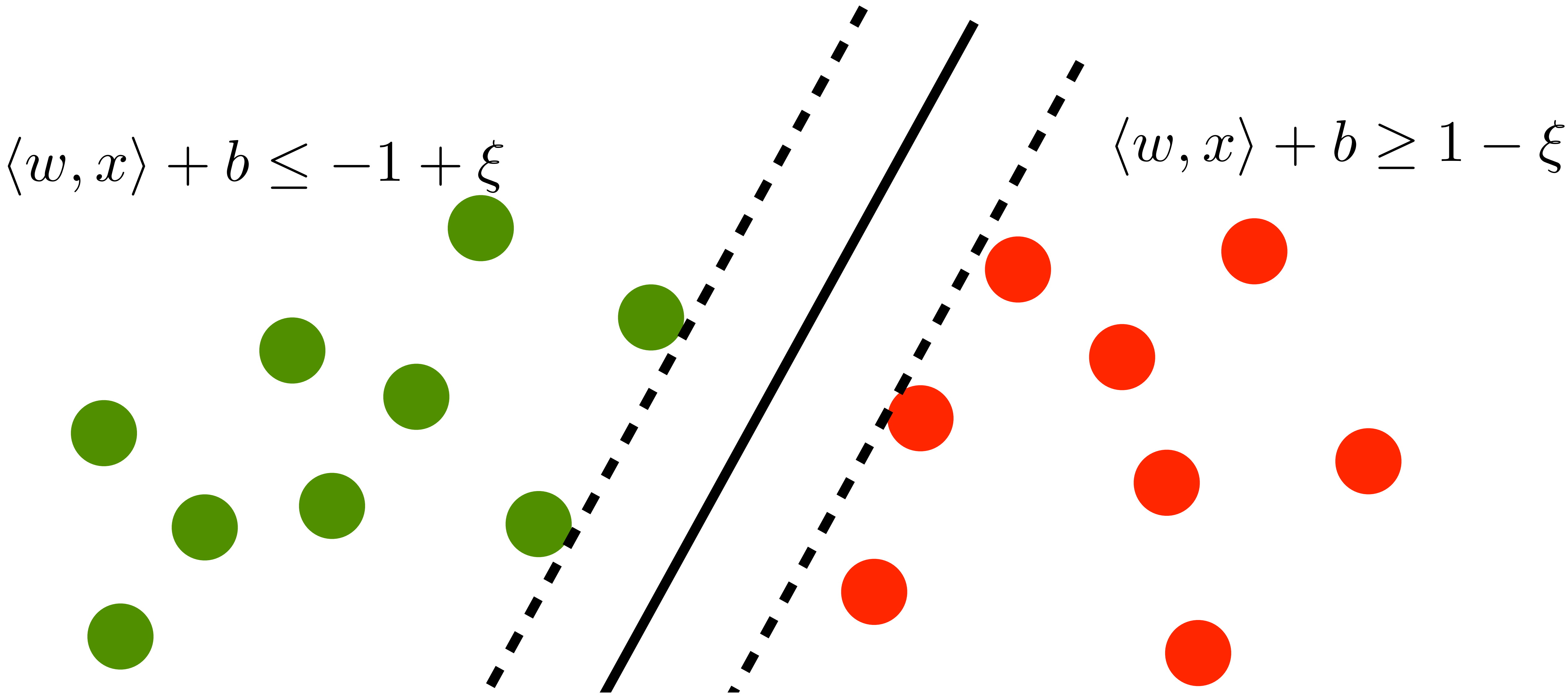
Large Margin Classifier



minimum error separator
is impossible

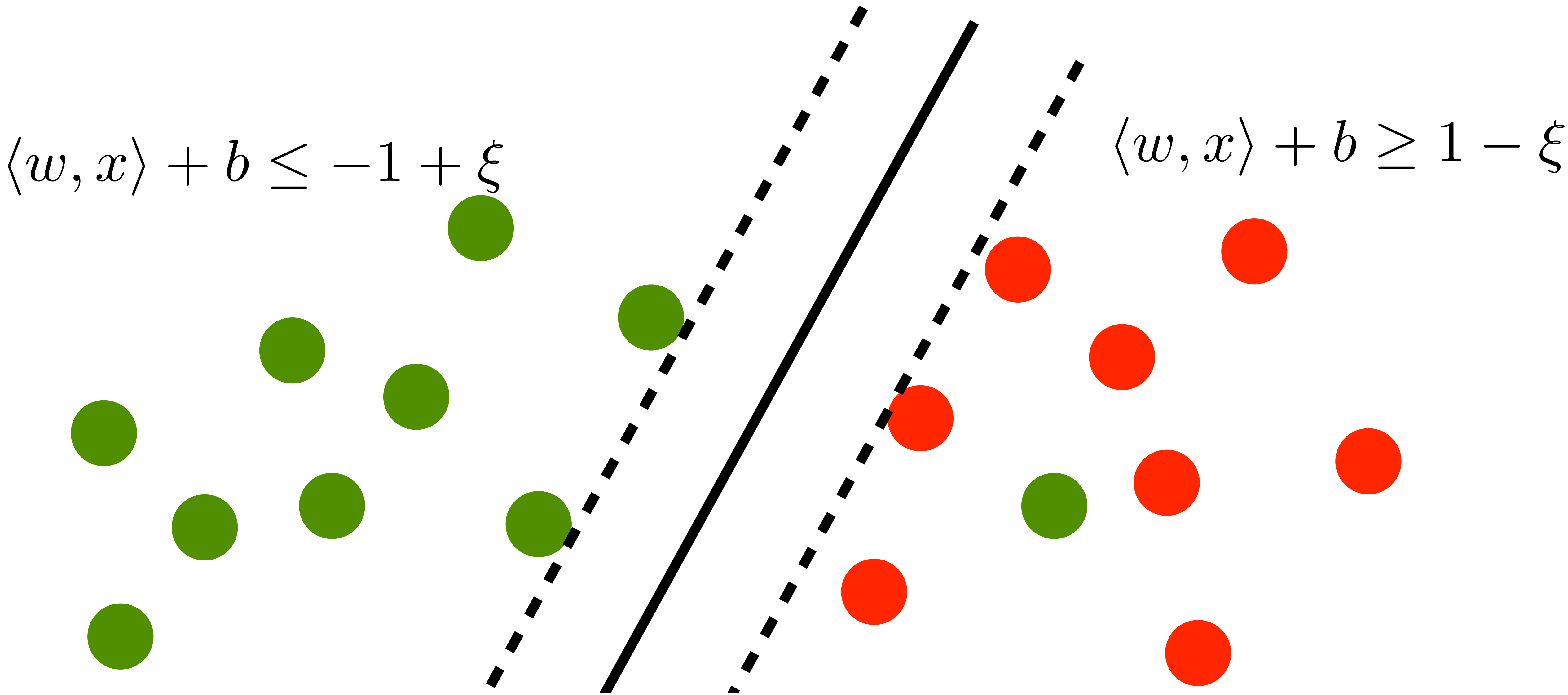
Theorem (Minsky & Papert)
Finding the minimum error separating hyperplane is NP hard

Adding slack variables



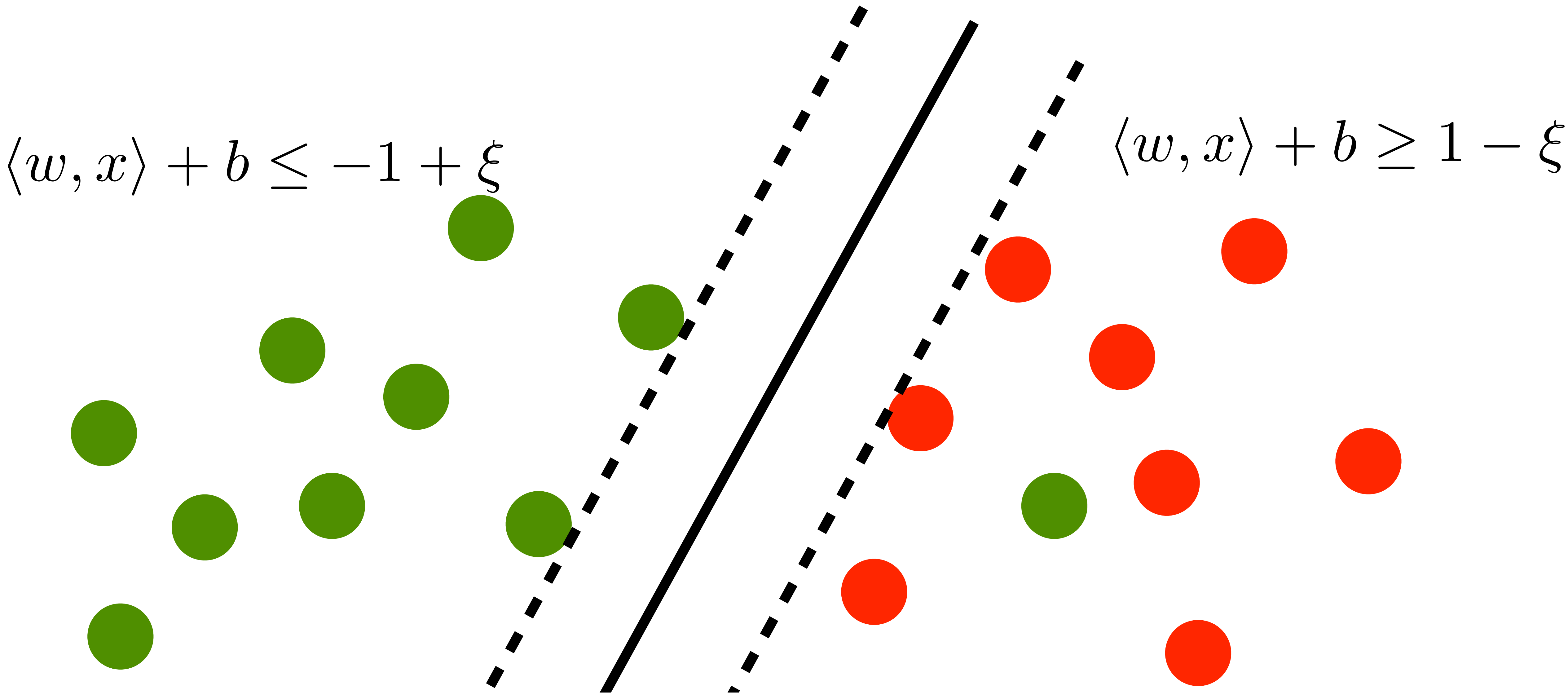
Convex optimization problem

Adding slack variables



Convex optimization problem

Adding slack variables



minimize amount of slack

Convex optimization problem

Intermezzo
Convex Programs for Dummies

- Primal optimization problem

$$\underset{x}{\text{minimize}}\, f(x) \text{ subject to } c_i(x) \leq 0$$

- Lagrange function

$$L(x, \alpha) = f(x) + \sum_i \alpha_i c_i(x)$$

- First order optimality conditions in x

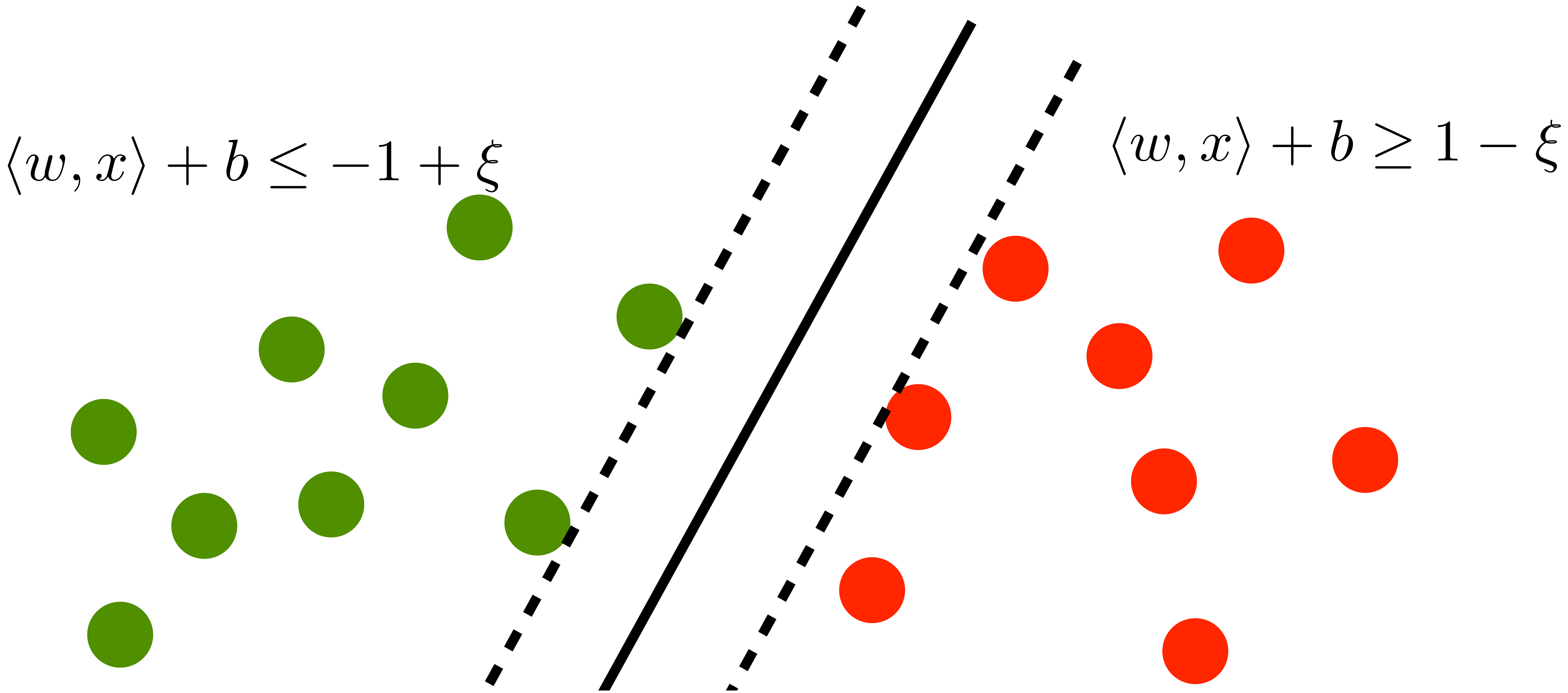
$$\partial_x L(x, \alpha) = \partial_x f(x) + \sum_i \alpha_i \partial_x c_i(x) = 0$$

- Solve for x and plug it back into L

$$\underset{\alpha}{\text{maximize}}\, L(x(\alpha), \alpha)$$

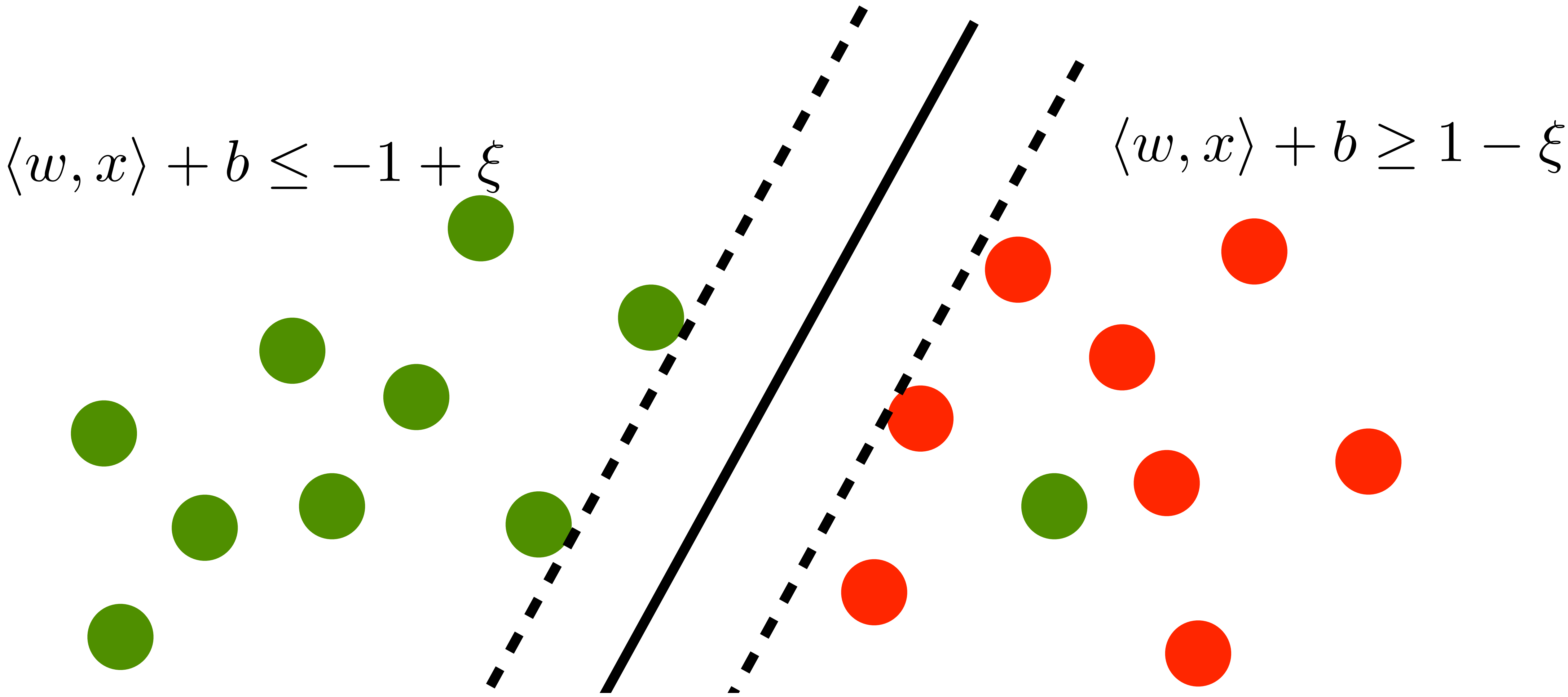
(keep explicit constraints)

Adding slack variables



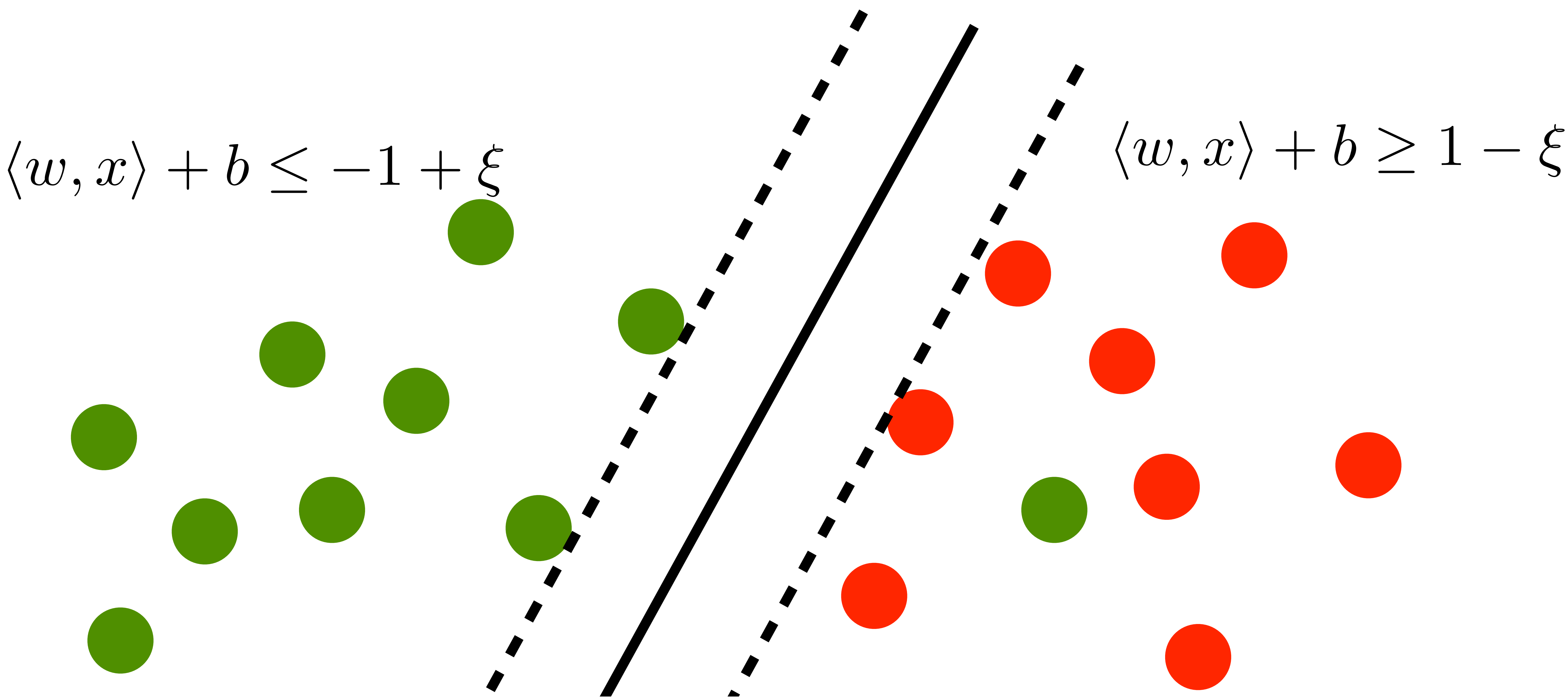
Convex optimization problem

Adding slack variables



Convex optimization problem

Adding slack variables



minimize amount of slack

Convex optimization problem

Adding slack variables

- Hard margin problem

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

- With slack variables

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

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

Problem is always feasible. Proof:

$w = 0 \text{ and } b = 0 \text{ and } \xi_i = 1$ (also yields upper bound)

Dual Problem

- Primal optimization problem

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

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

- Lagrange function

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

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

- Derivatives in w,b,ξ need to vanish

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

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

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

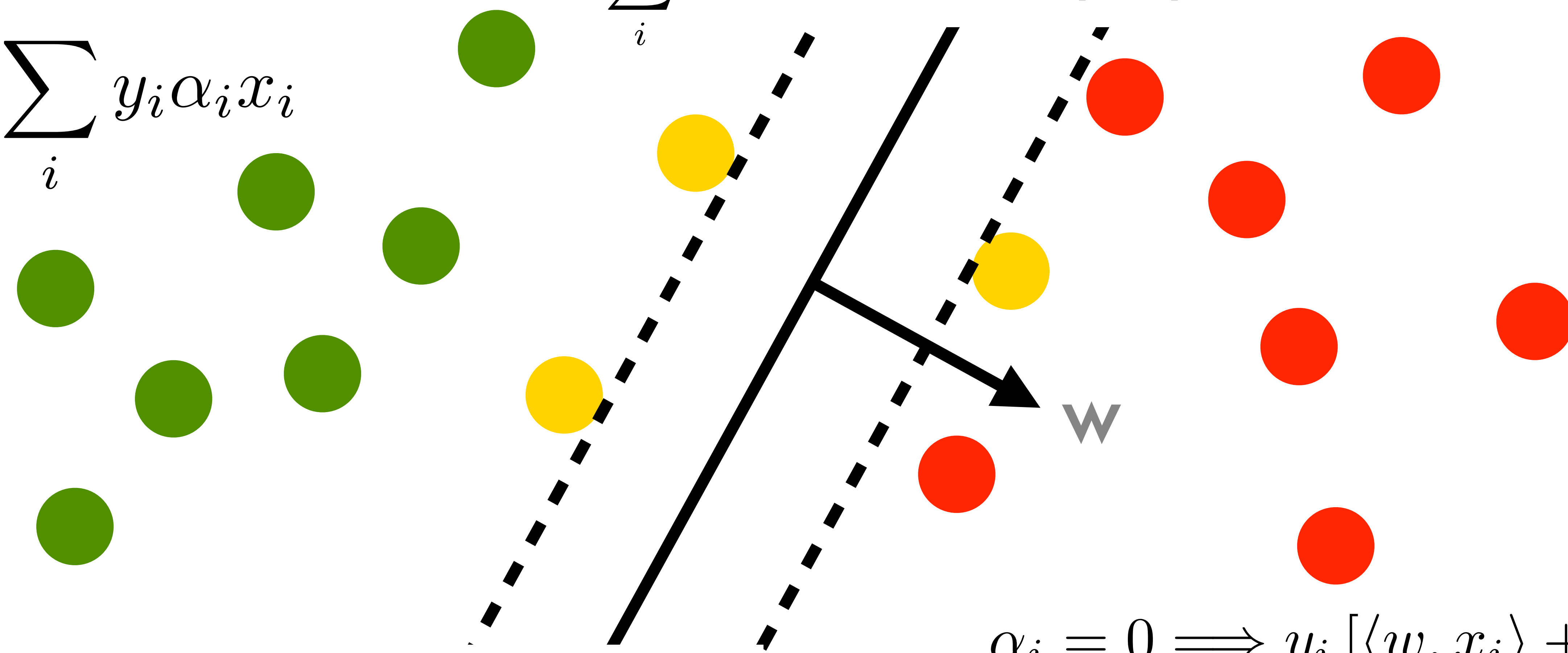
bound influence

Karush Kuhn Tucker Conditions

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

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

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



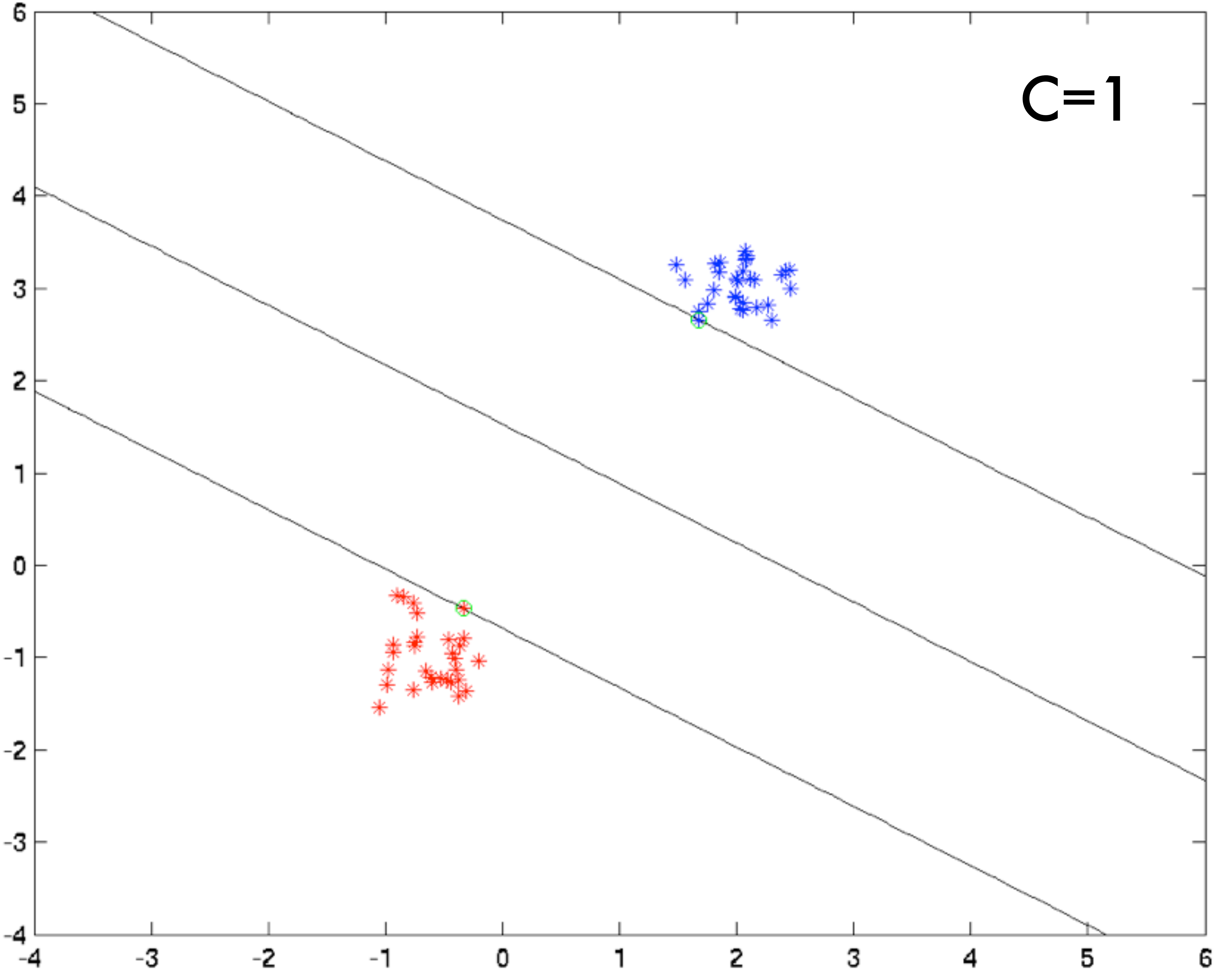
$$\alpha_i \left[y_i \left[\langle w, x_i\rangle + b\right] + \xi_i - 1\right] = 0$$

$$\eta_i \xi_i = 0$$

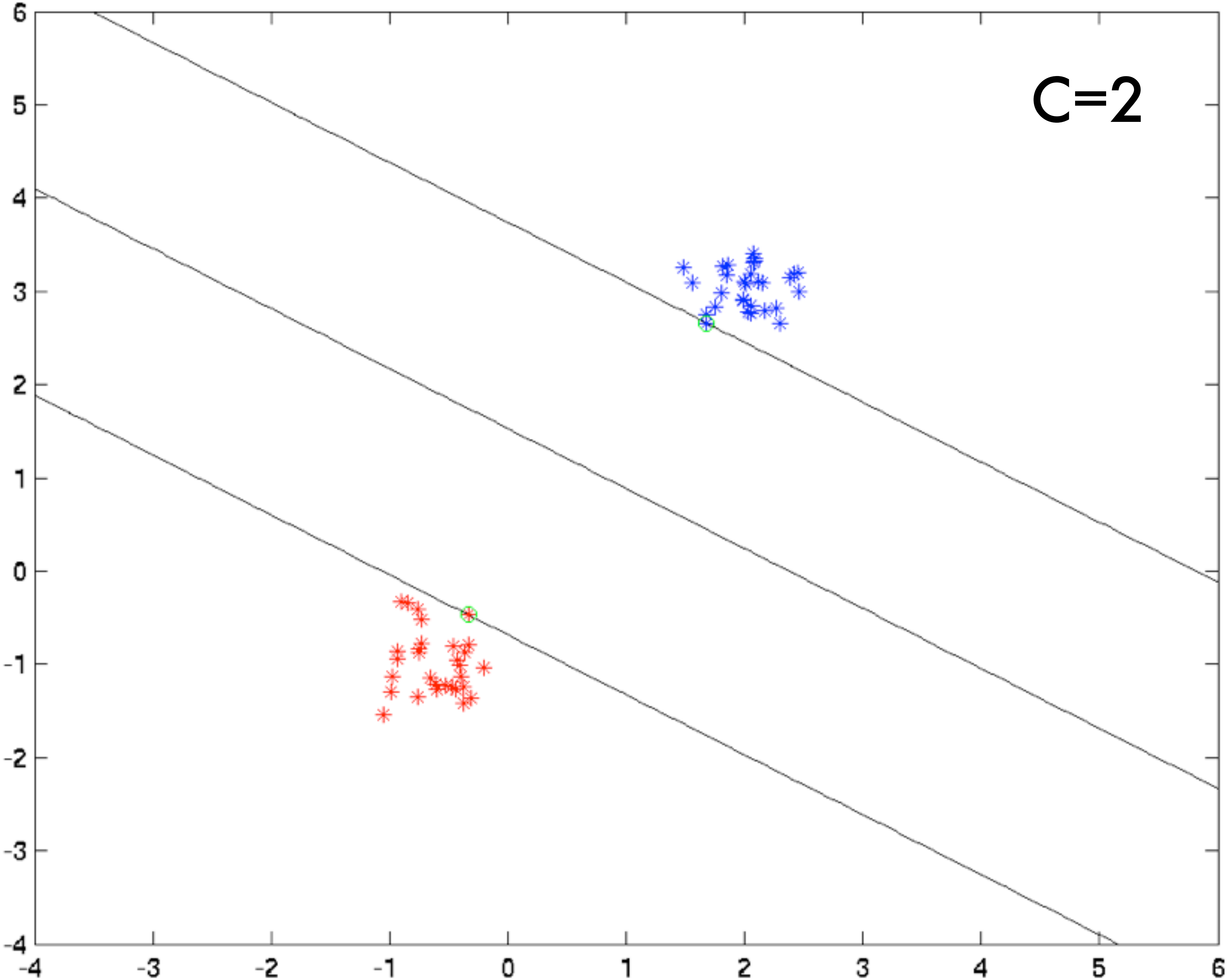
$$\alpha_i = 0 \Longrightarrow y_i \left[\langle w, x_i\rangle + b\right] \geq 1$$

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

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



C=1
6
5
4
3
2
1
0
-1
-2
-3
-4
-4
-3
-2
-1
0
1
2
3
4
5
6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-2
-1
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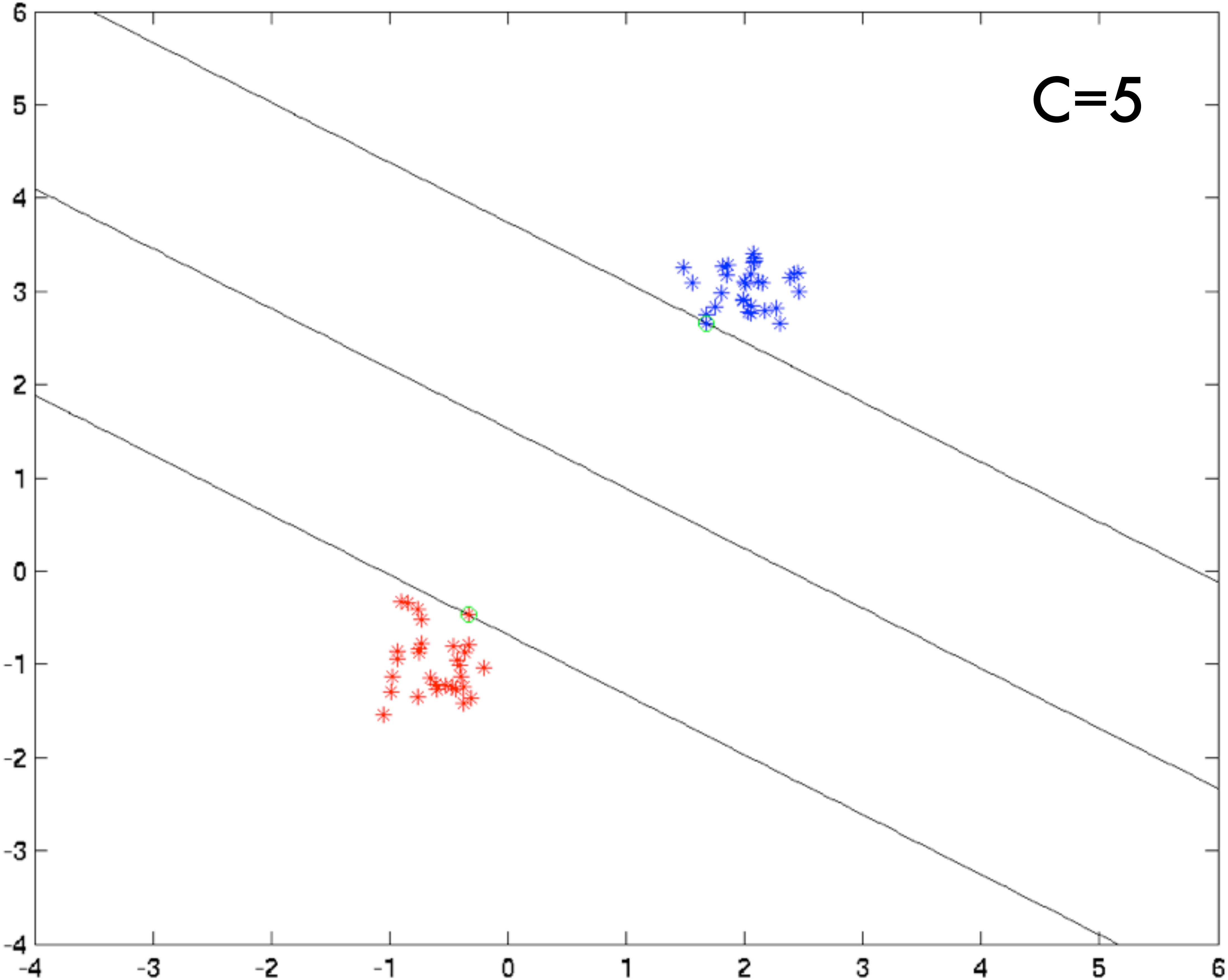
2
3
4
5
6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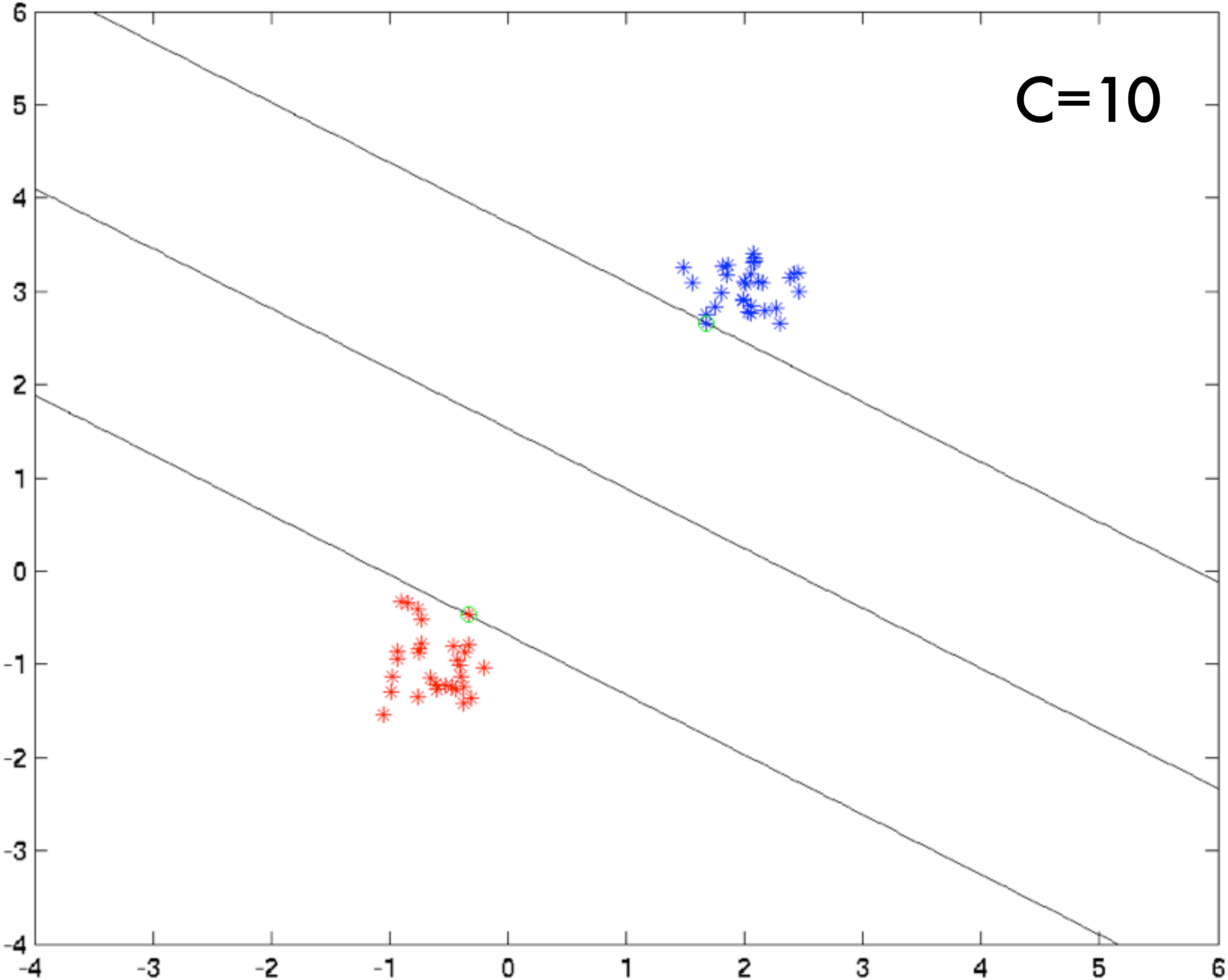
2
3
4
5
6



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-1
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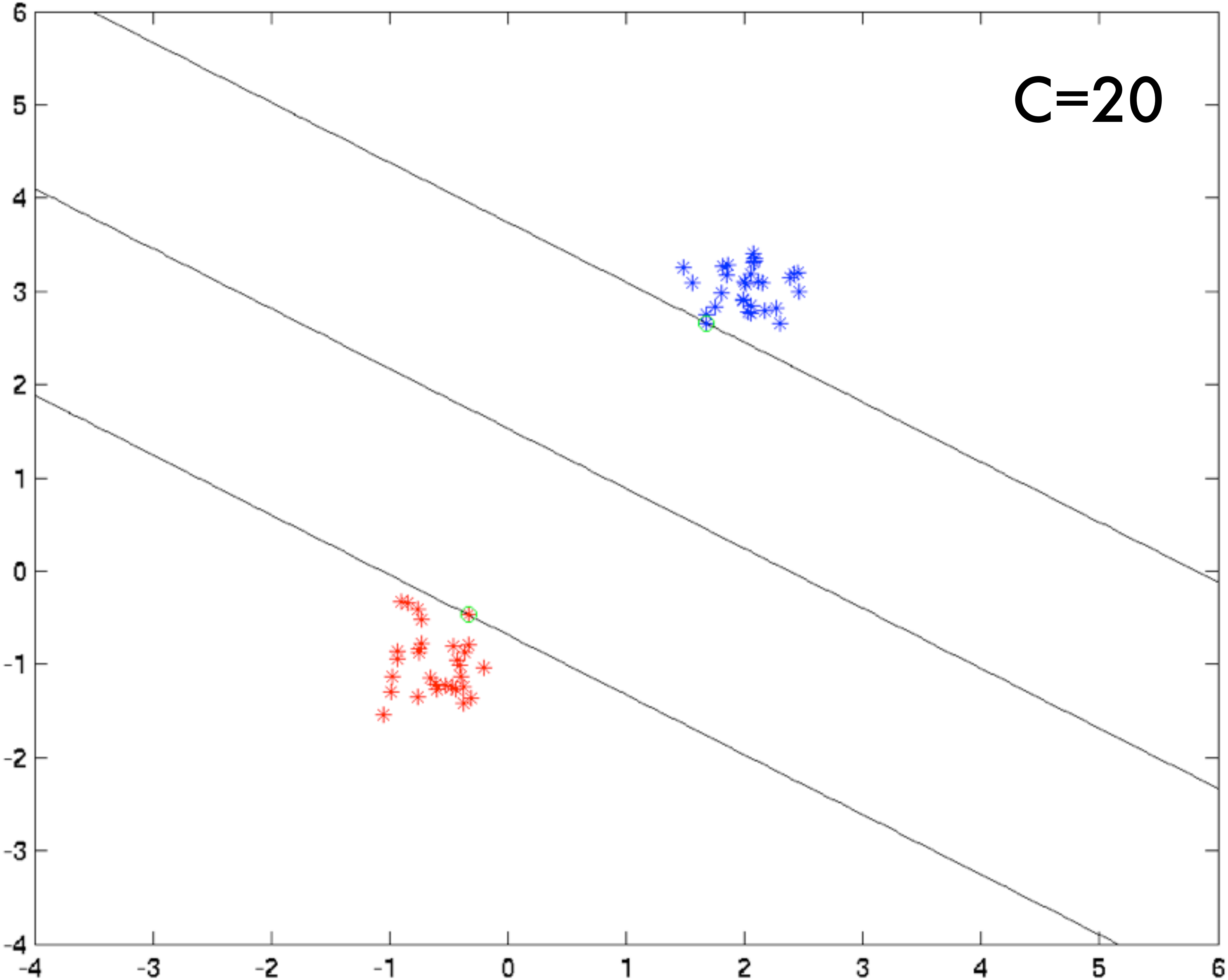
5
6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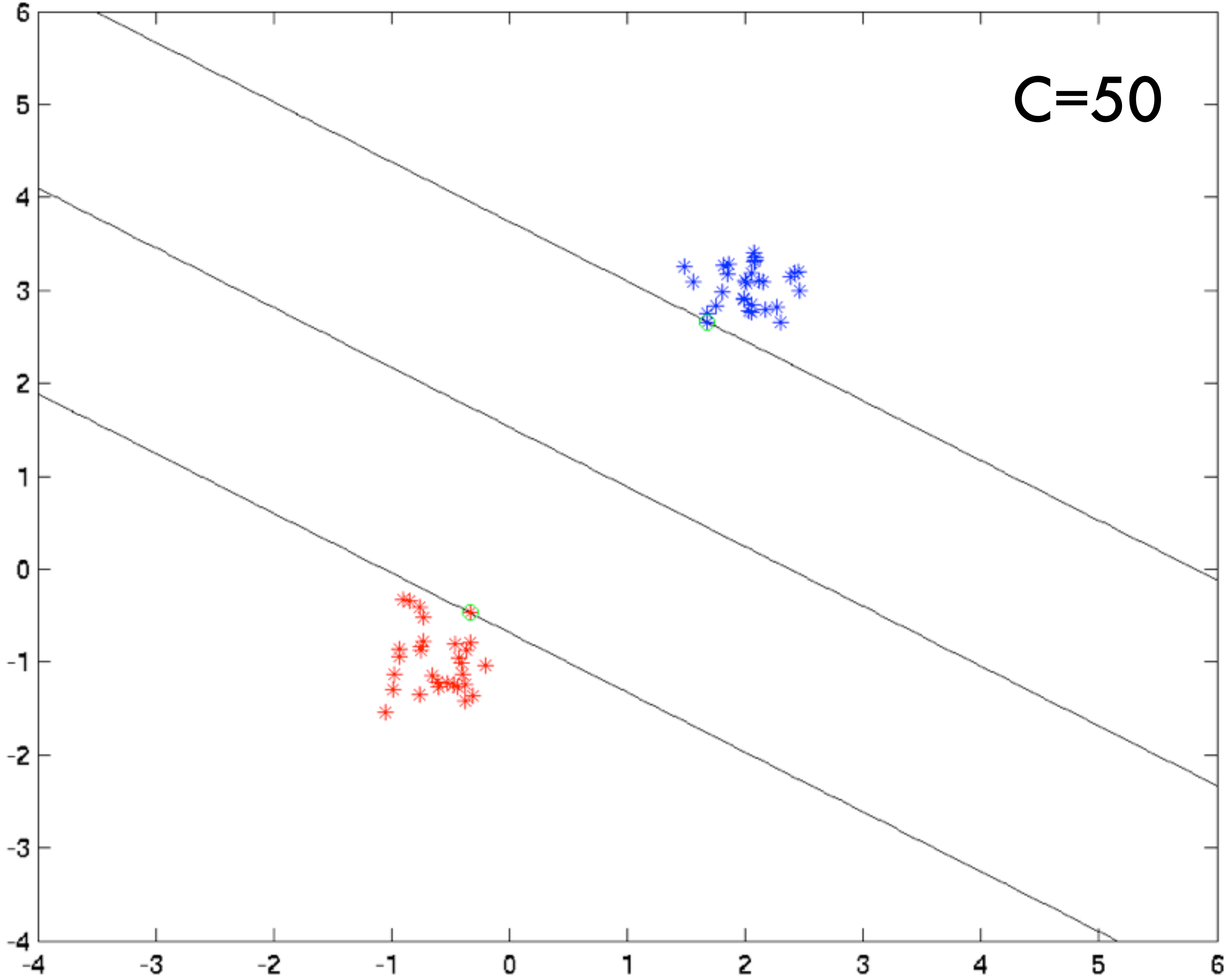
6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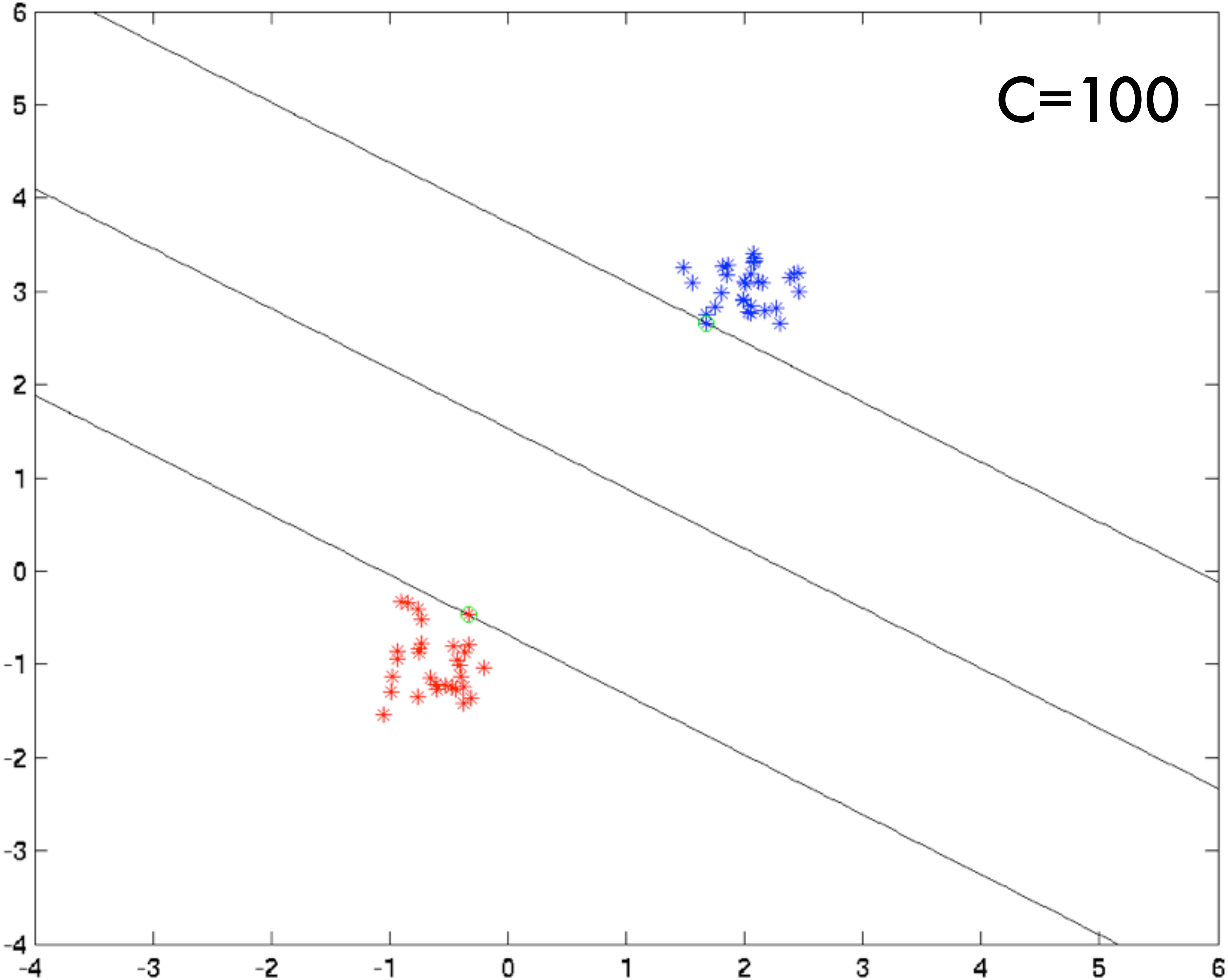
6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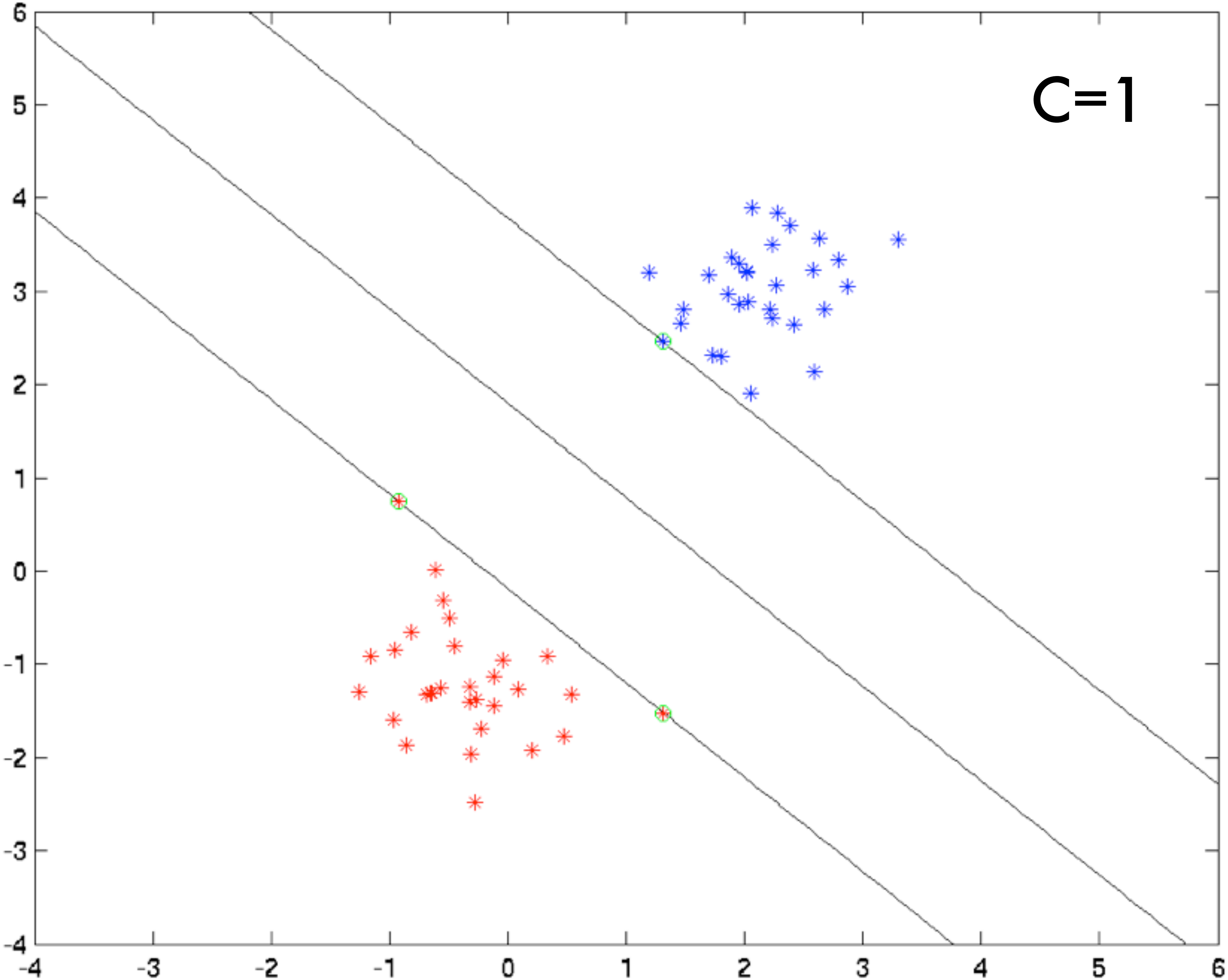
C=1
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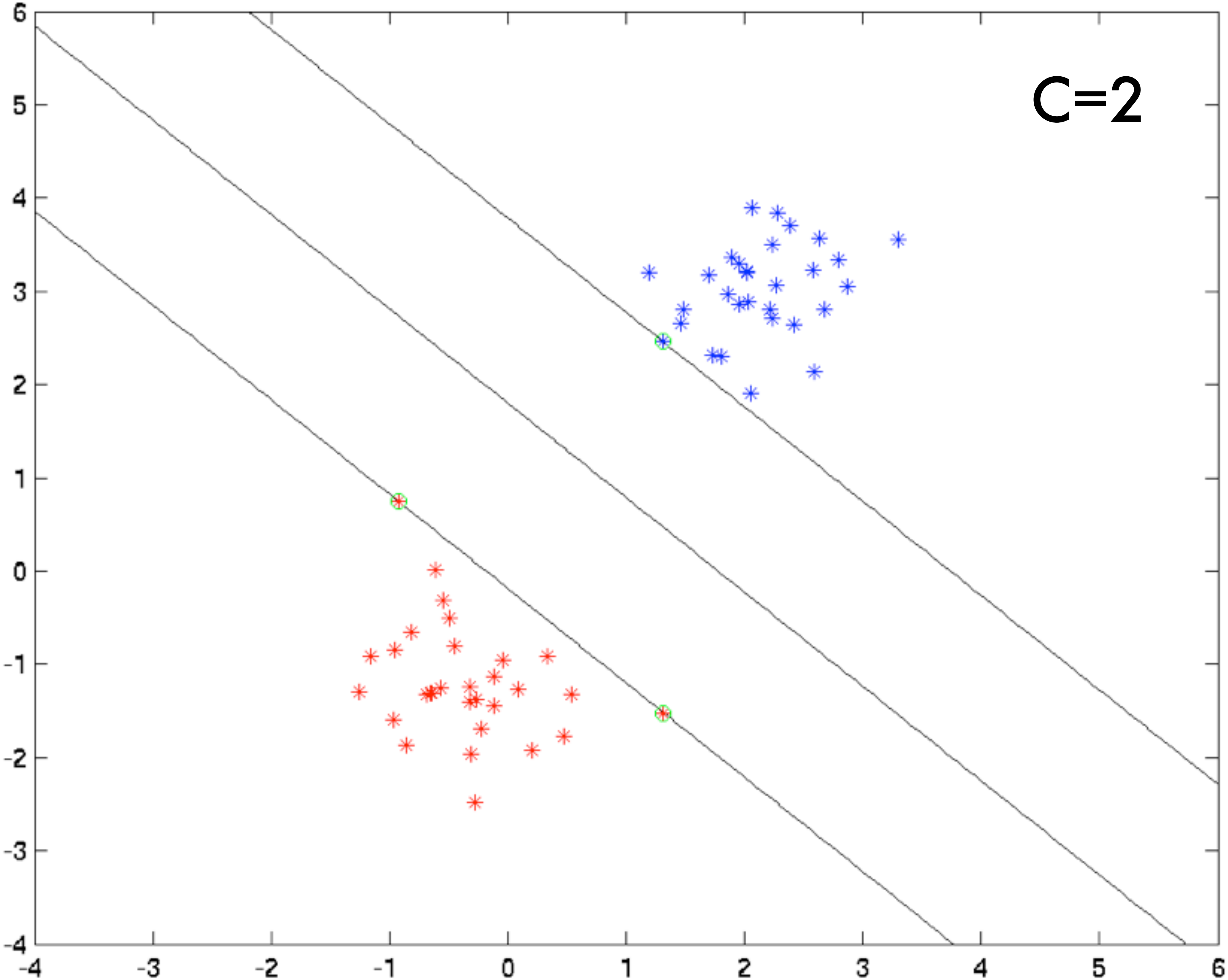
C=2
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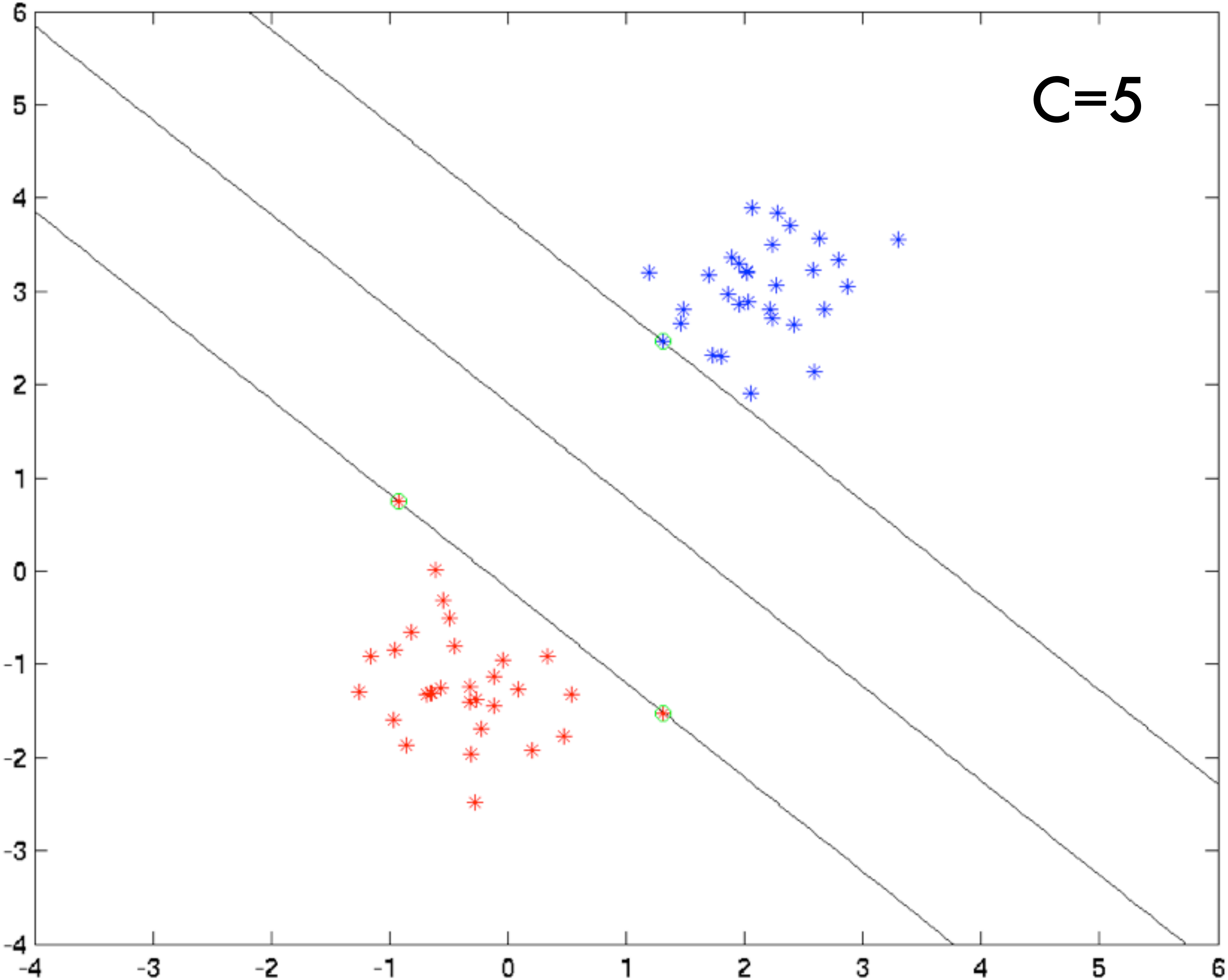
C=5
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-3
-4
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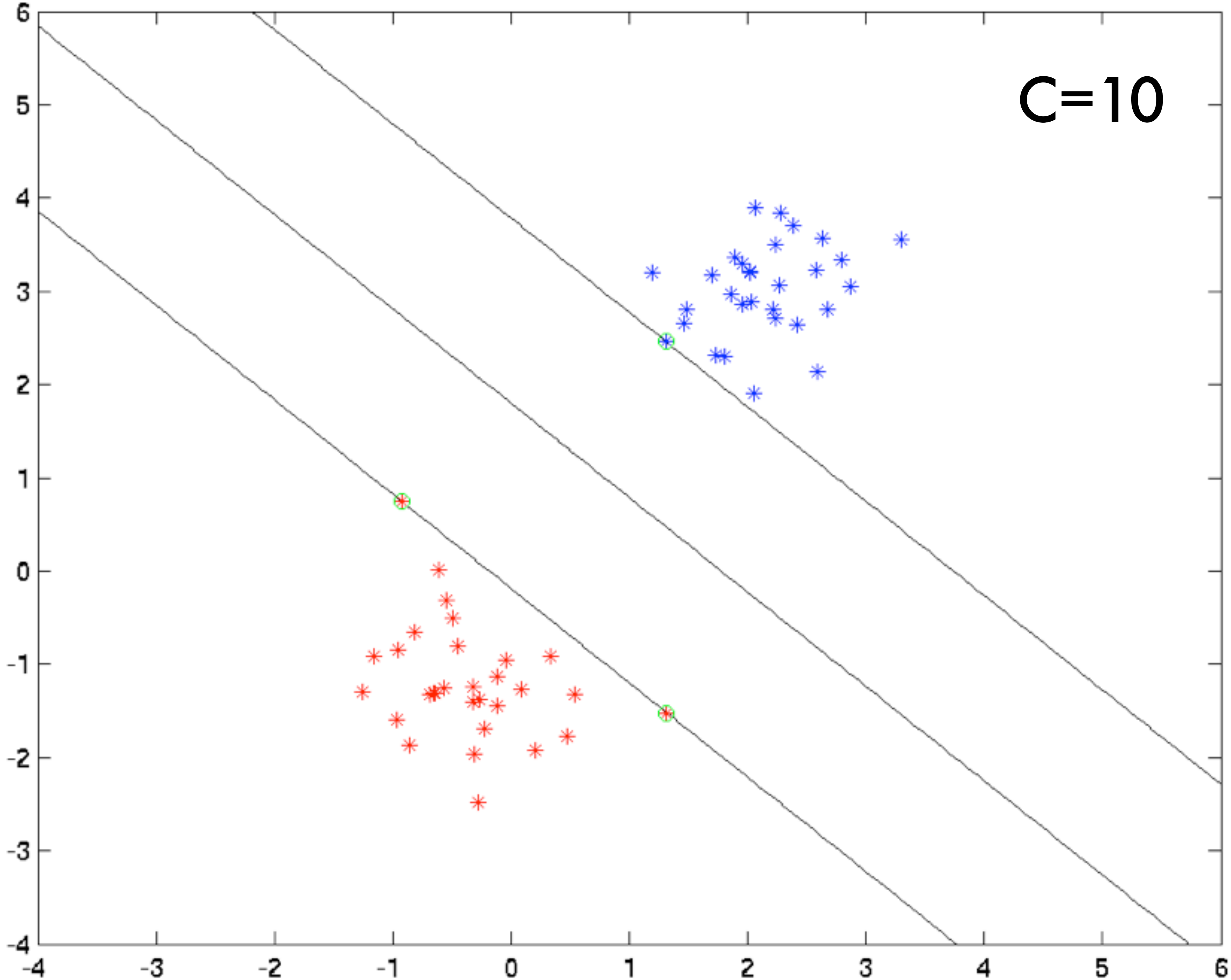
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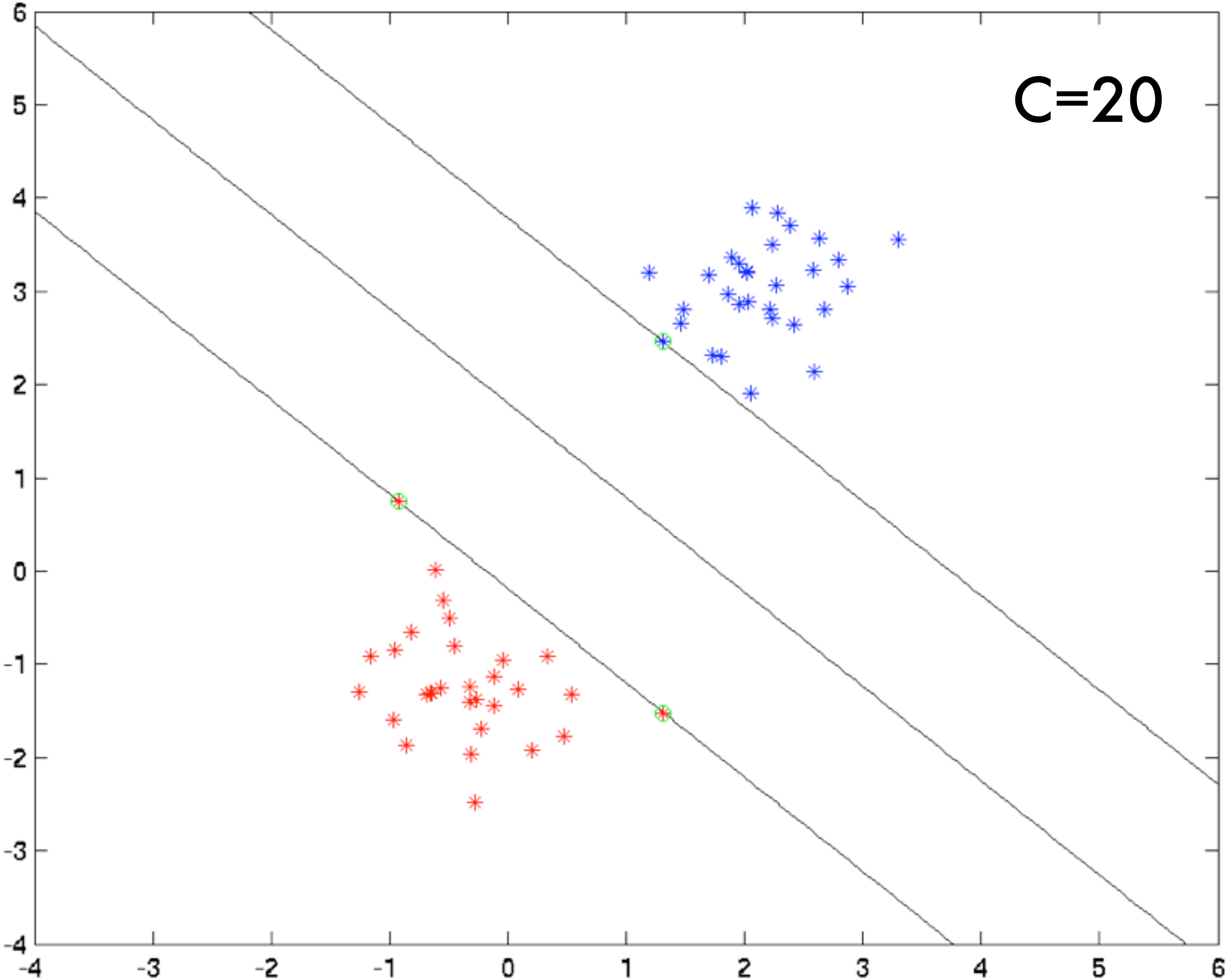
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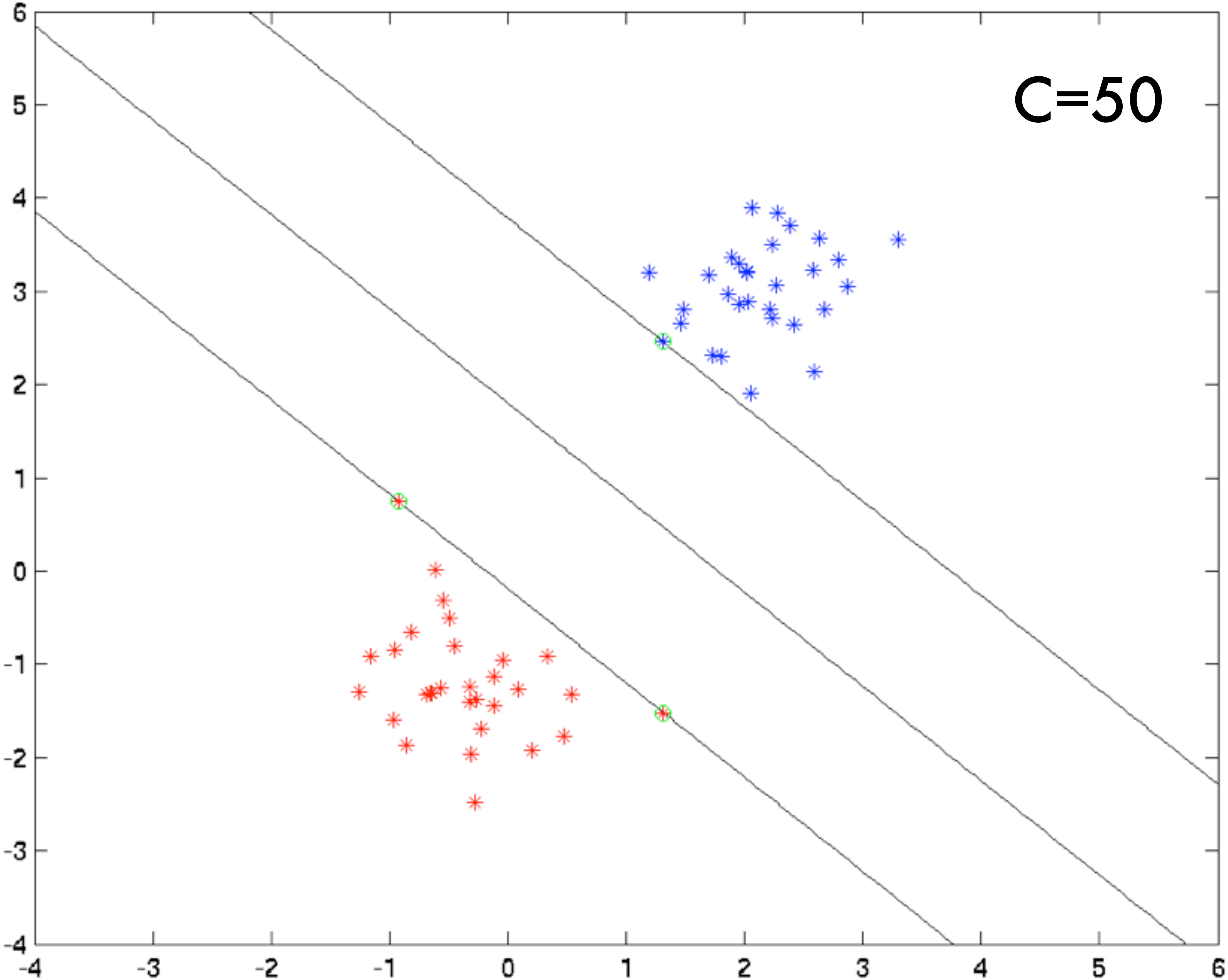
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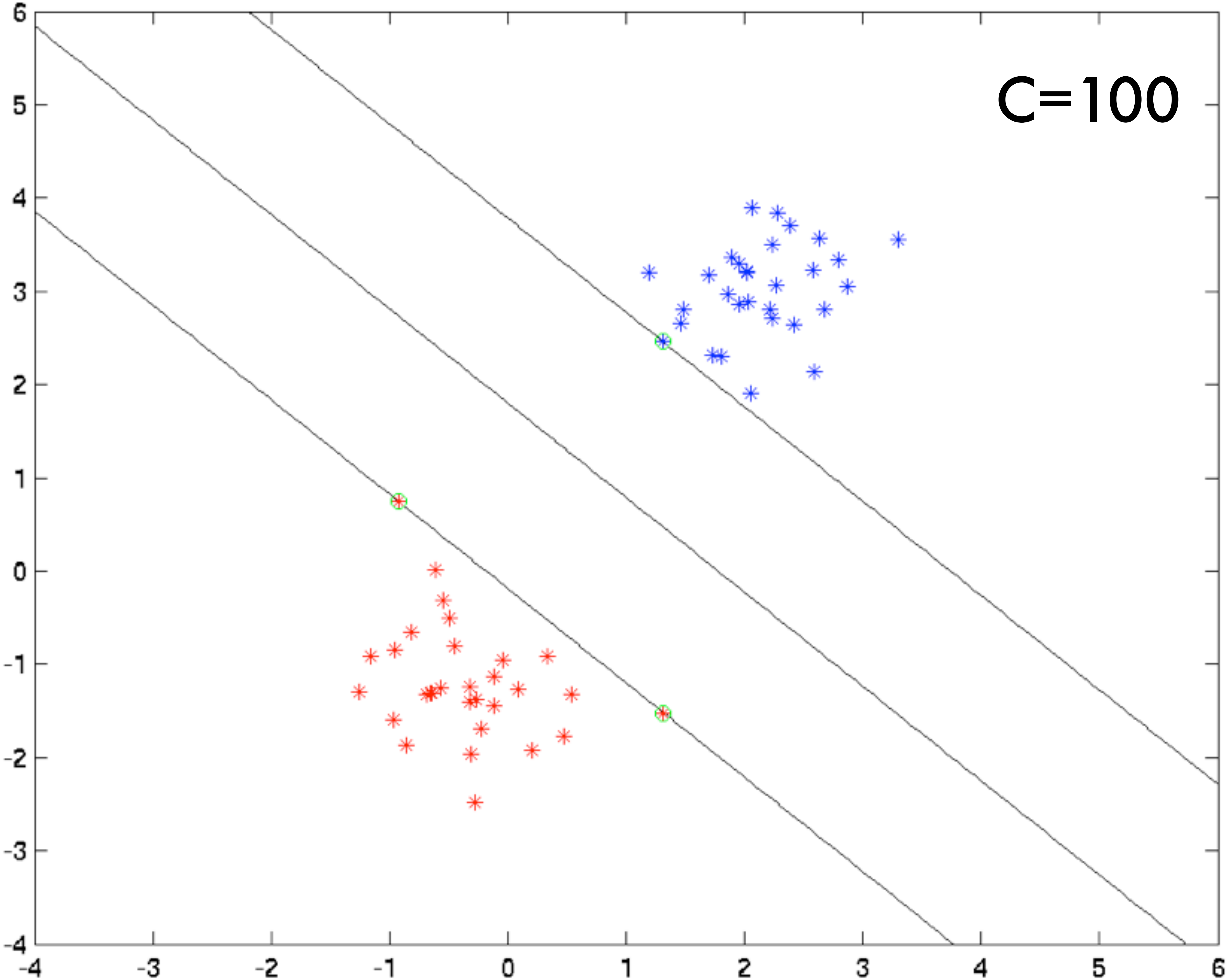
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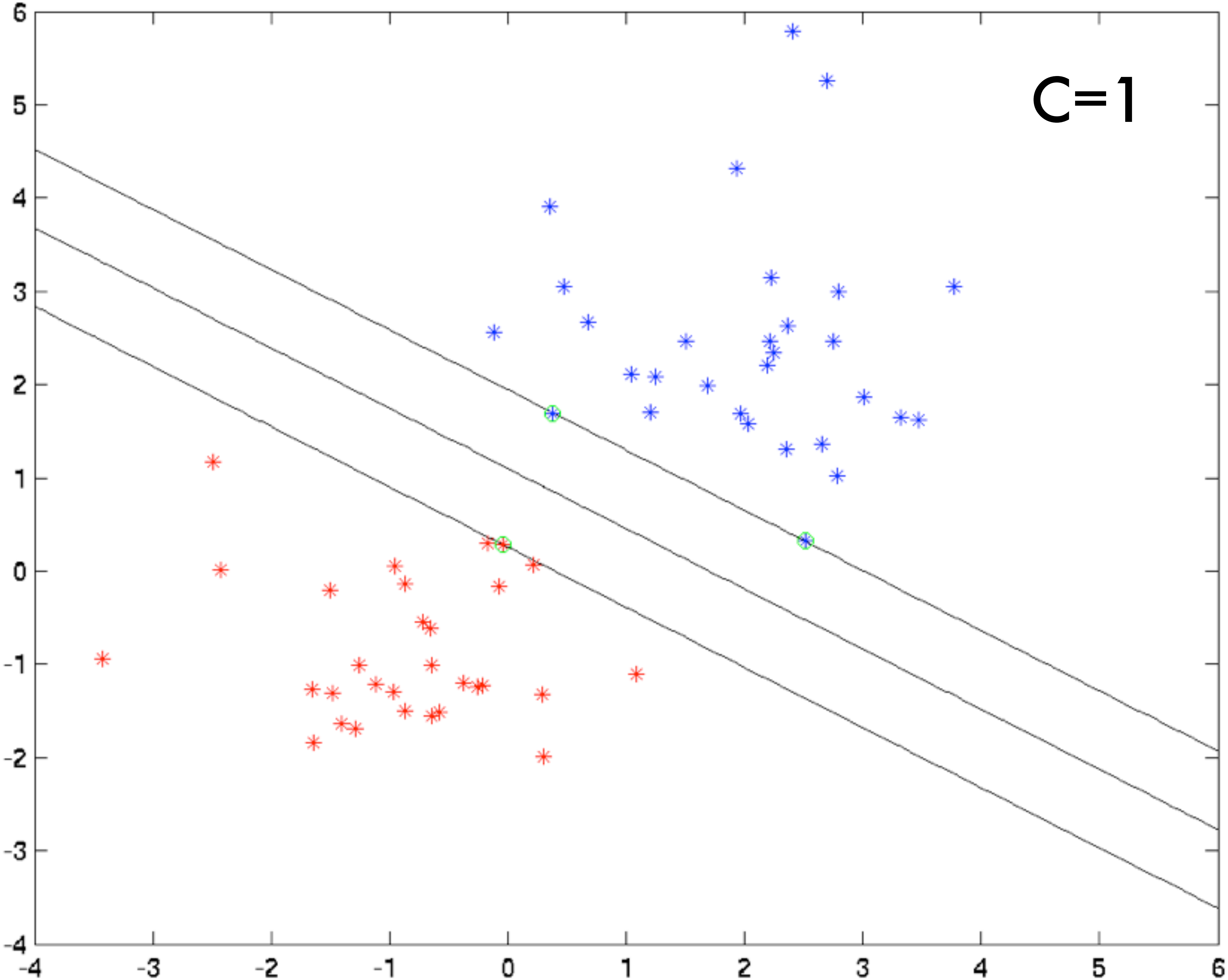
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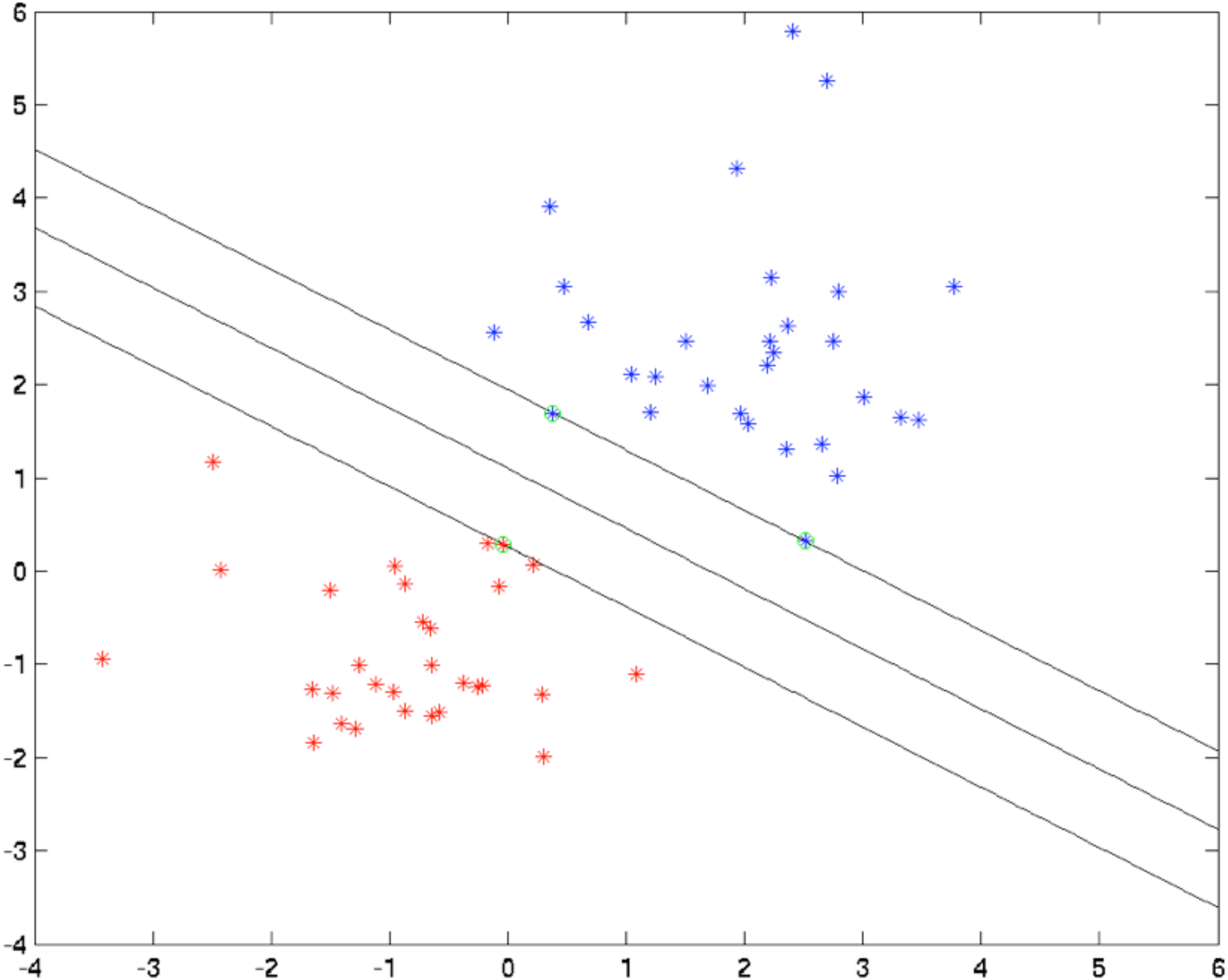
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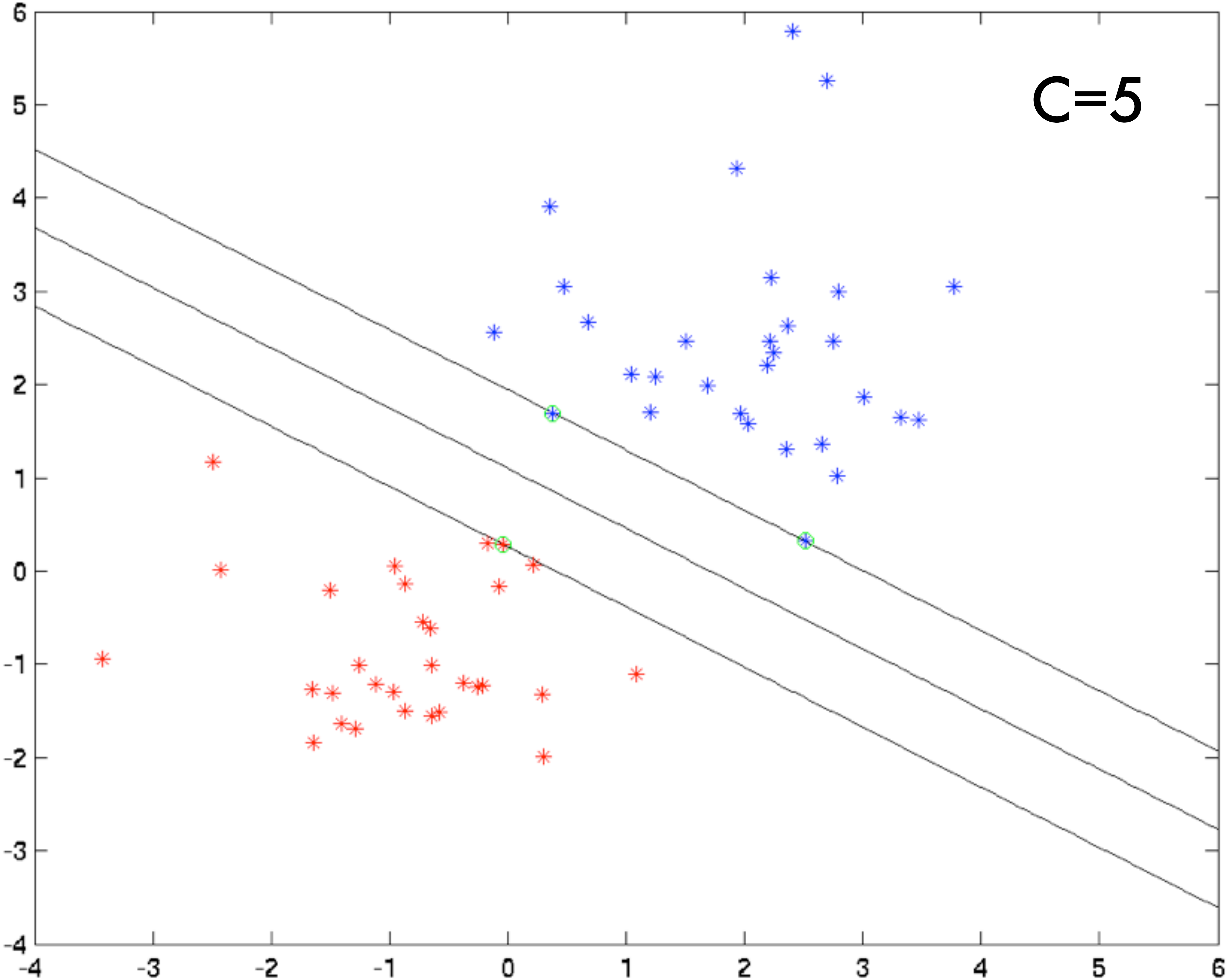
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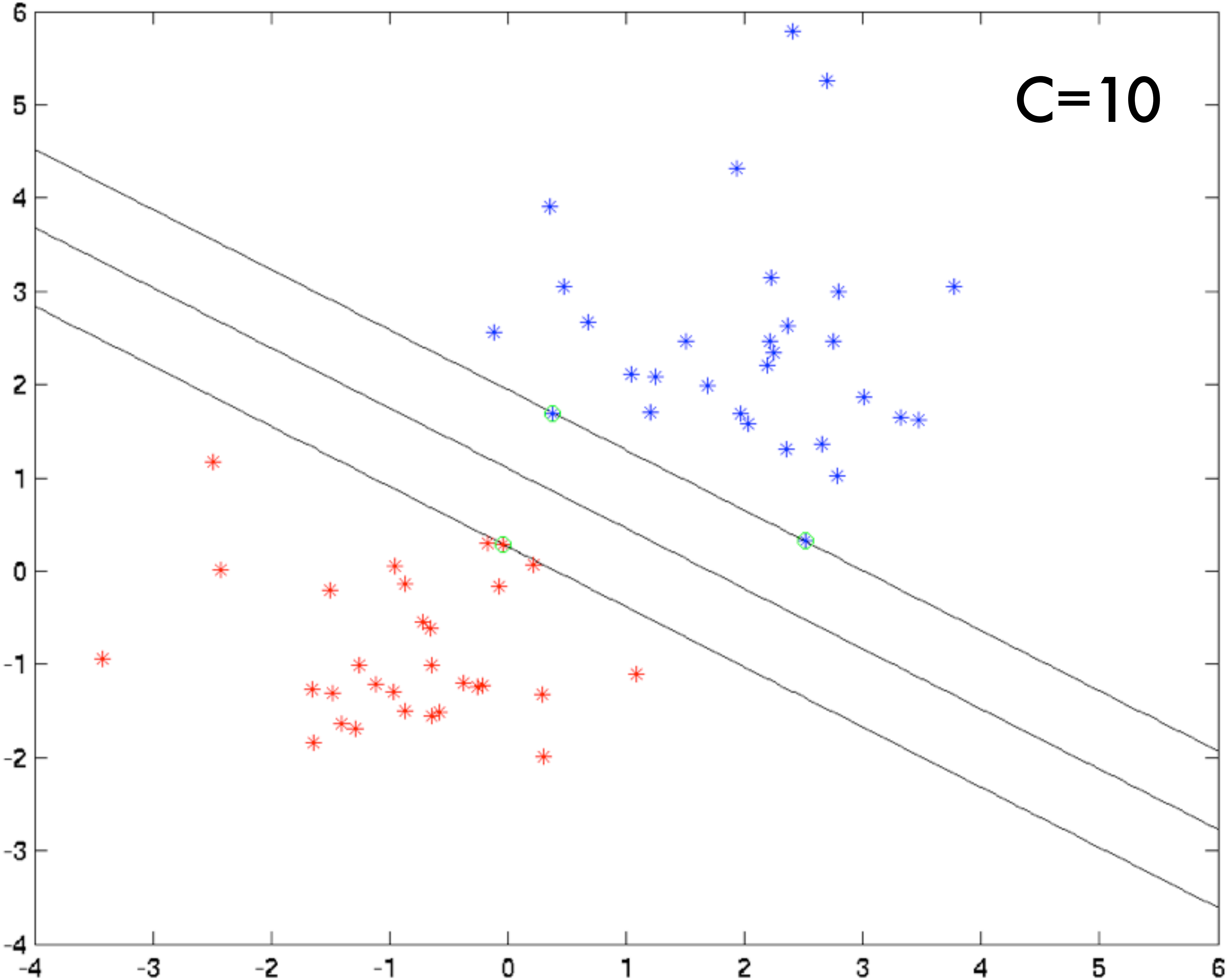
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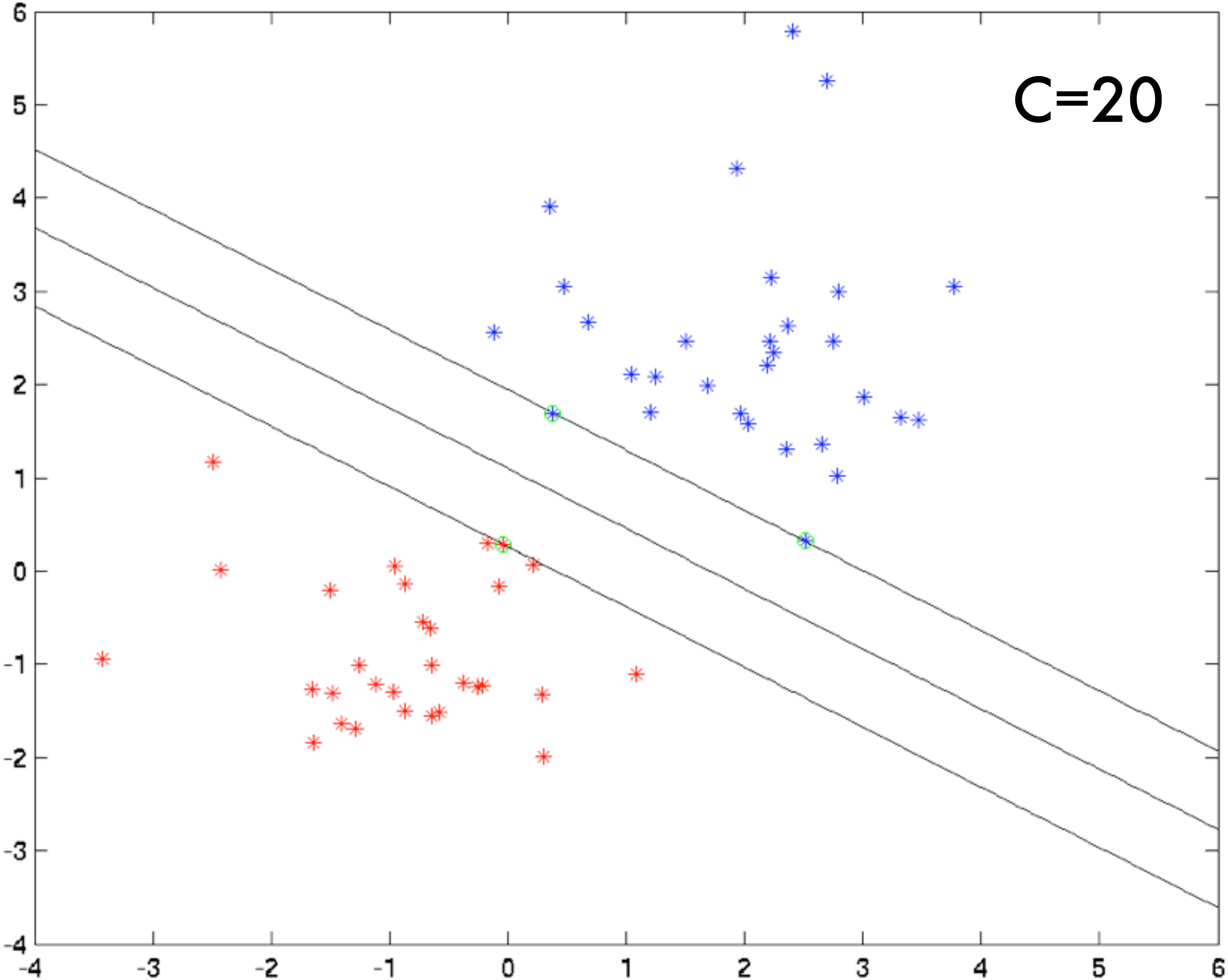
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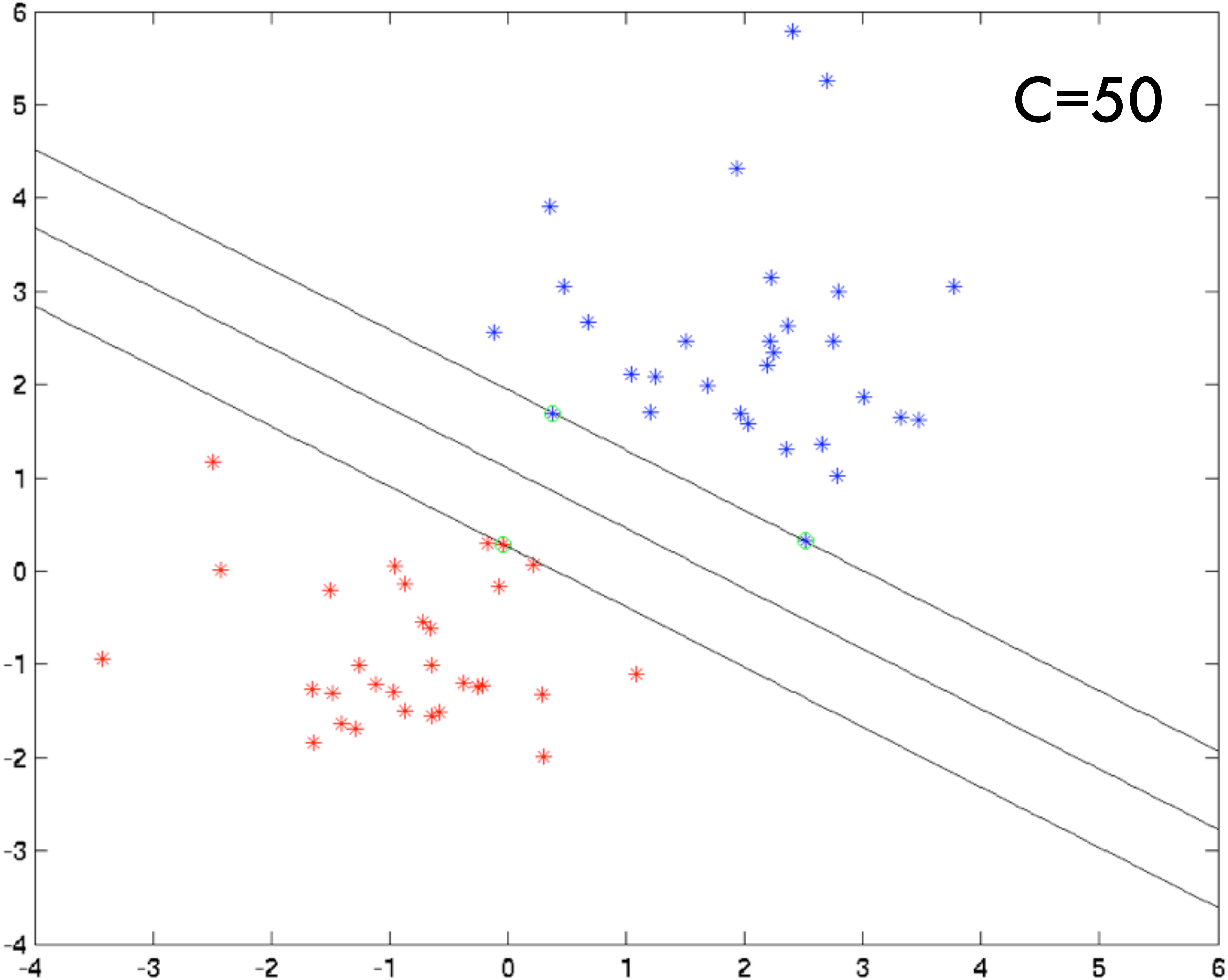

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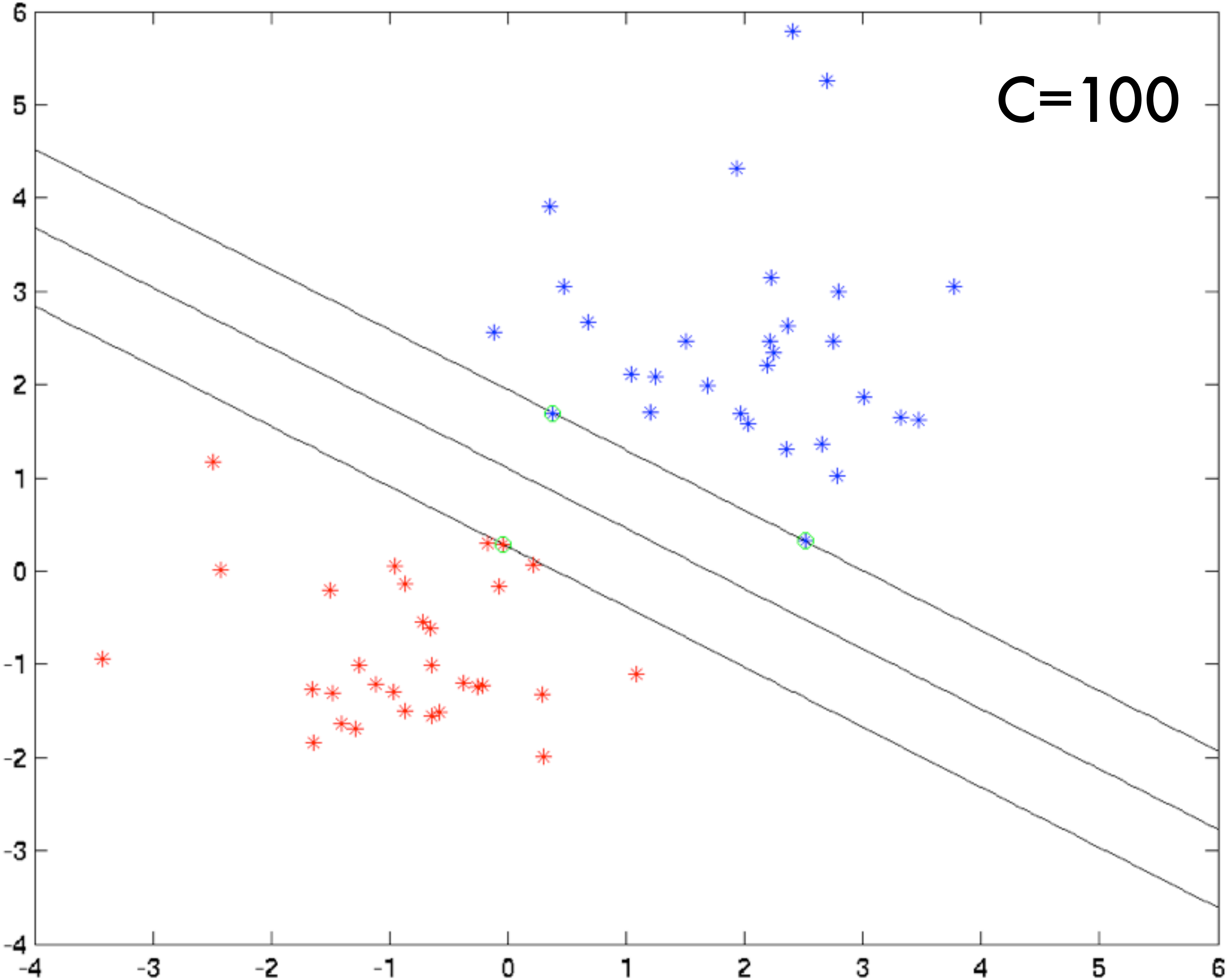

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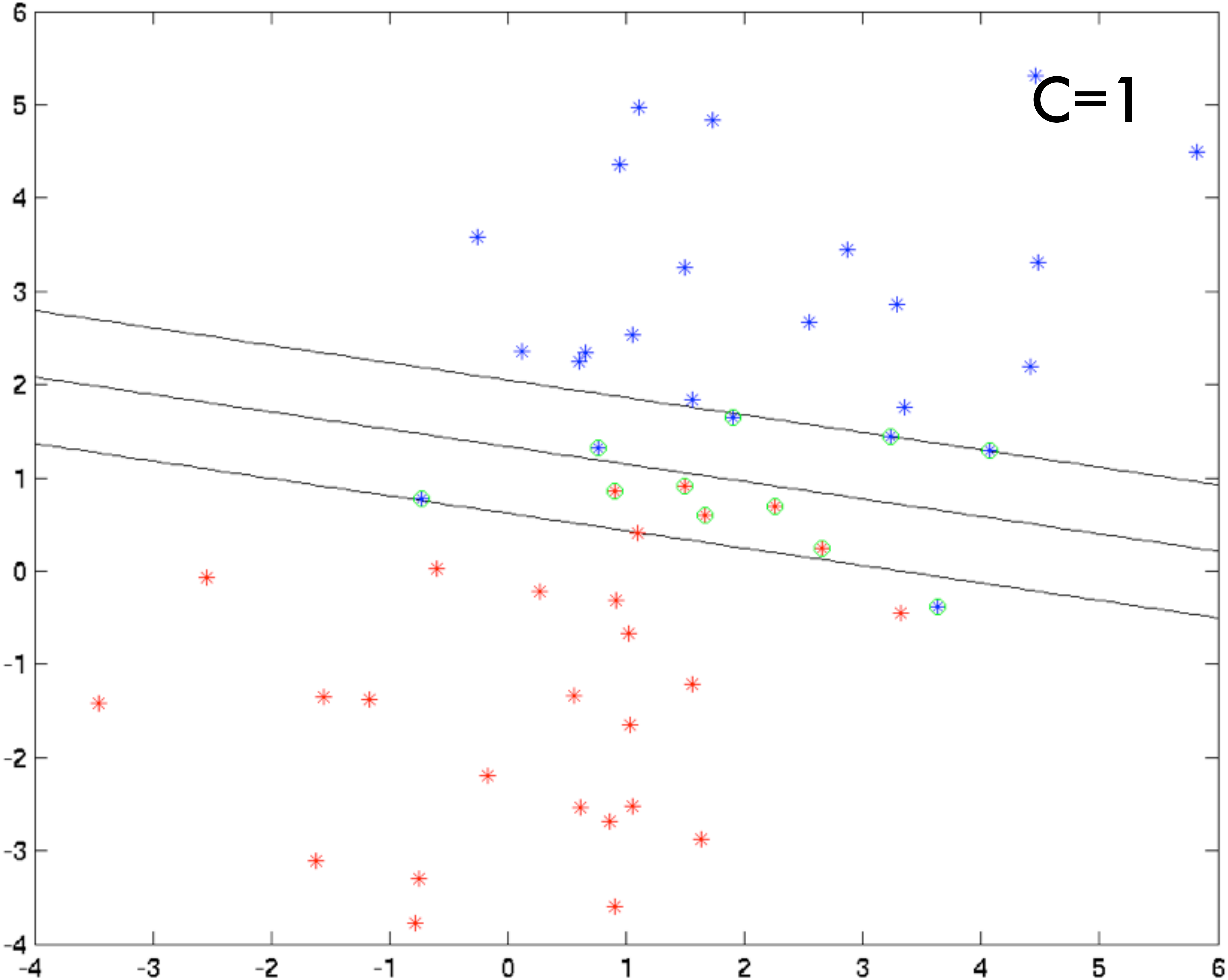
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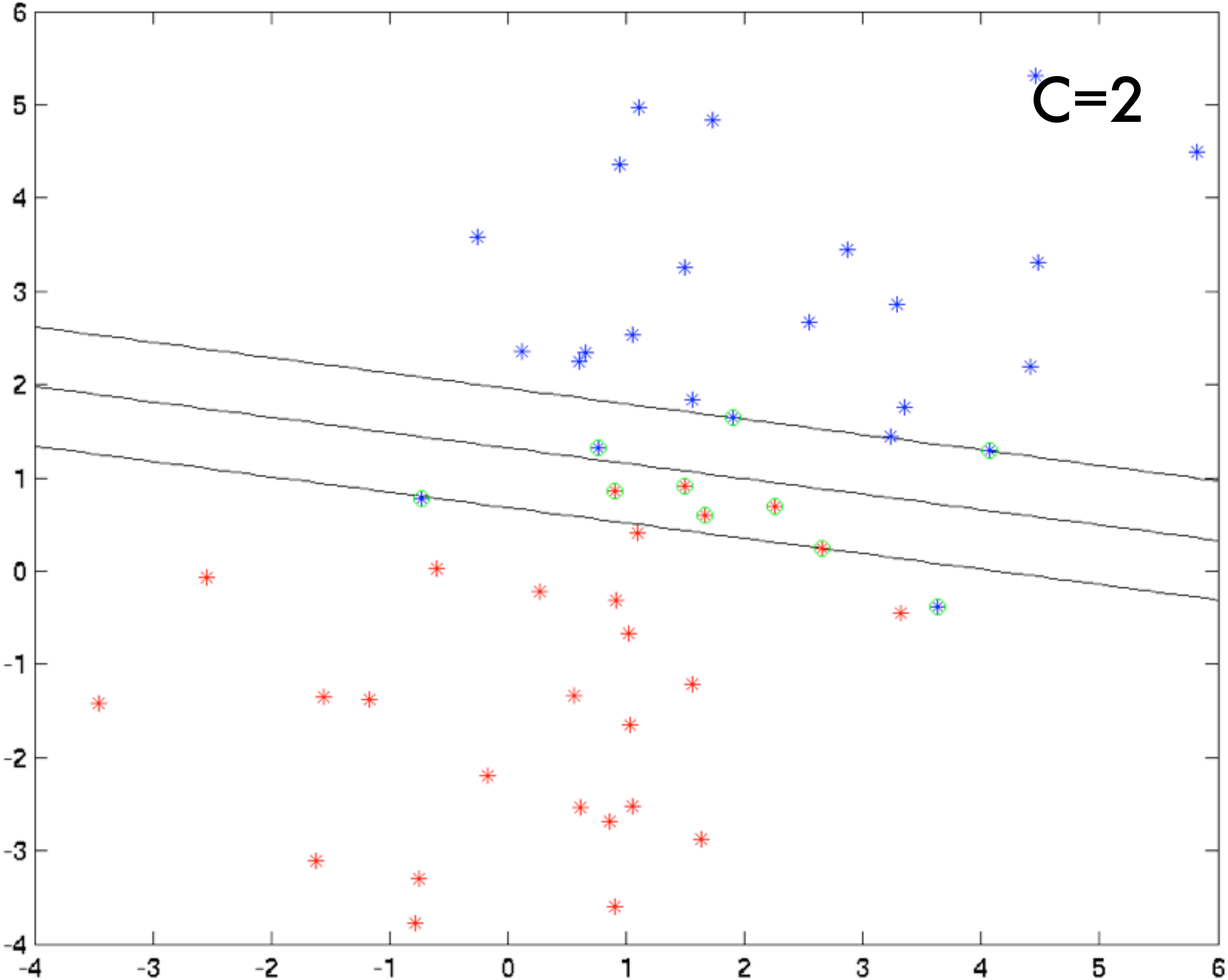
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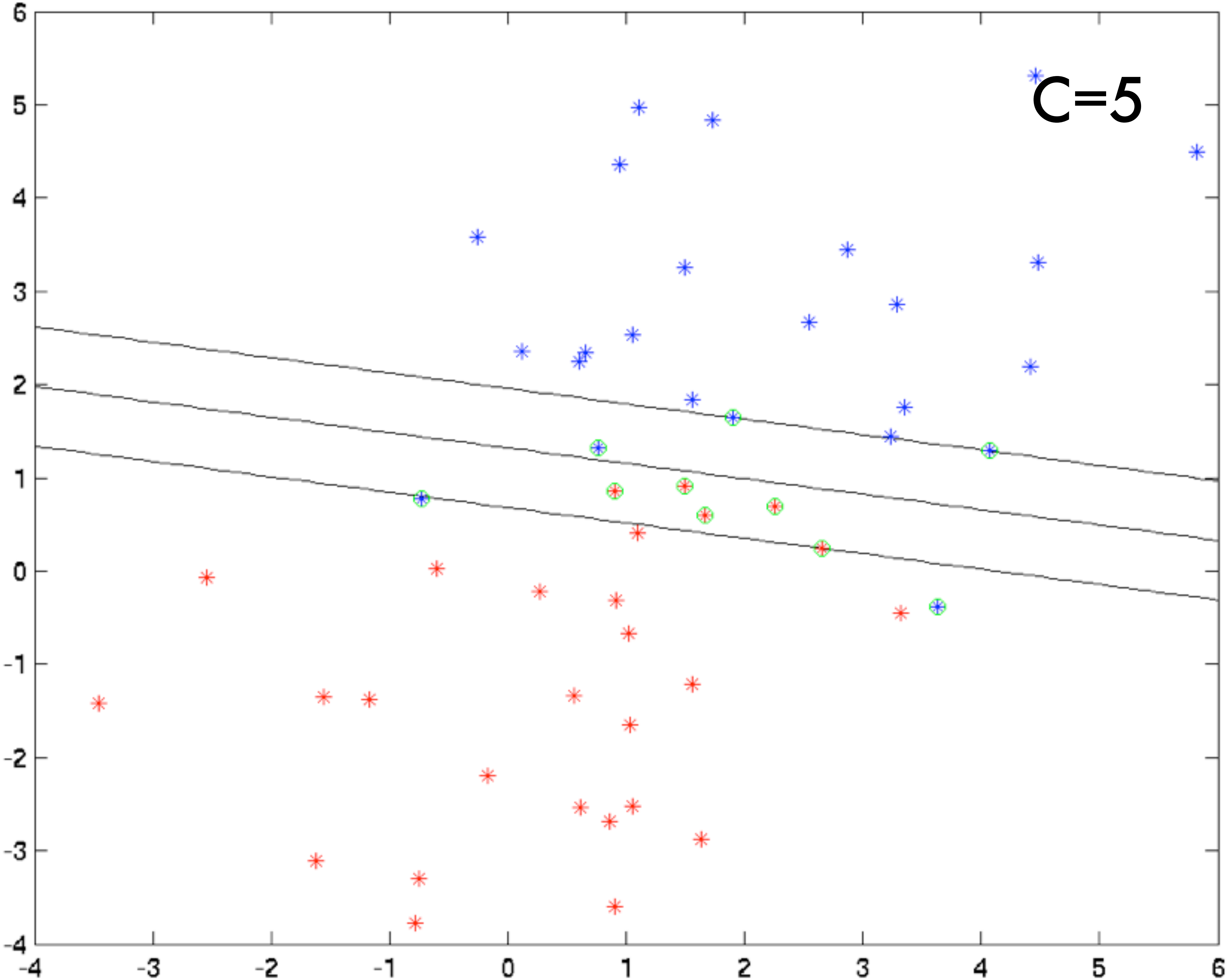

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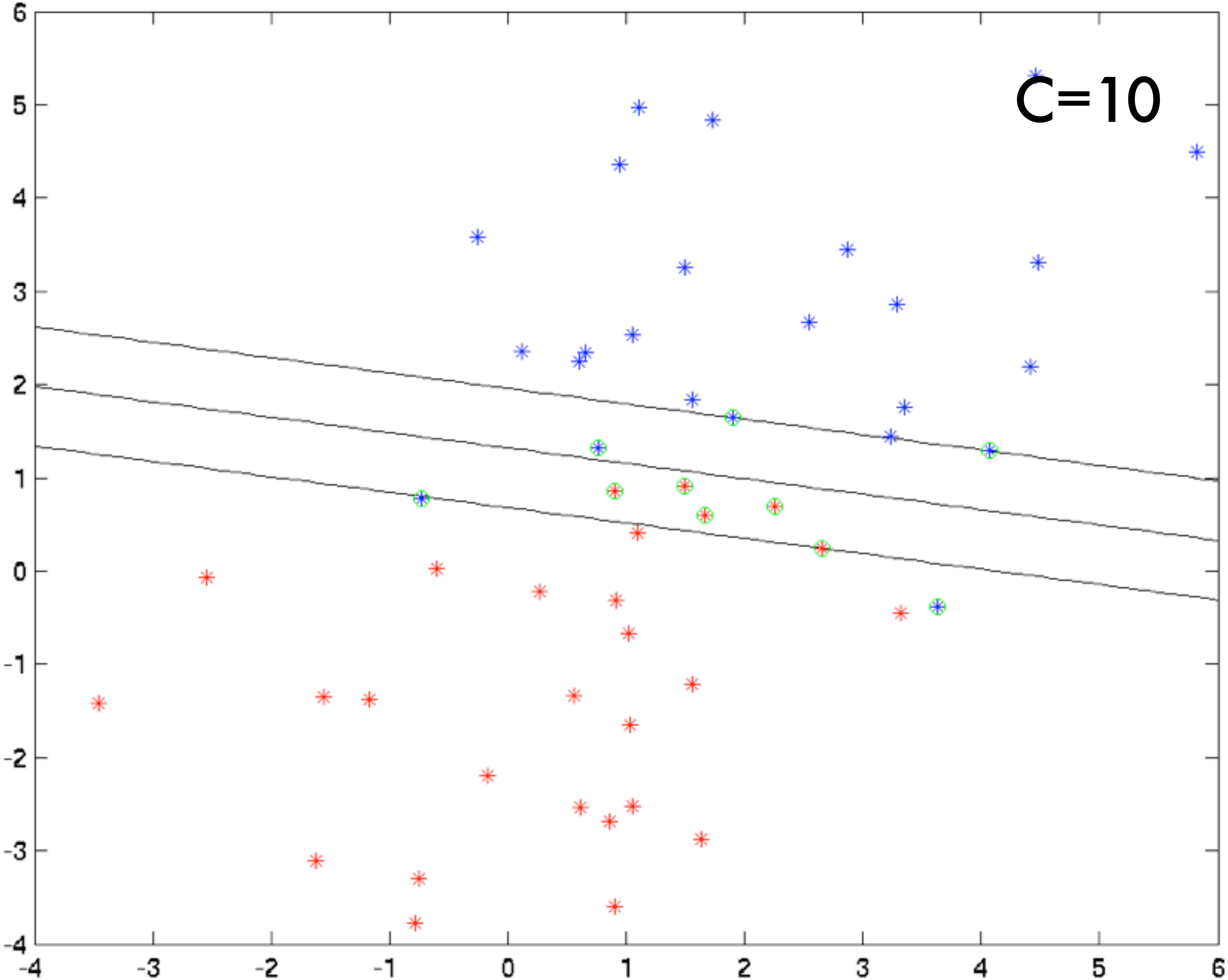
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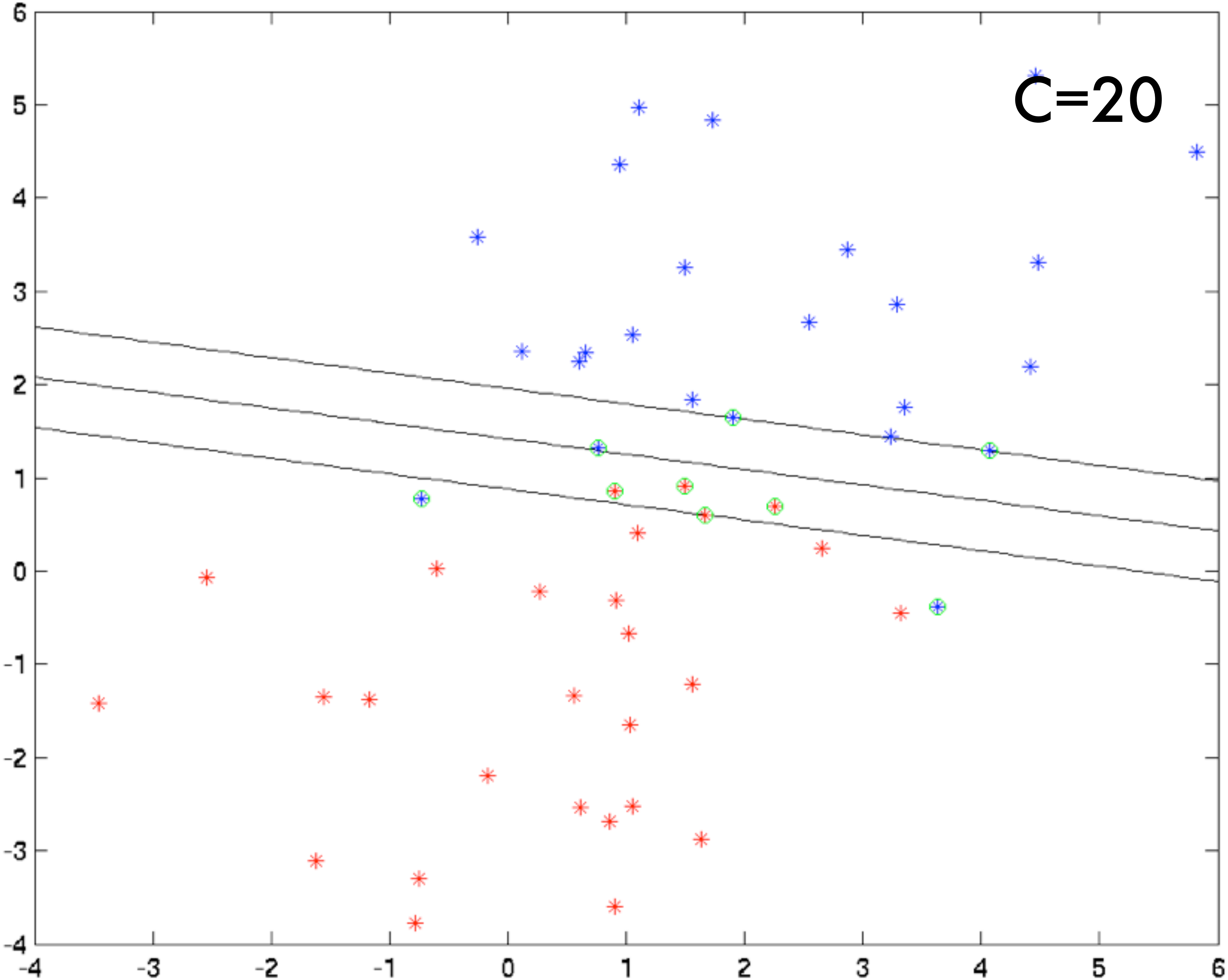
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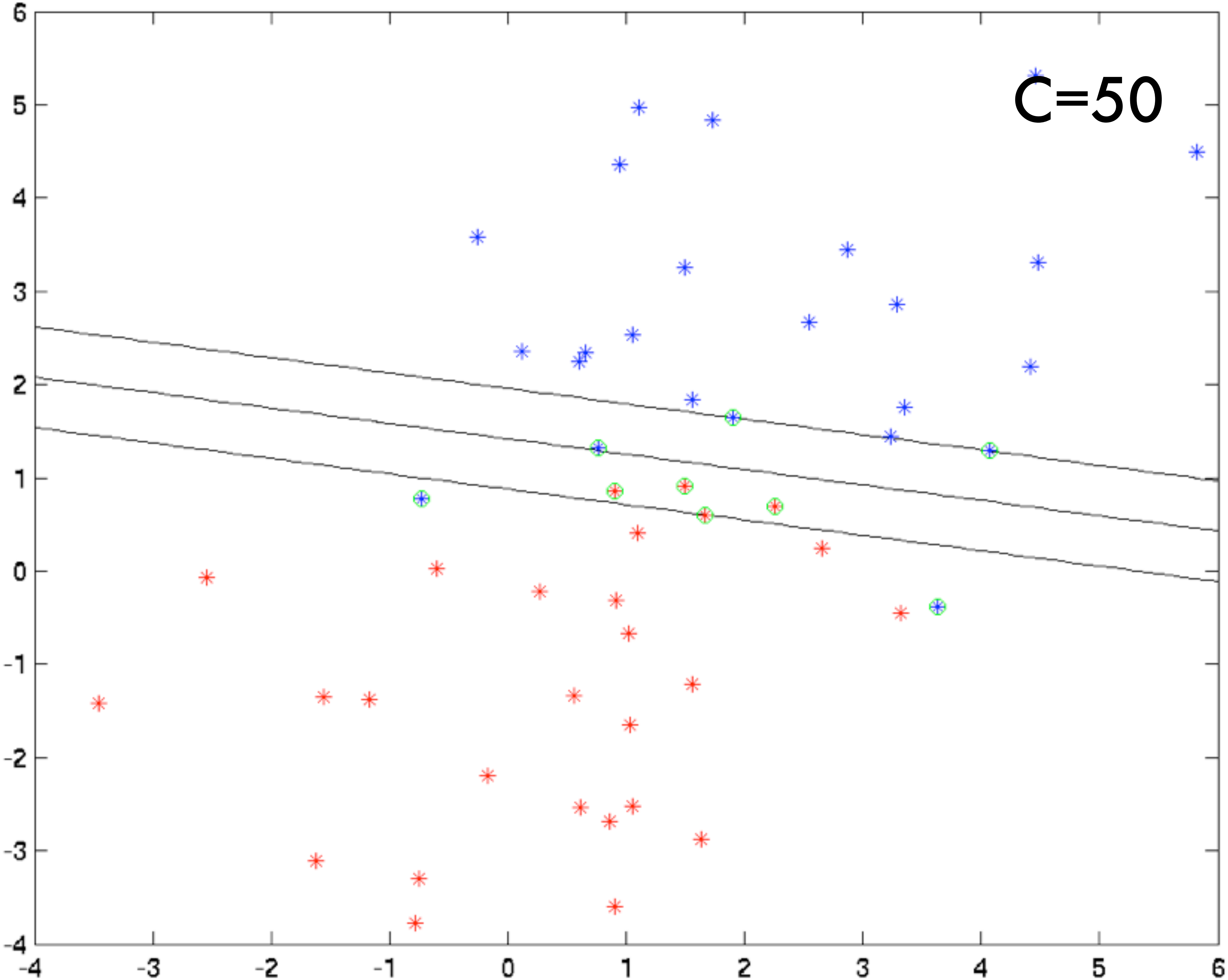
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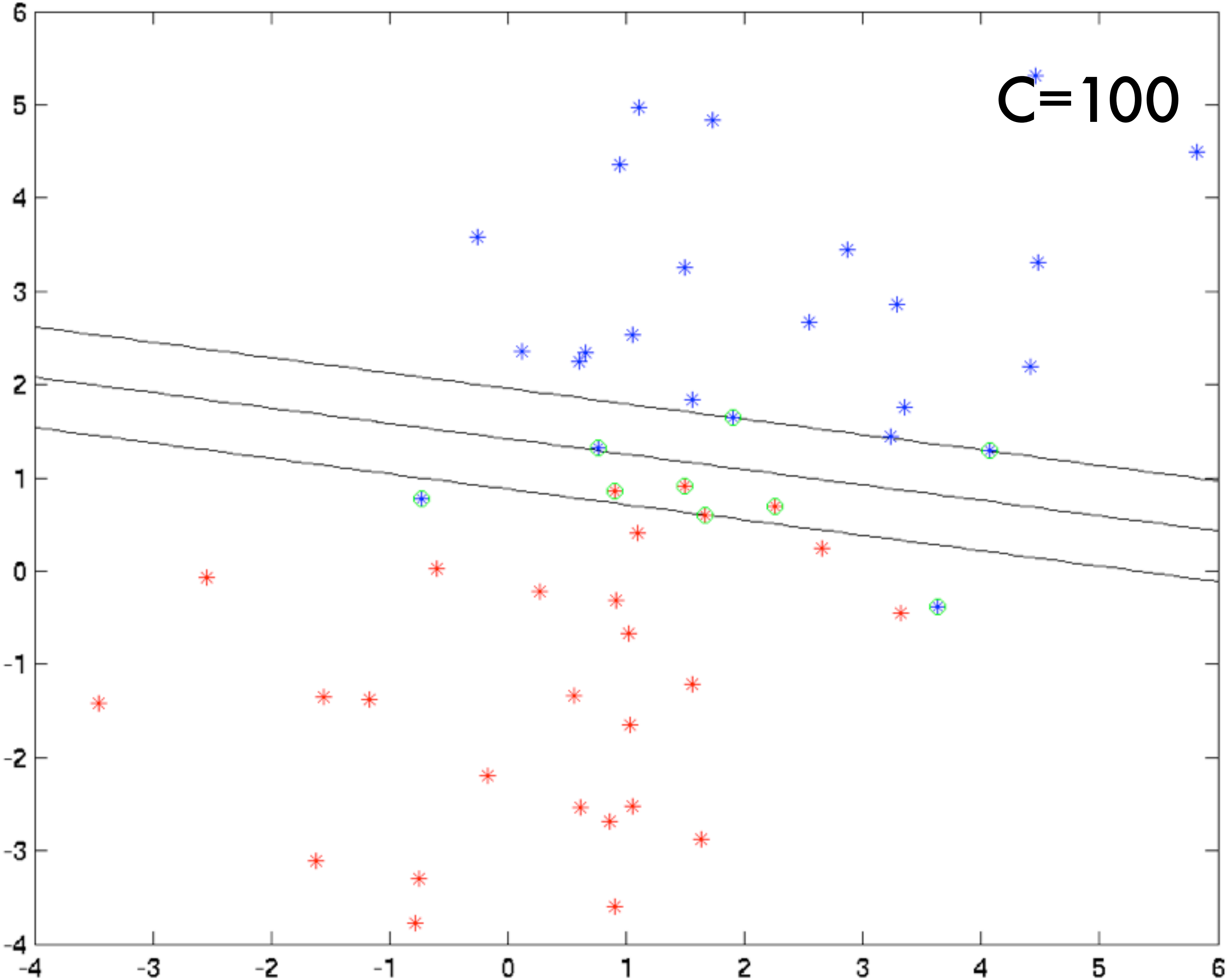
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Solving the optimization problem

- Dual problem

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

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

- If problem is small enough (1000s of variables) we can use off-the-shelf solver (CVXOPT, CPLEX, OOQP, LOQO)
- For larger problem use fact that only SVs matter and solve in blocks (active set method).

Nonlinear Separation

The Kernel Trick

- **Linear soft margin problem**

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

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

- **Dual problem**

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

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

- **Support vector expansion**

$$f(x) = \sum_i \alpha_i y_i \langle x_i, x\rangle + b$$

The Kernel Trick

- **Linear soft margin problem**

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

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

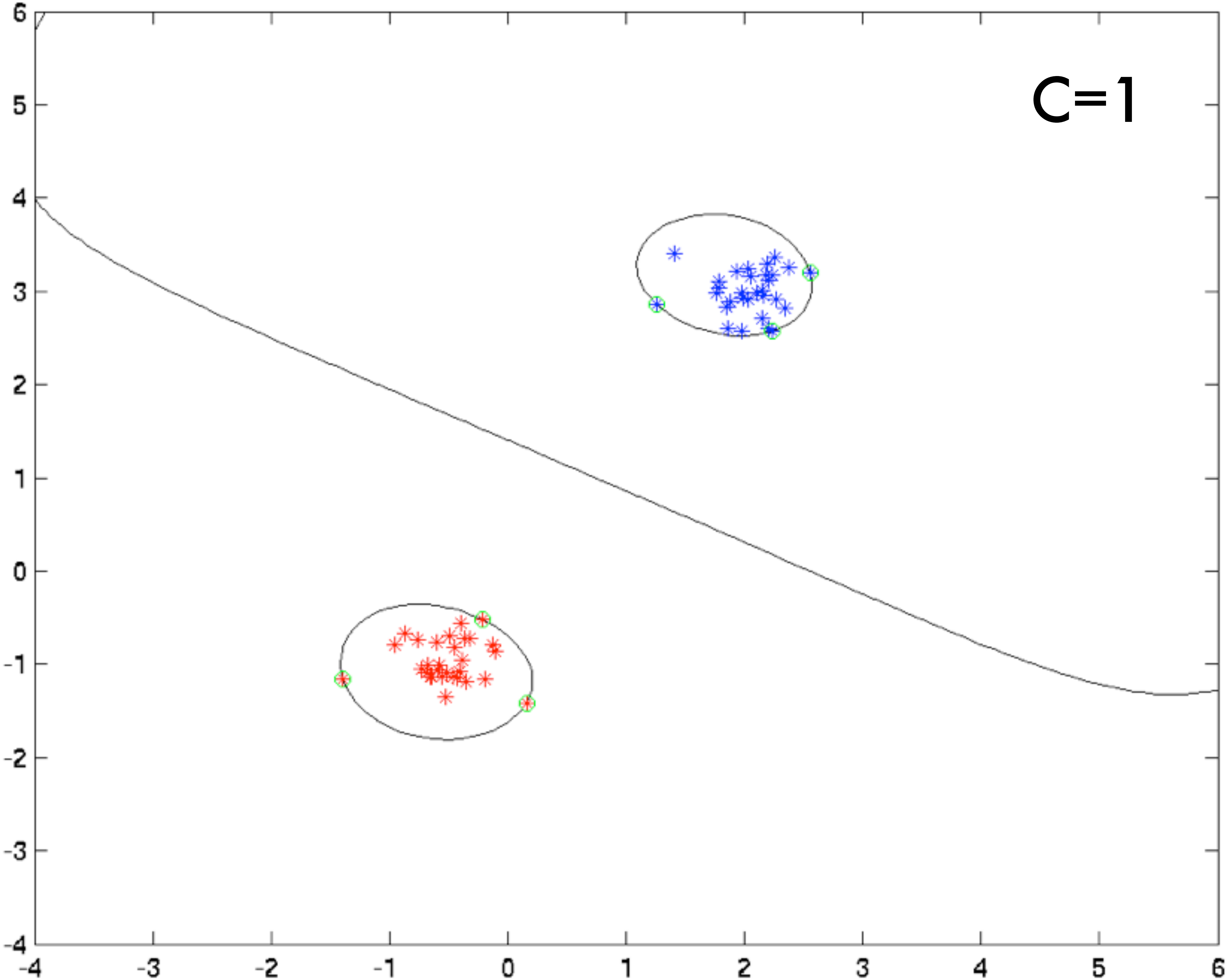
- **Dual problem**

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

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

- **Support vector expansion**

$$f(x) = \sum_i \alpha_i y_i k(x_i, x) + b$$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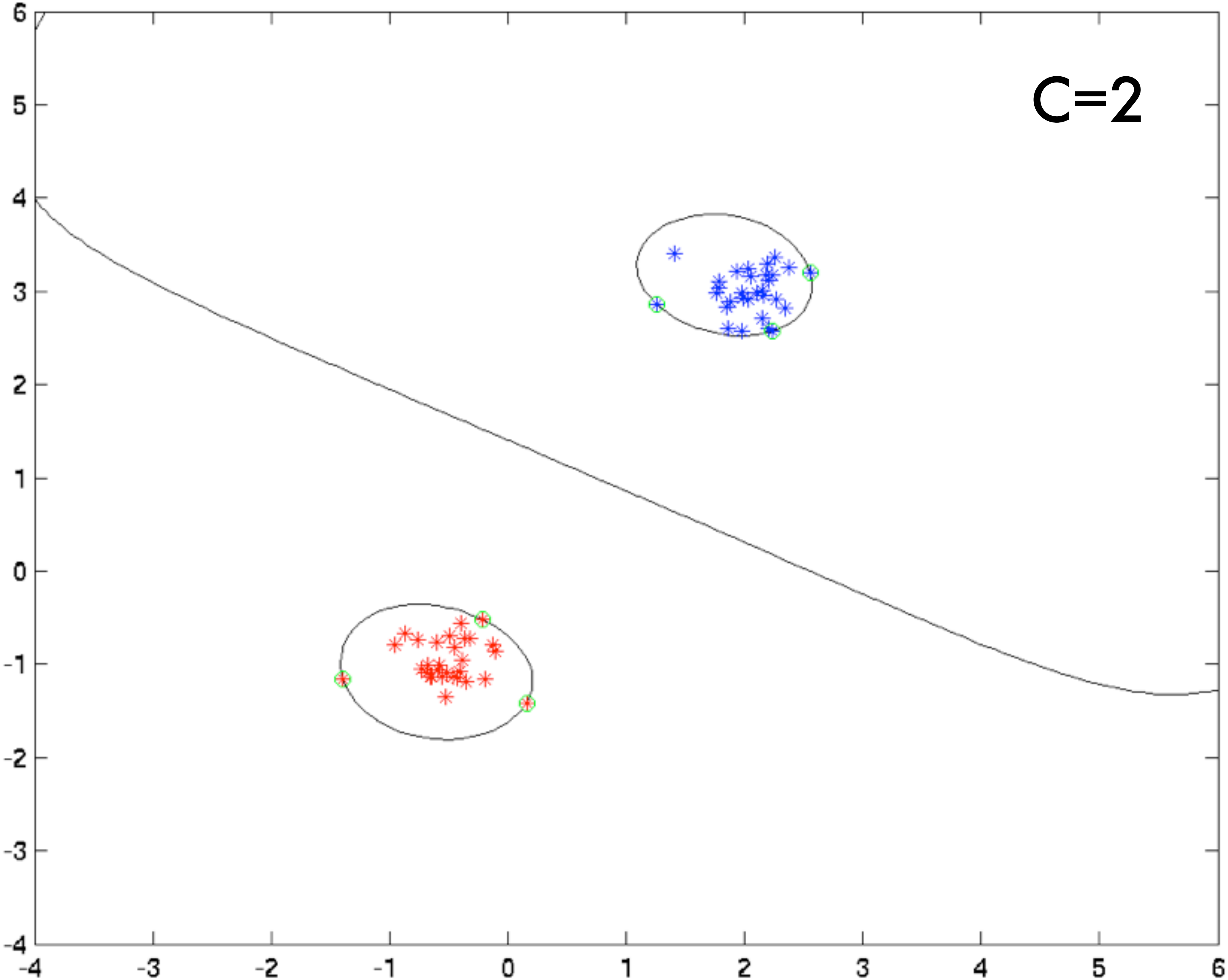

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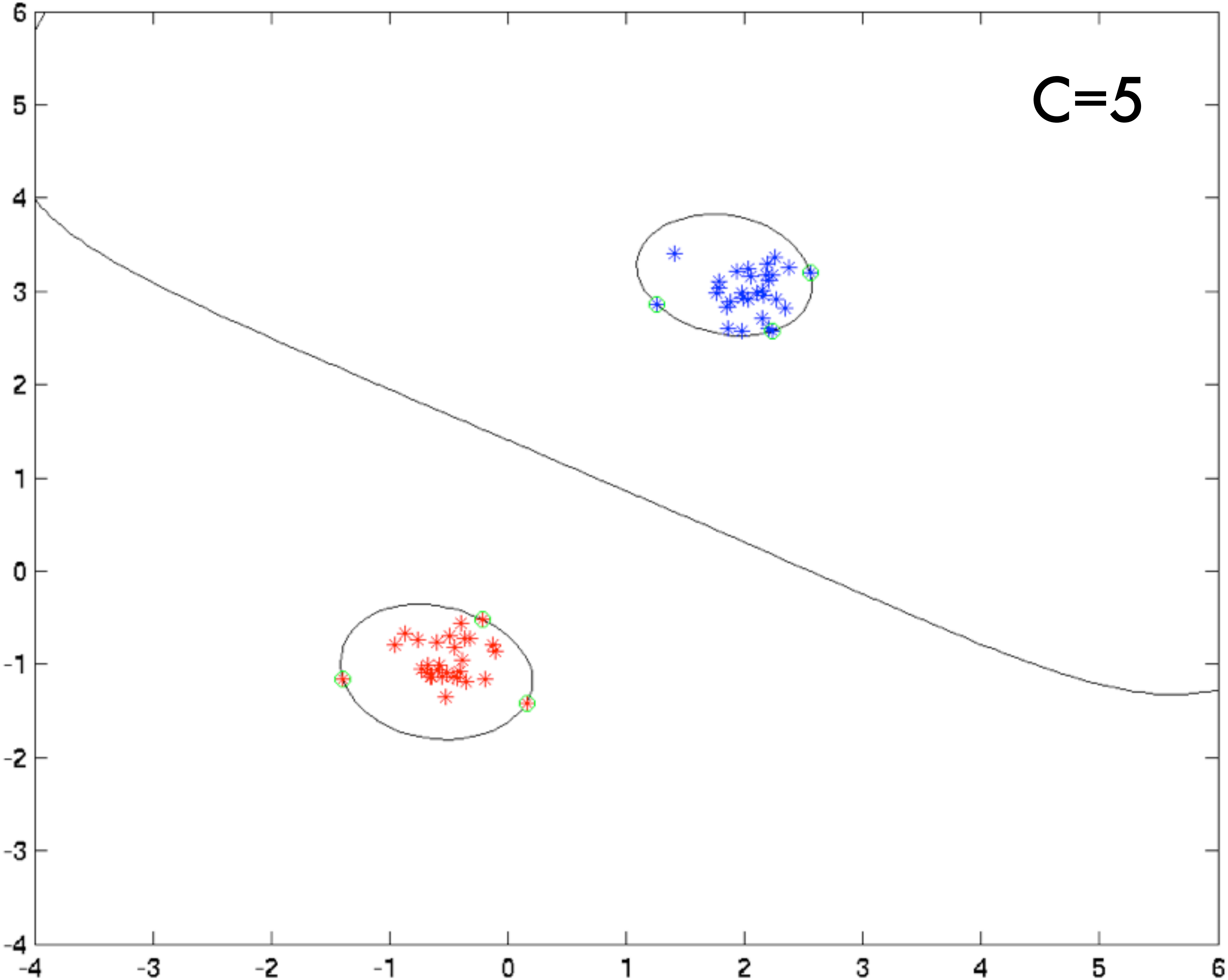
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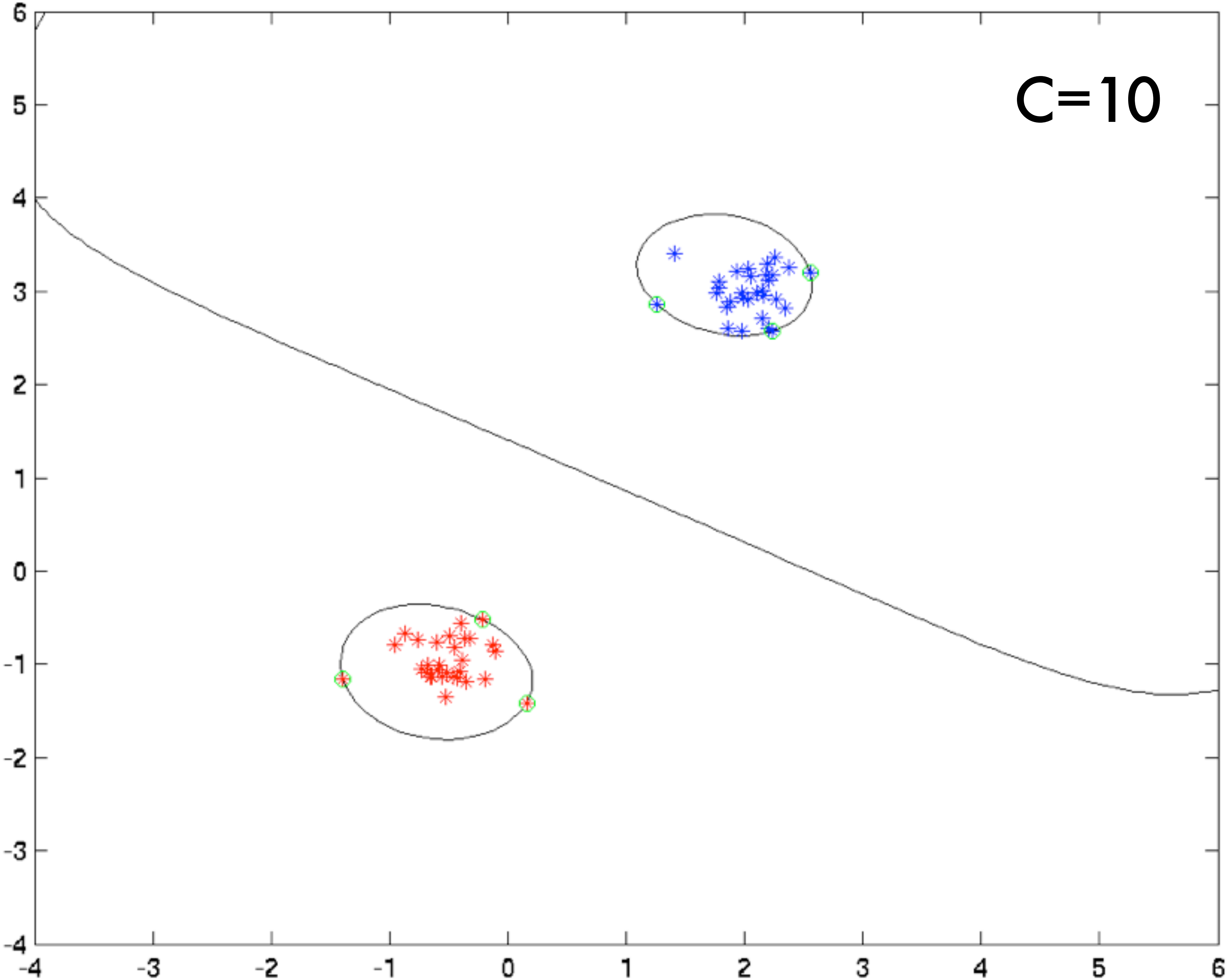
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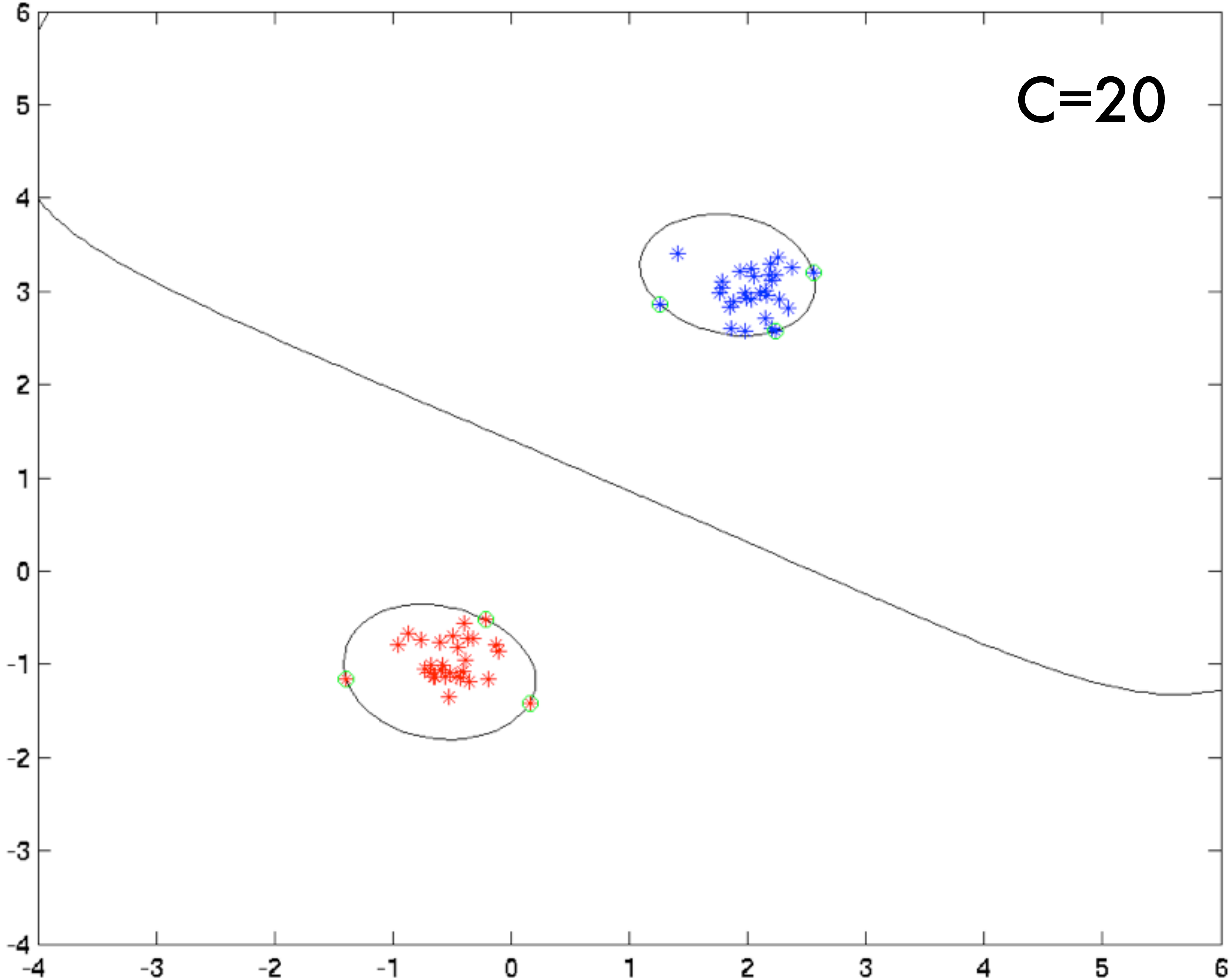
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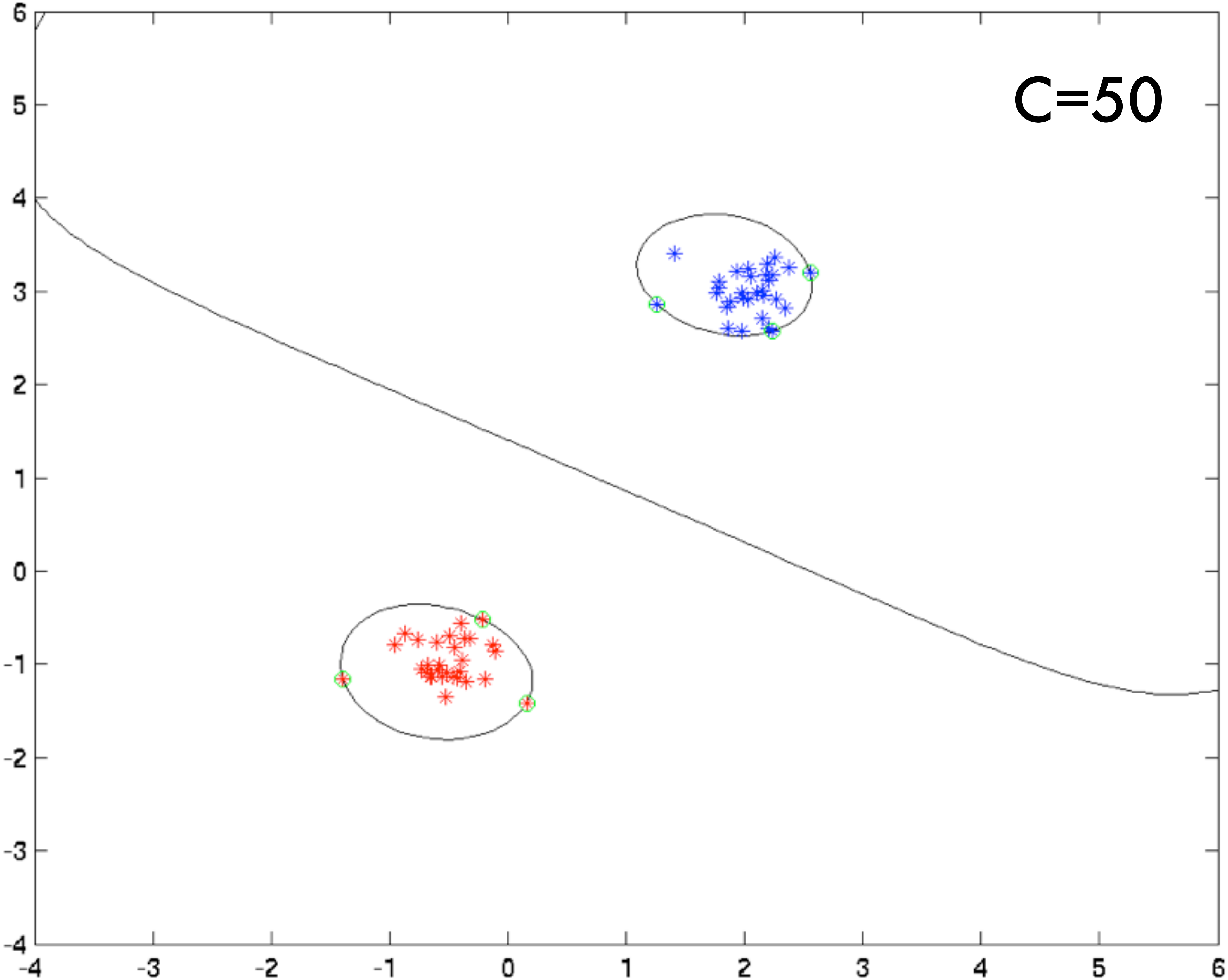

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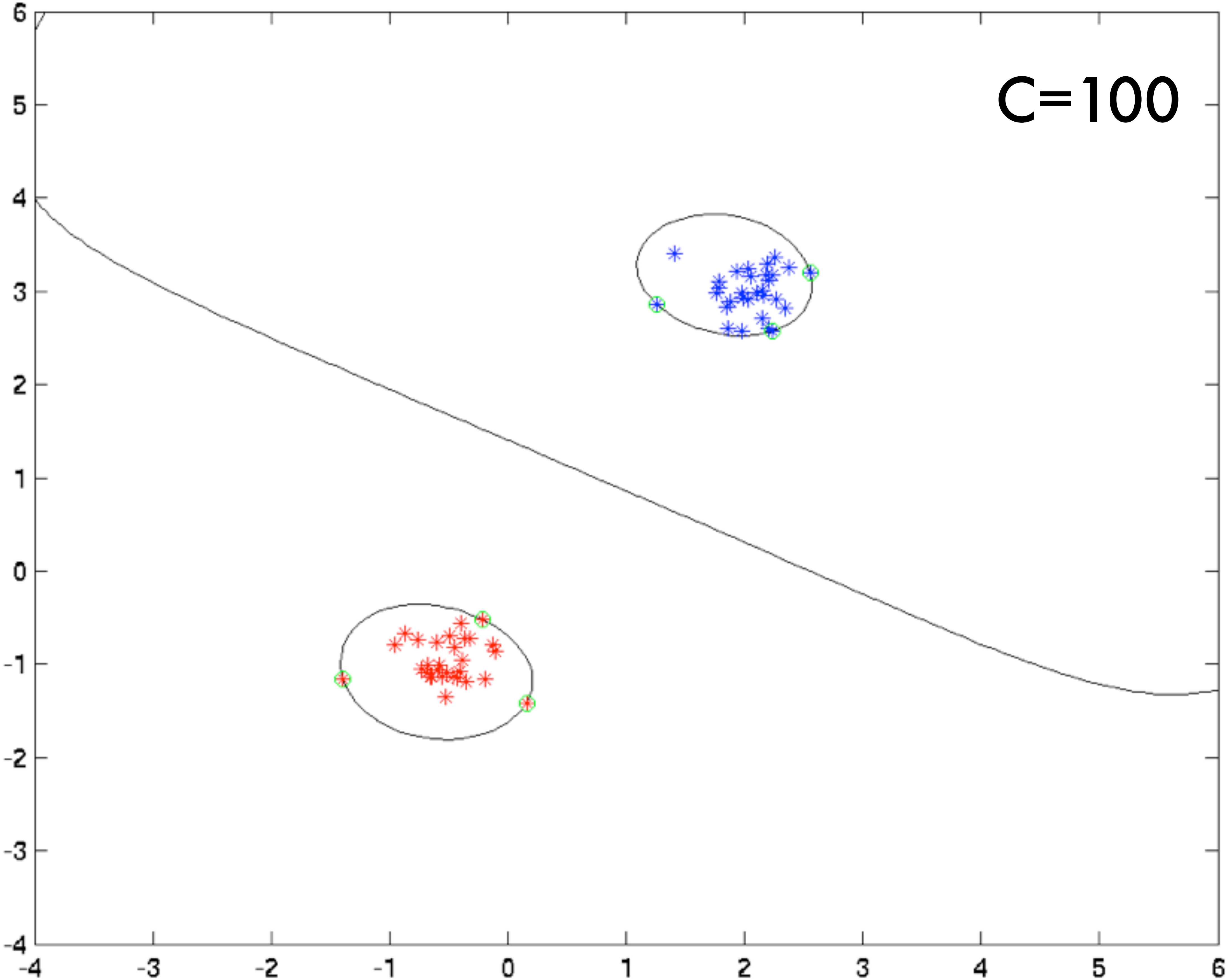
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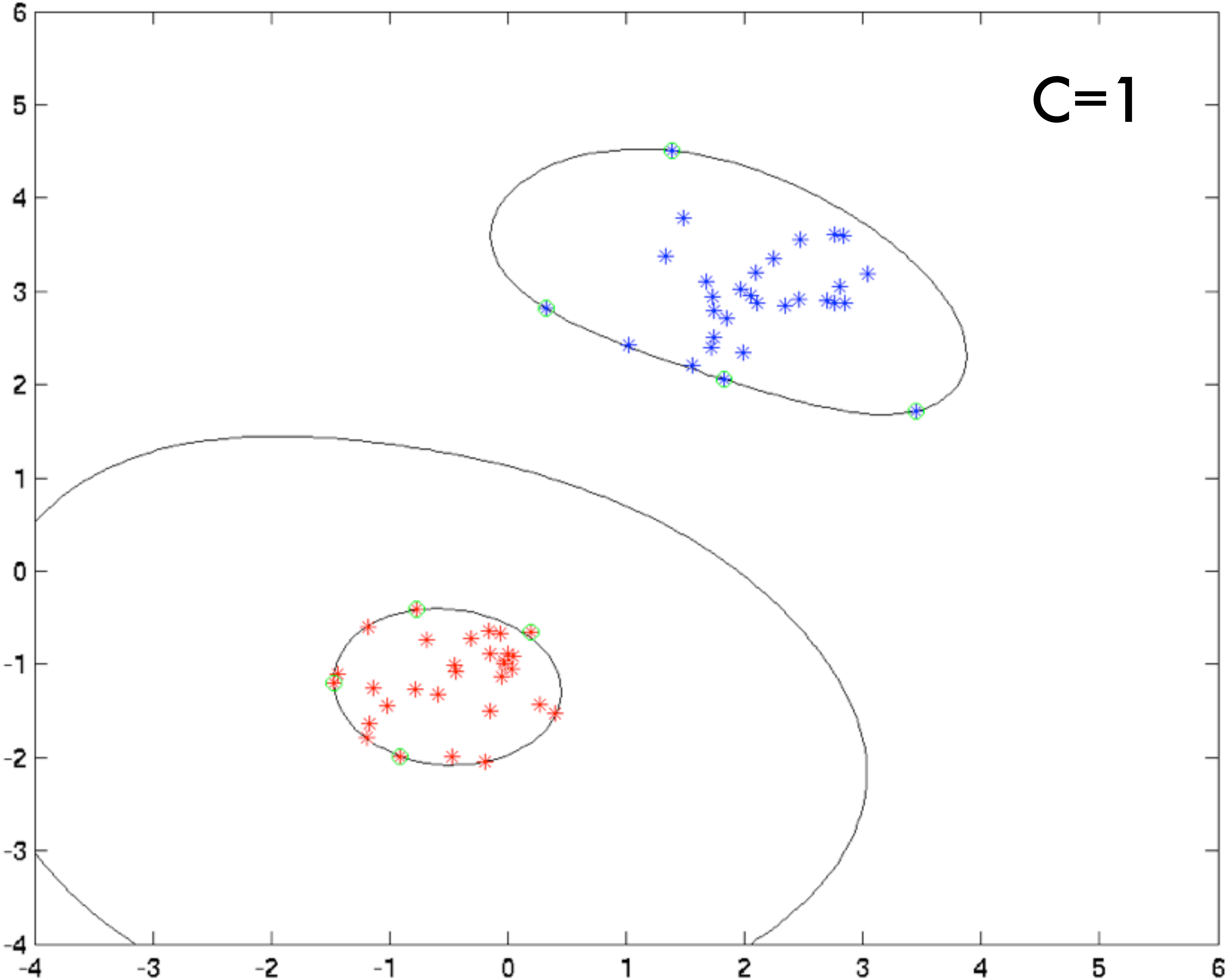
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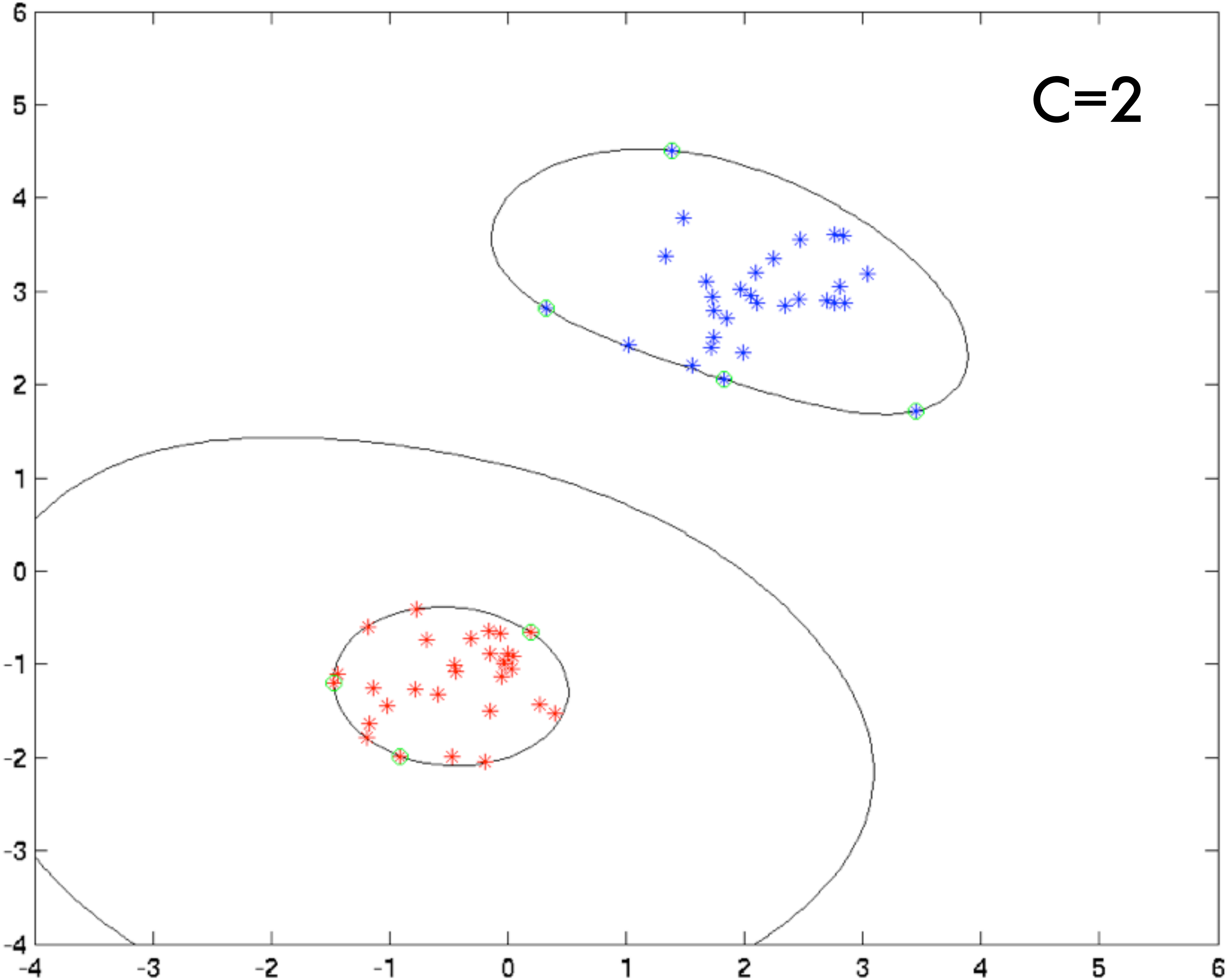
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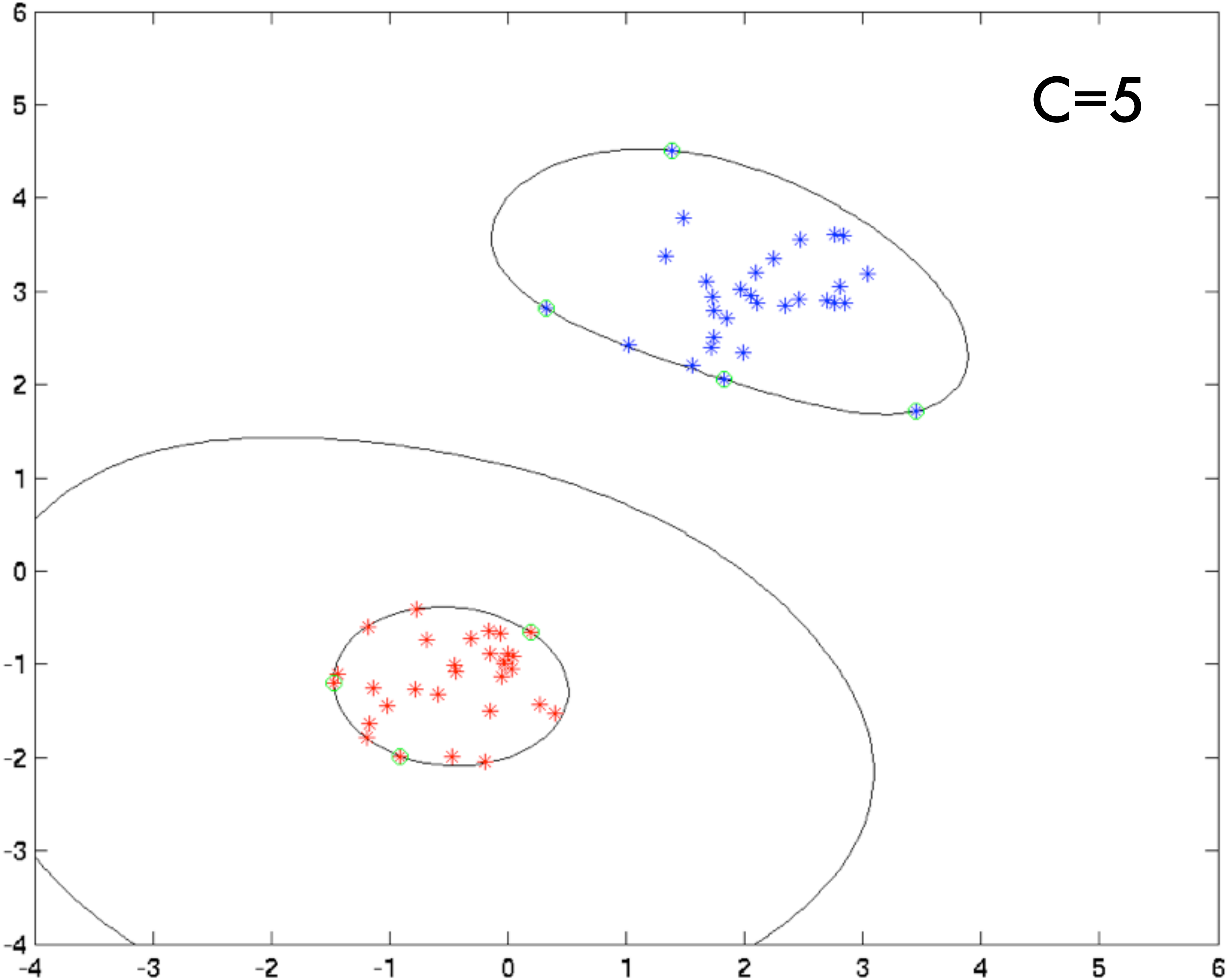
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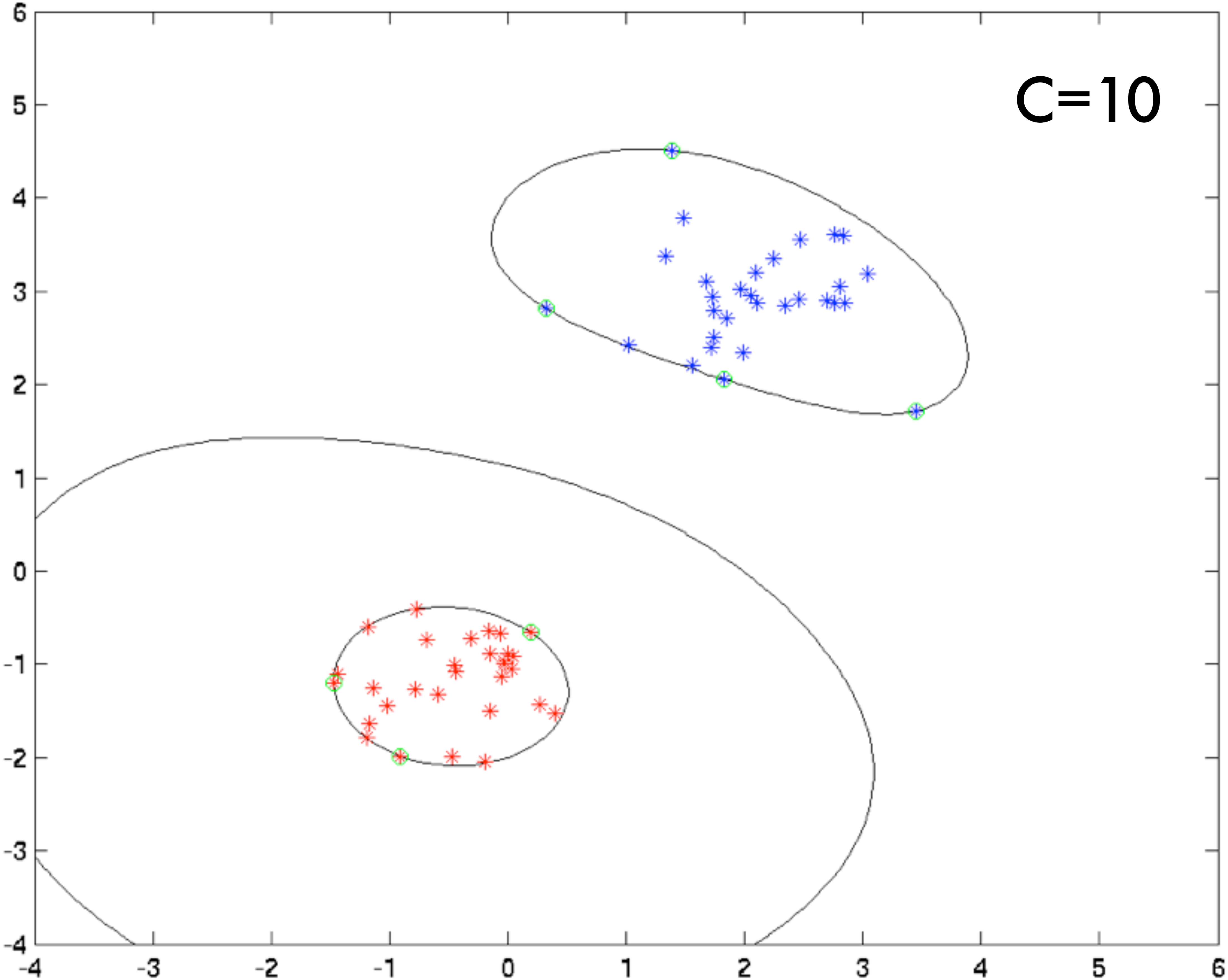

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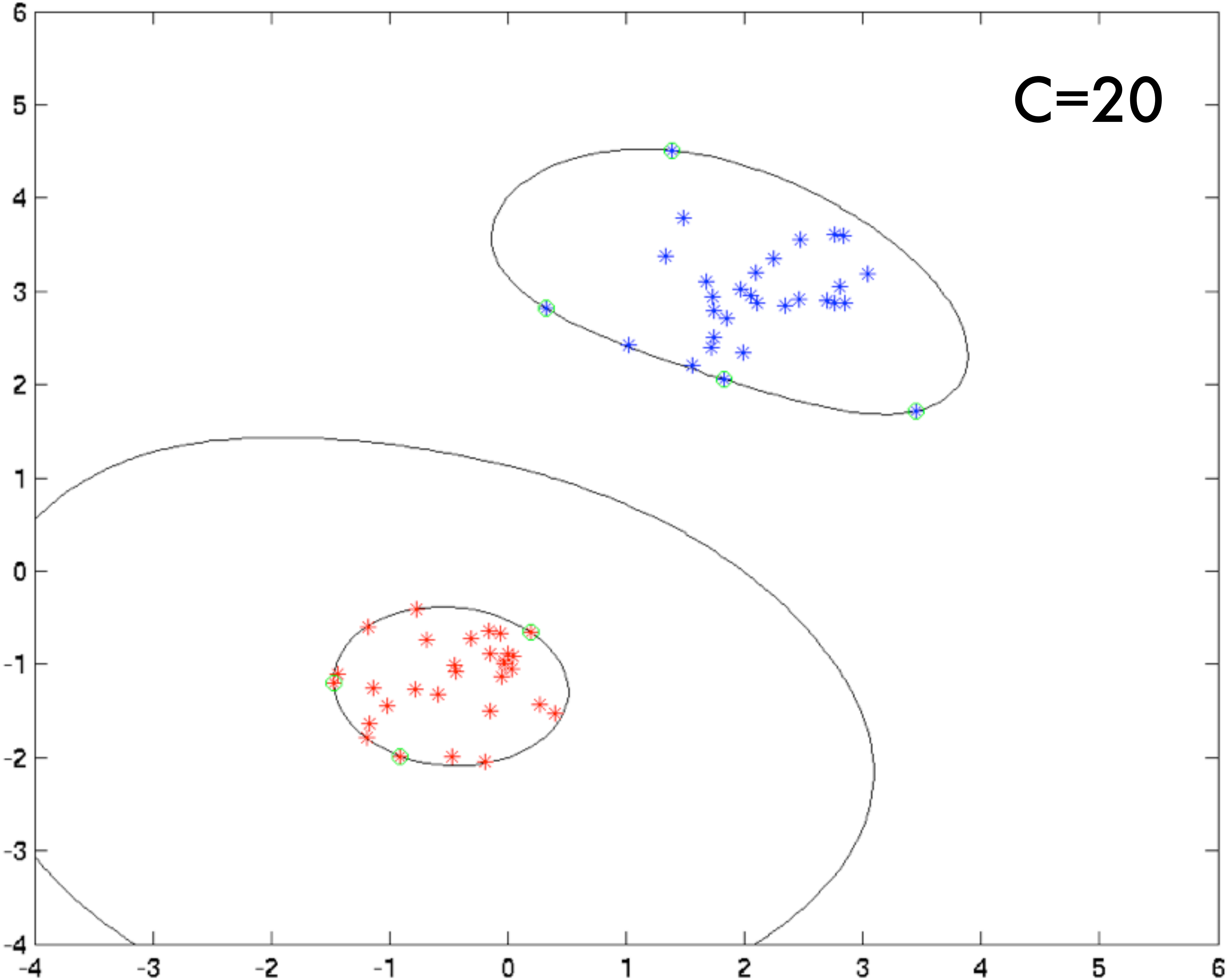
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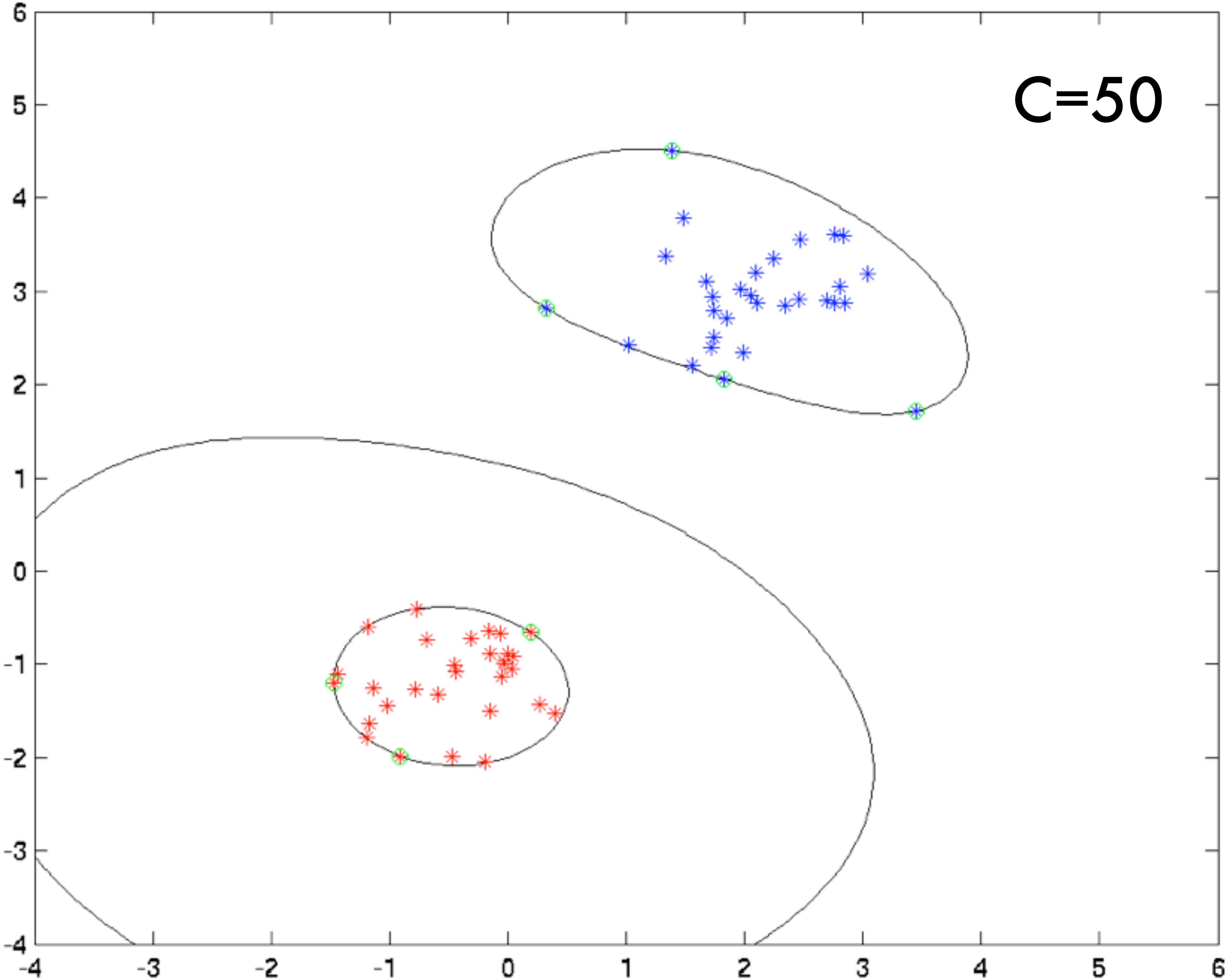
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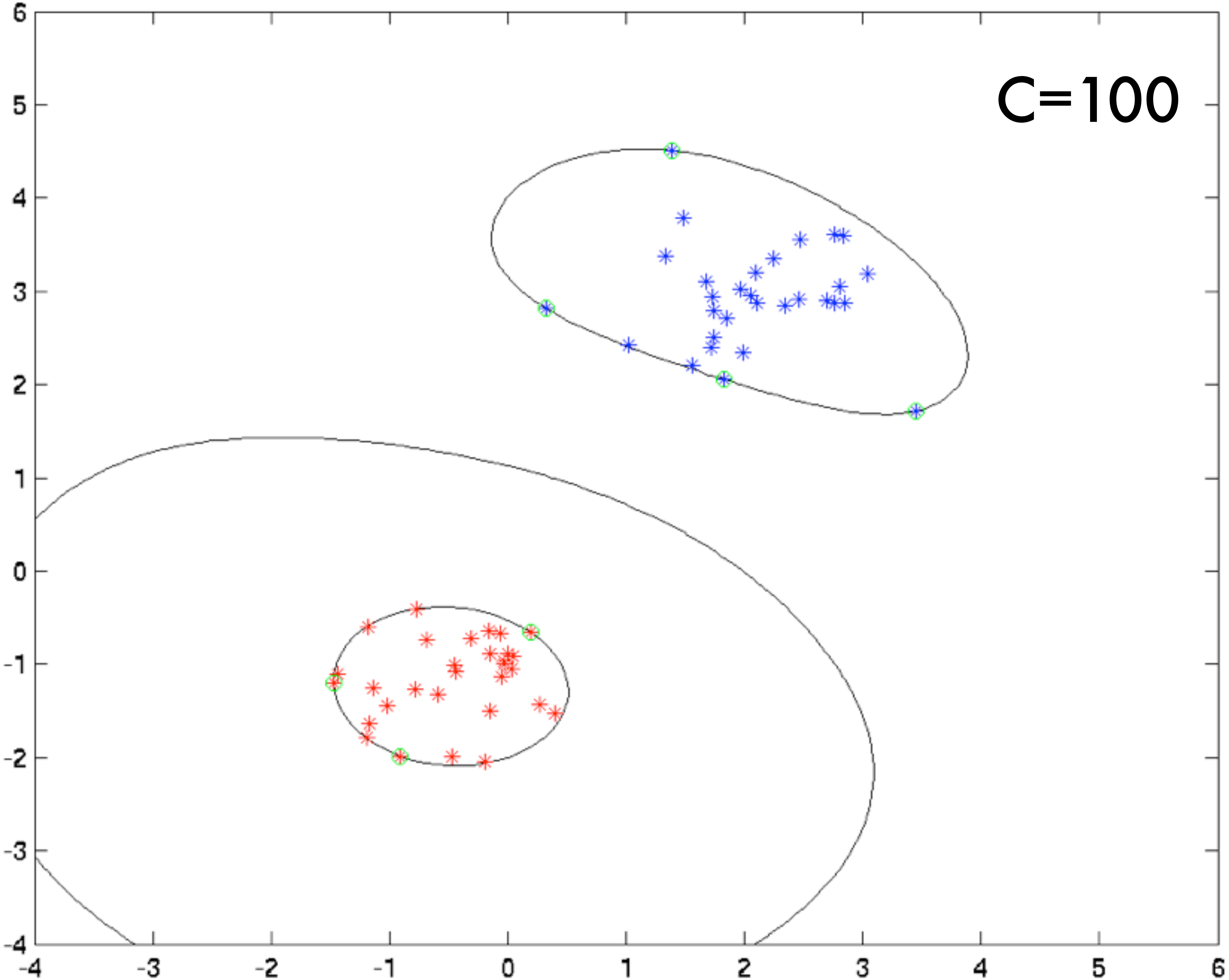
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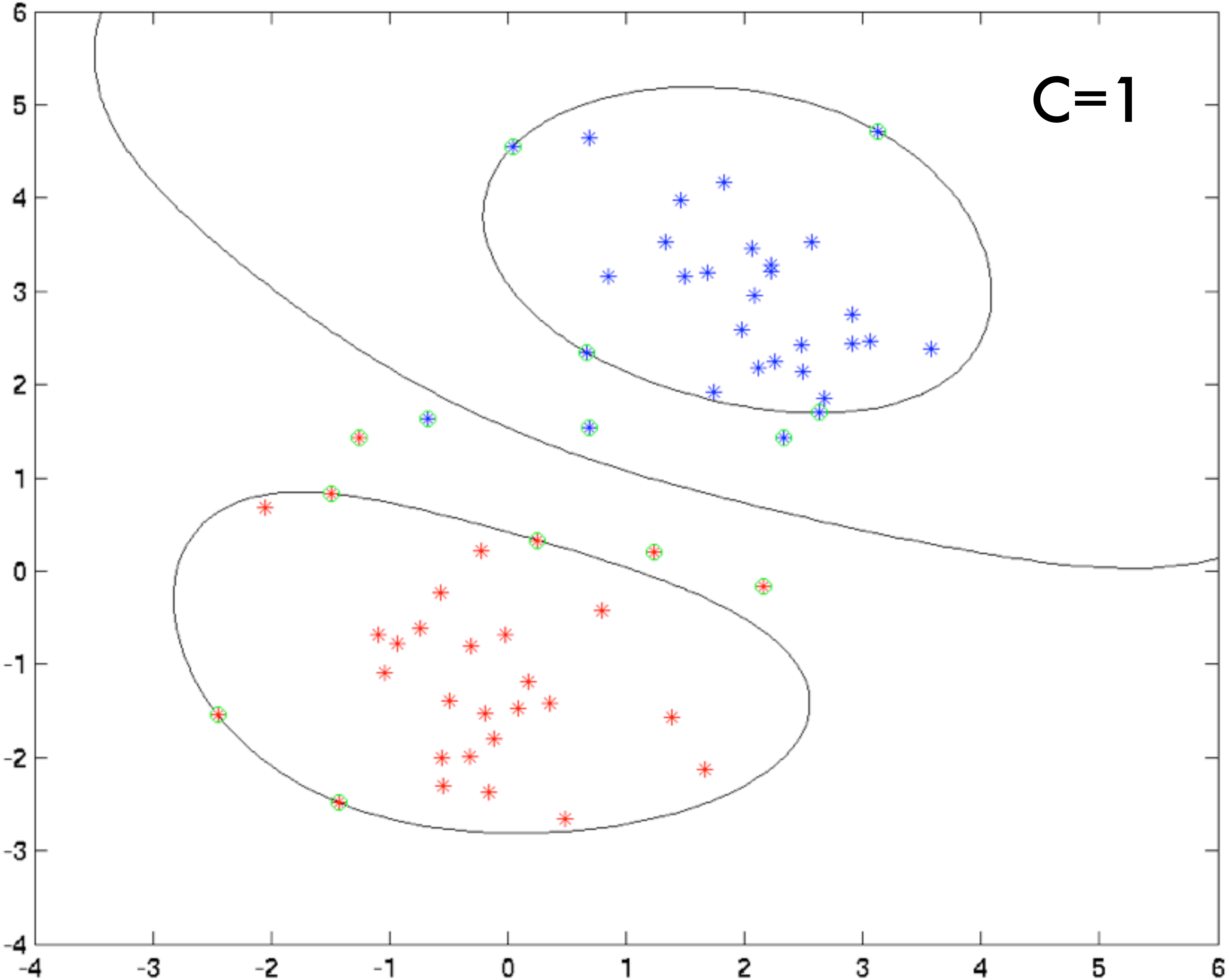
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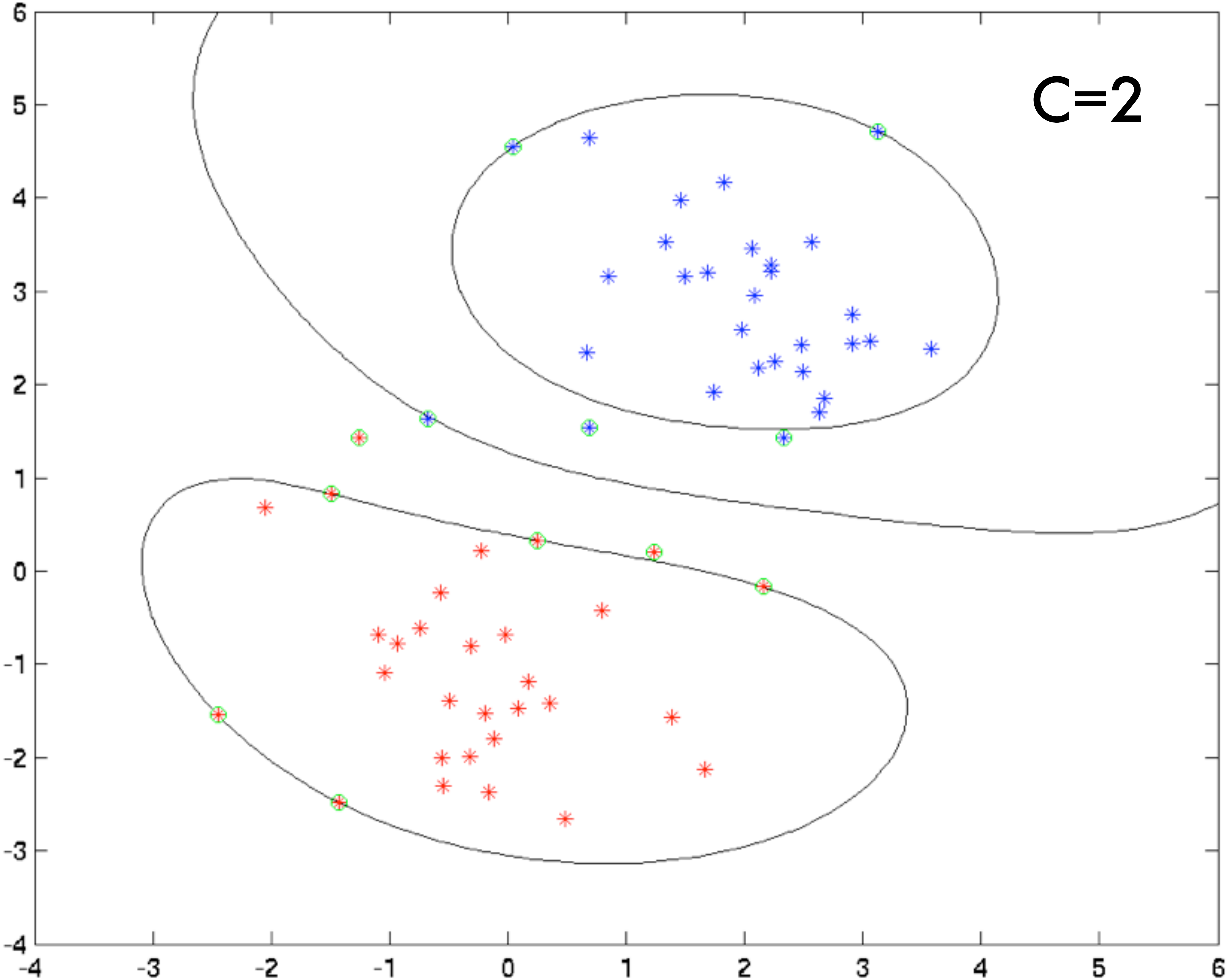
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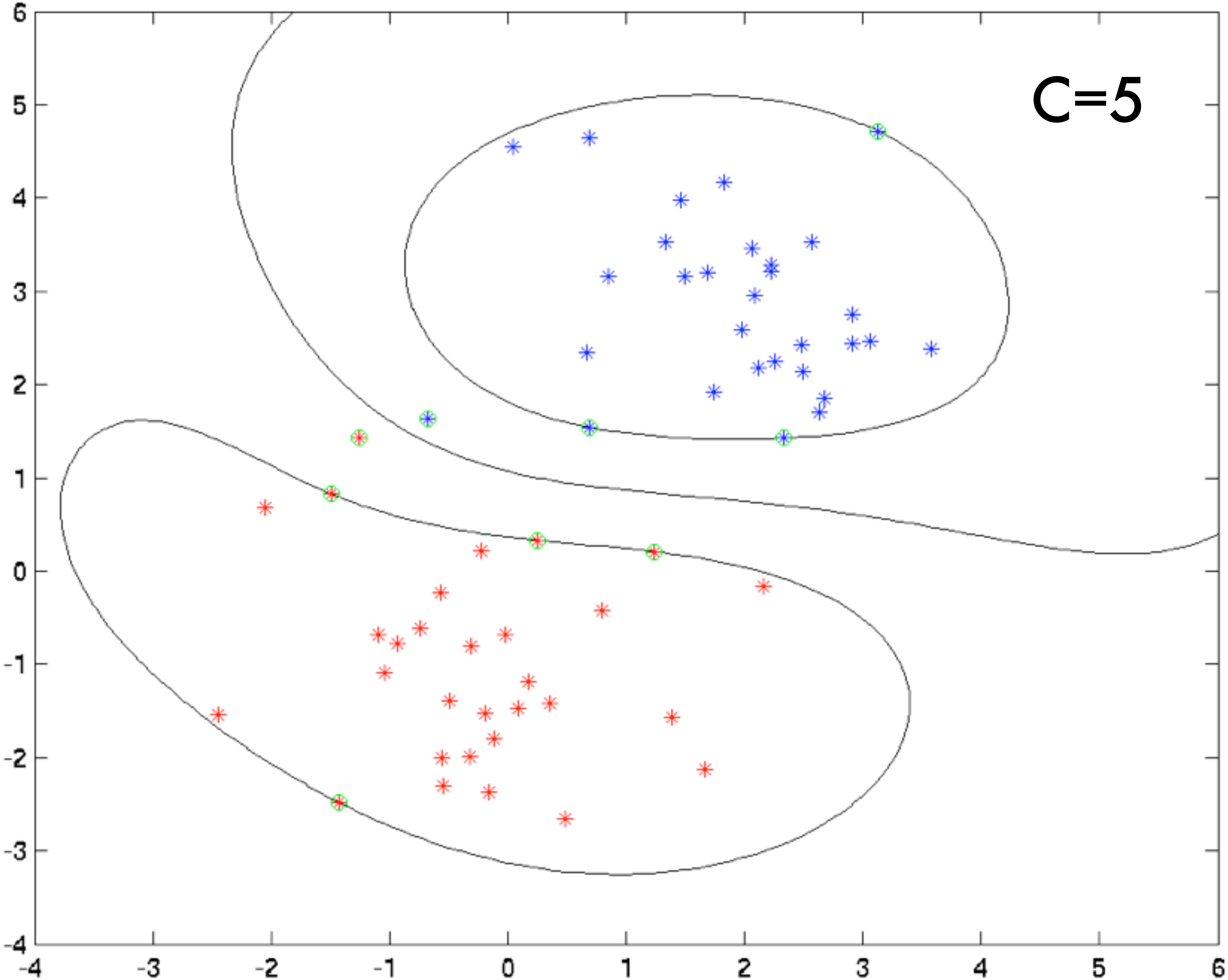

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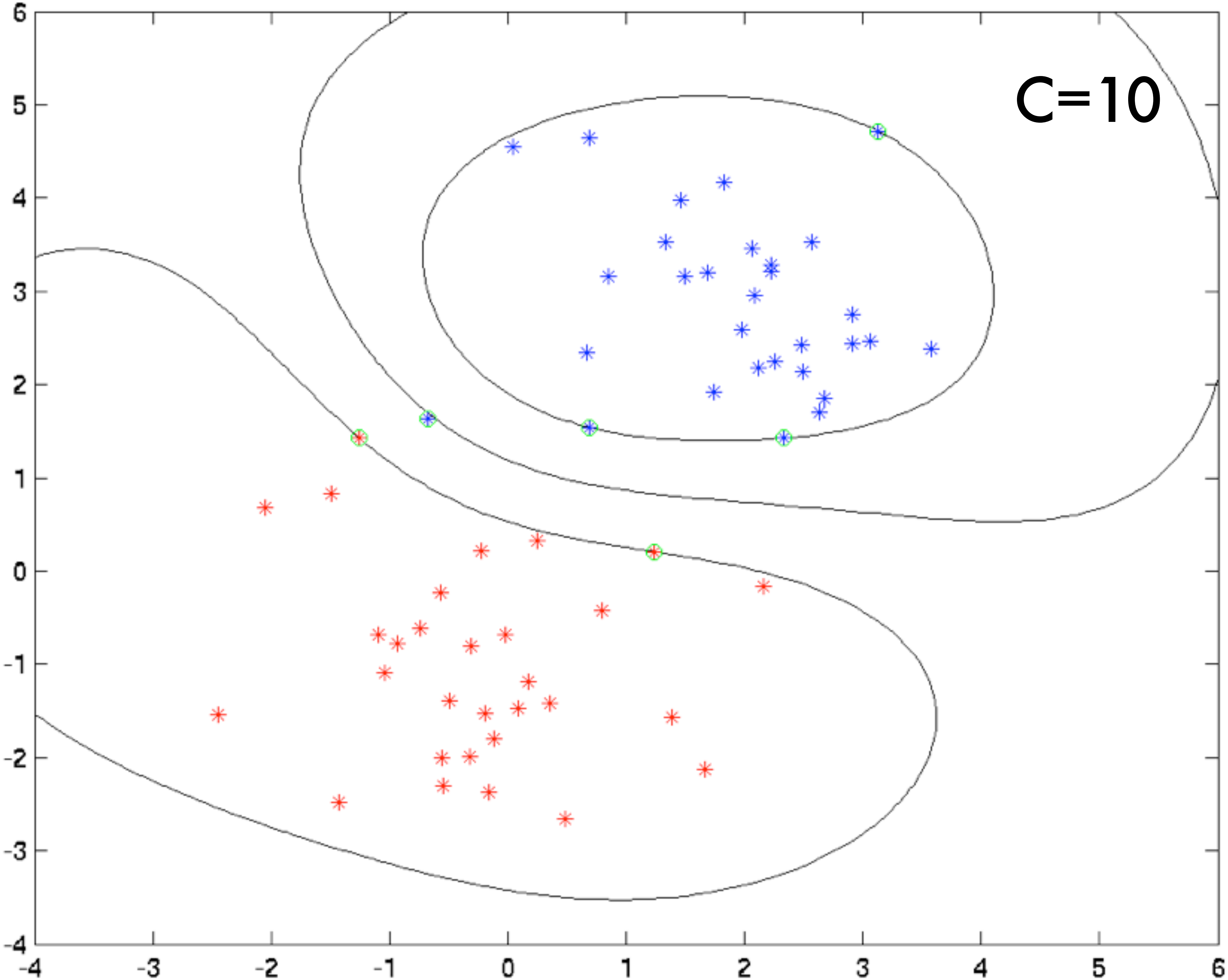
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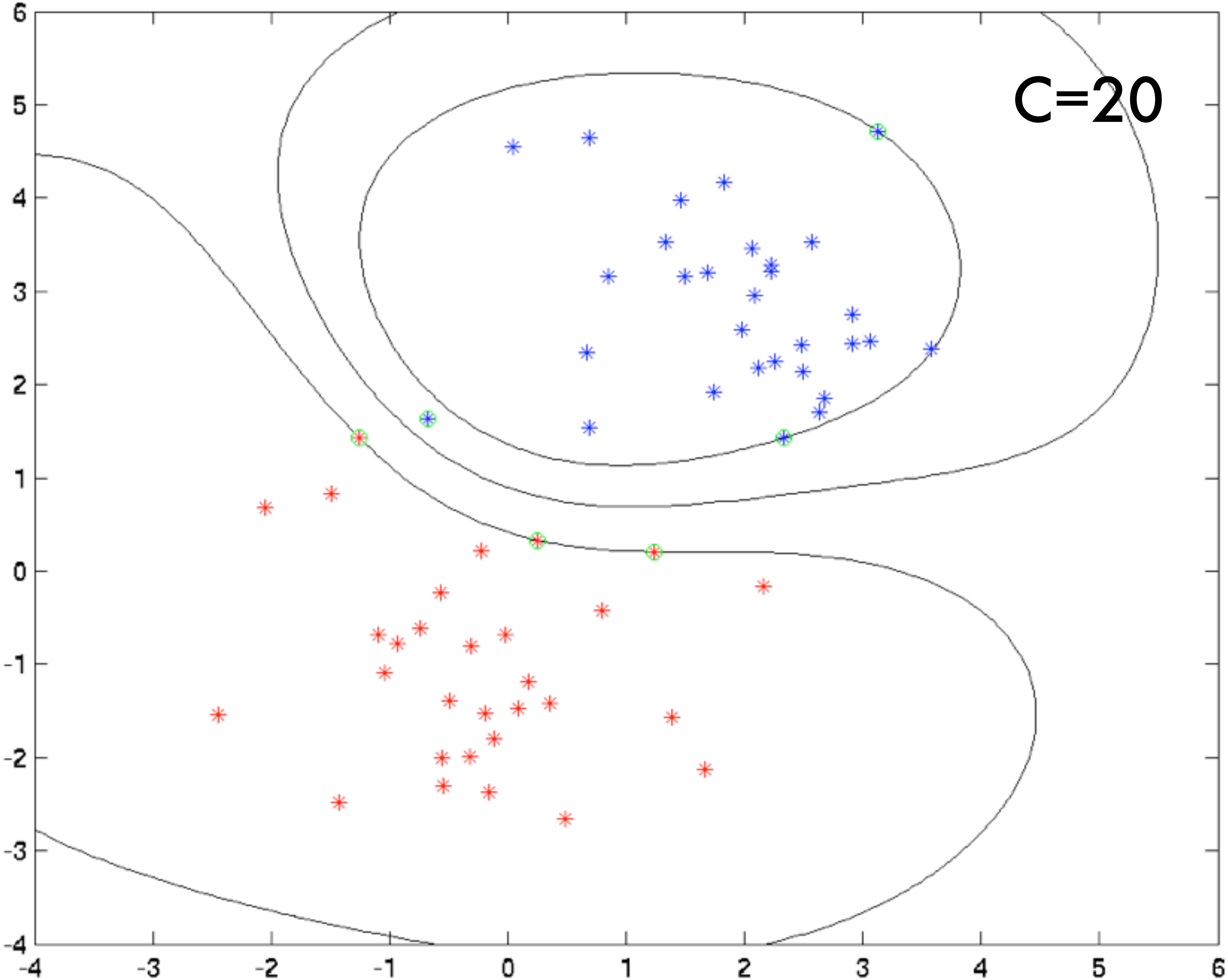

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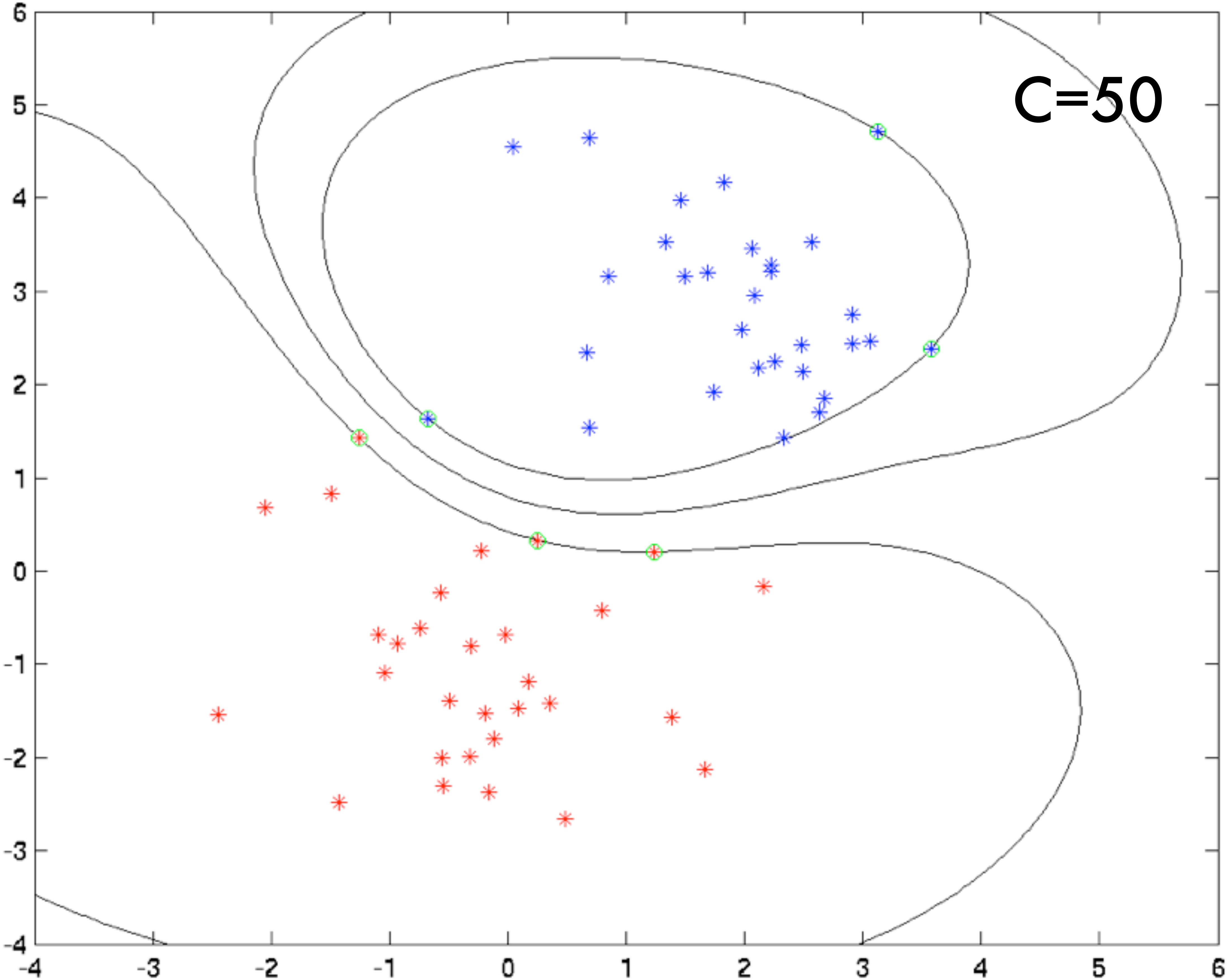
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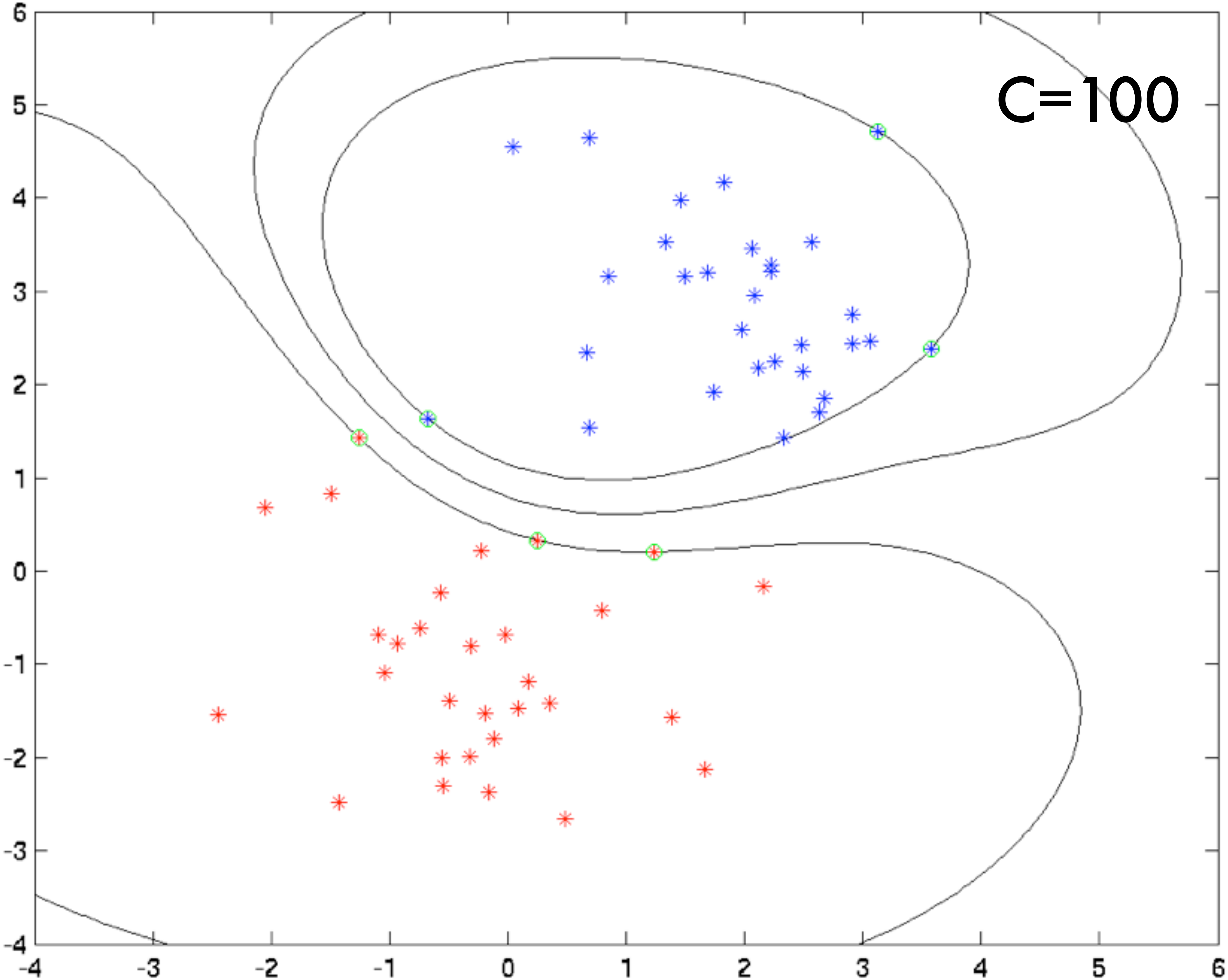
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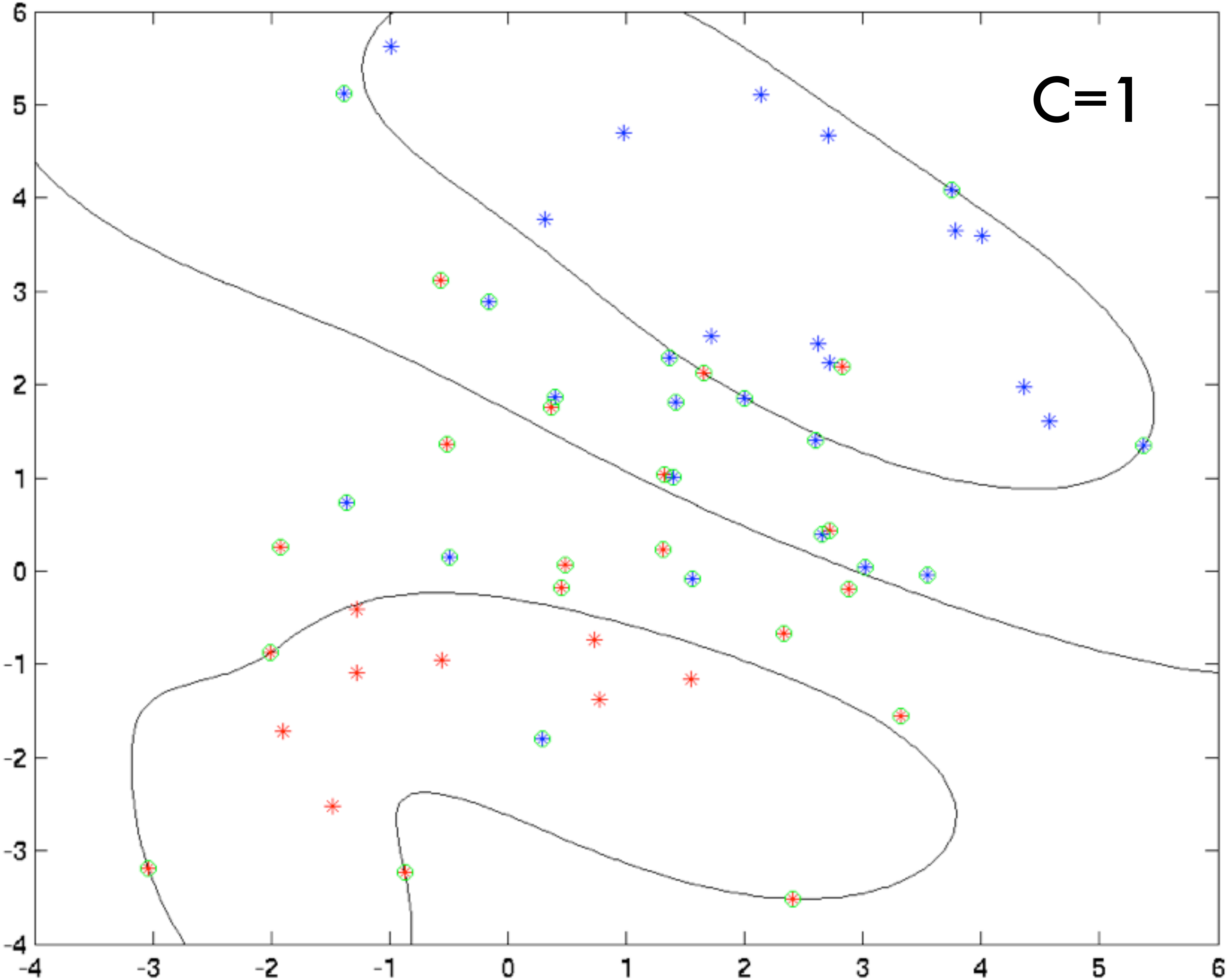

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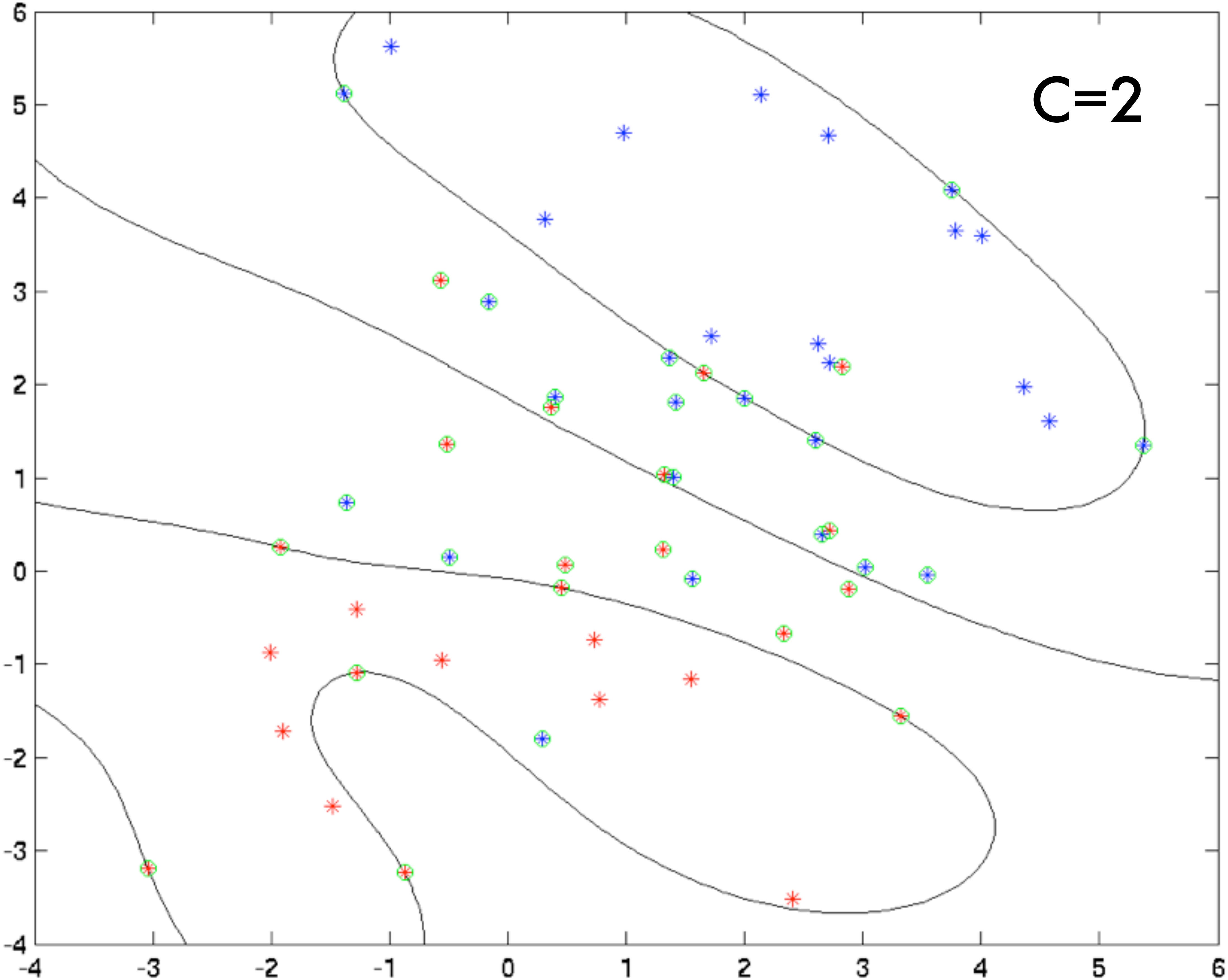

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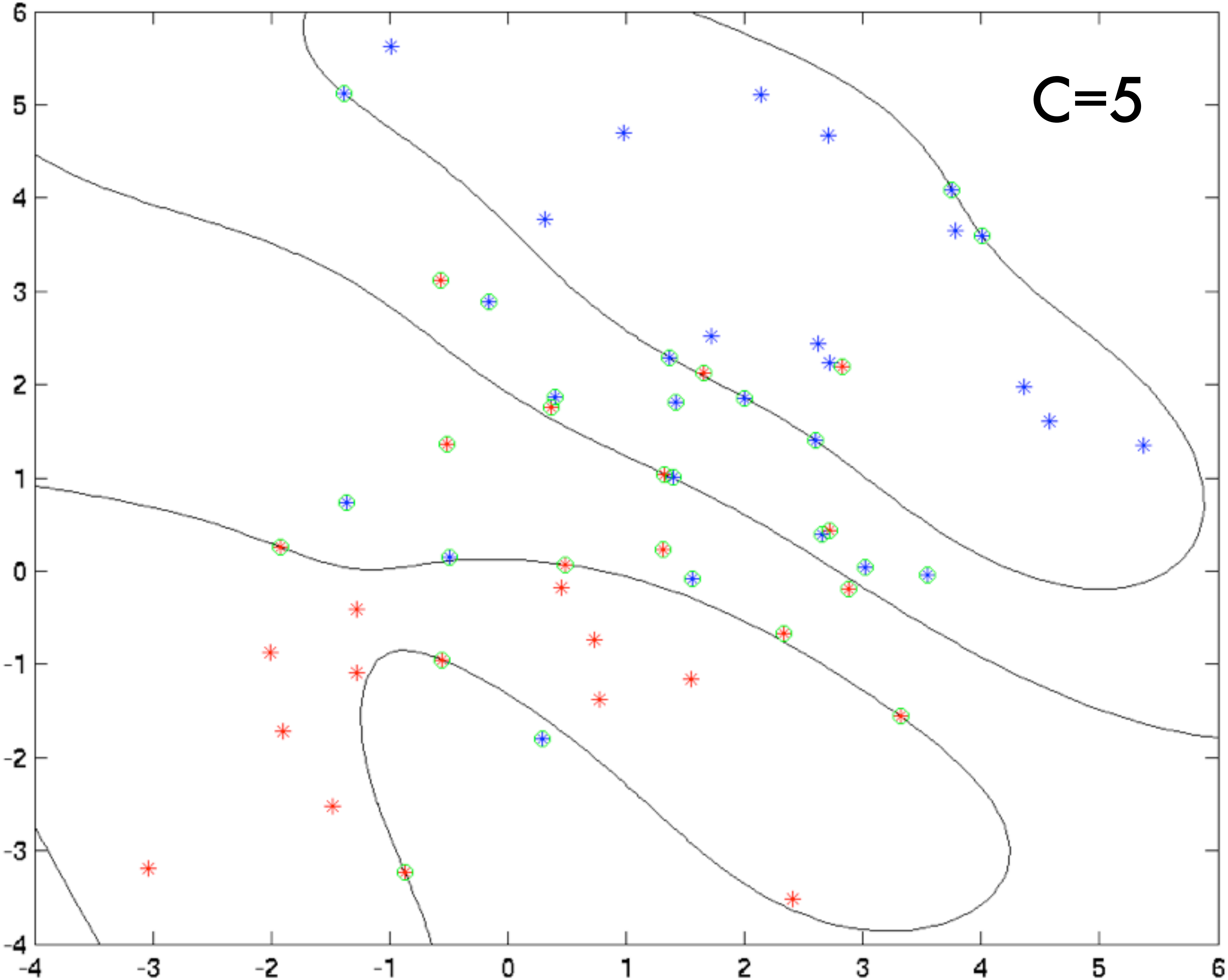
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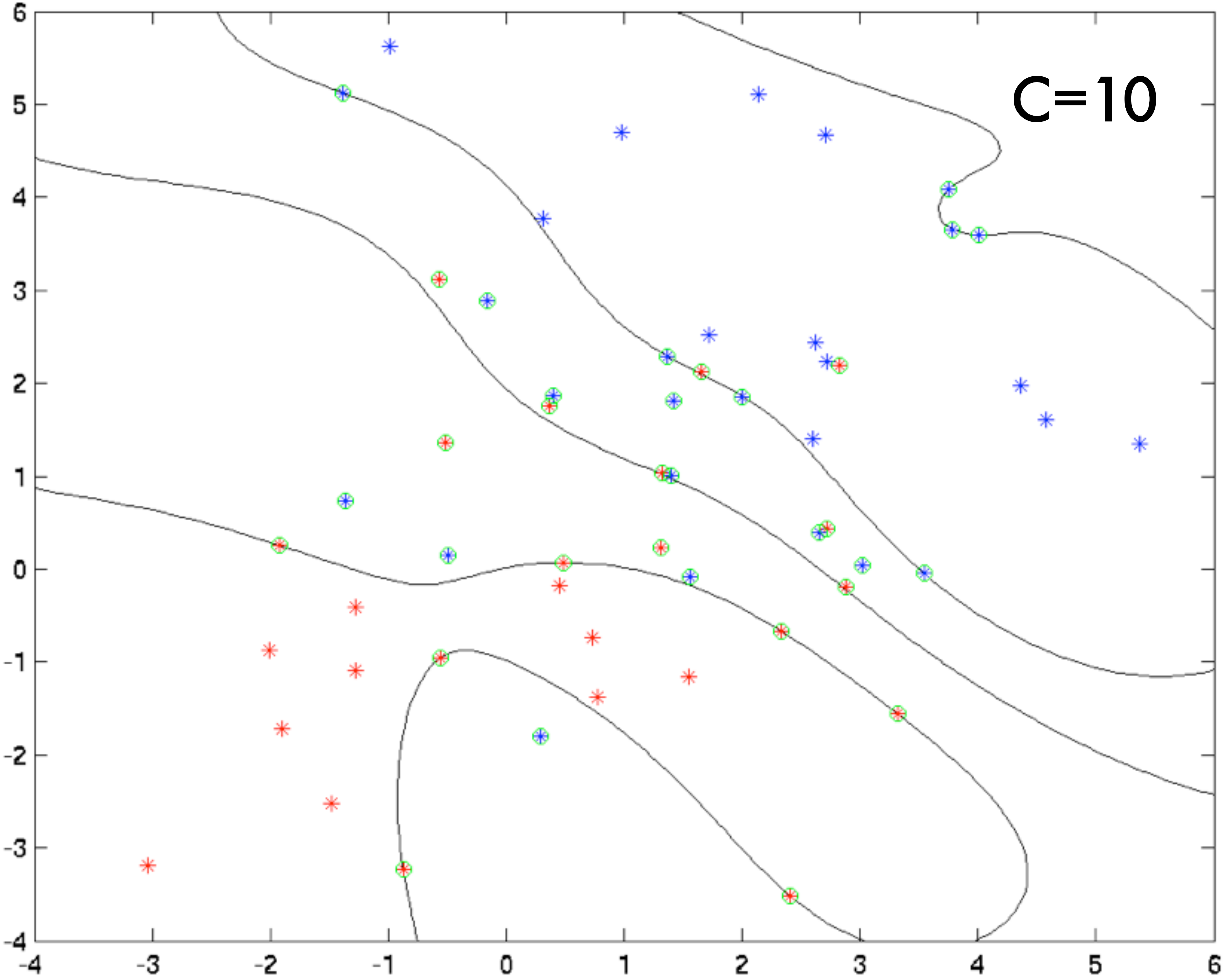
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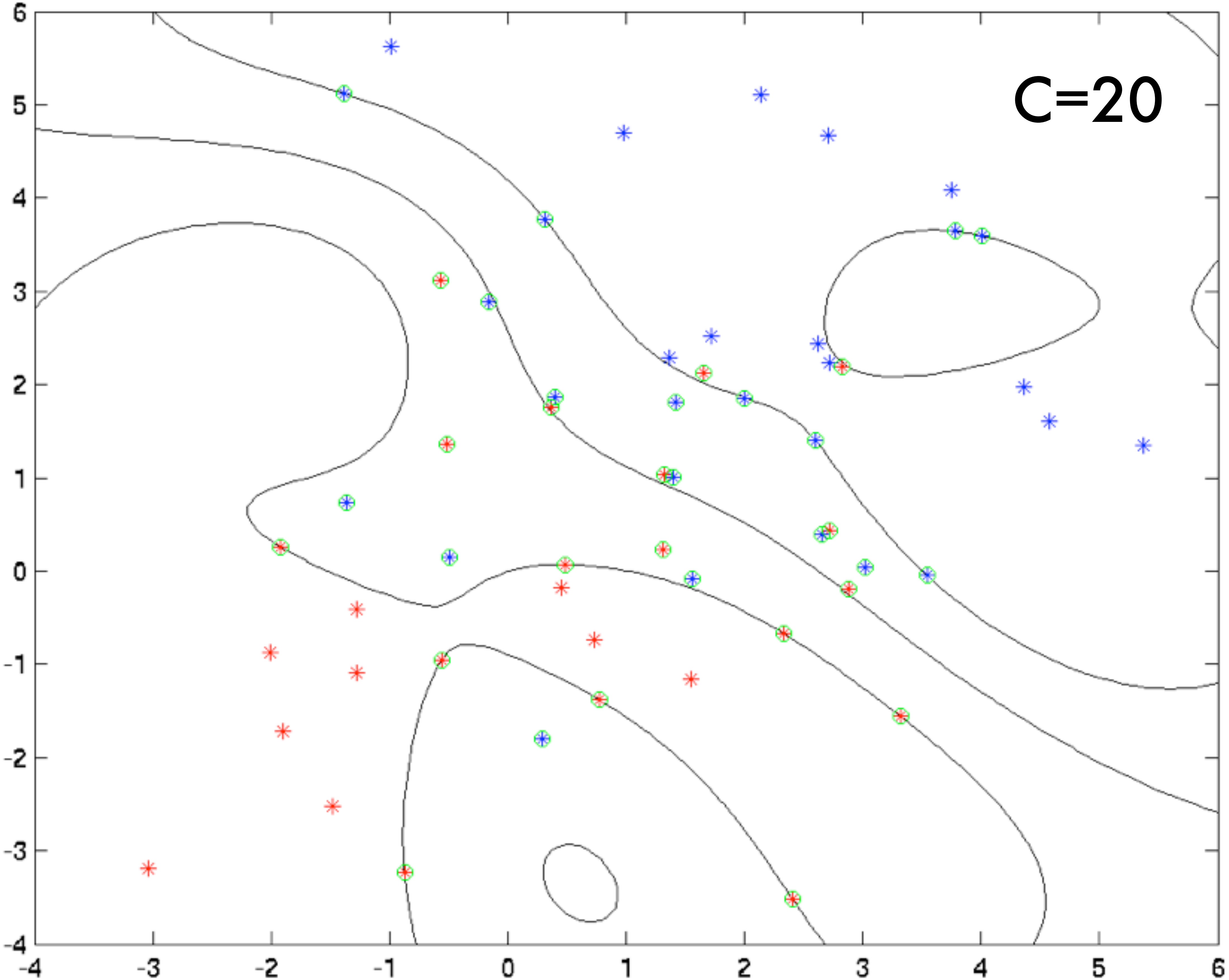
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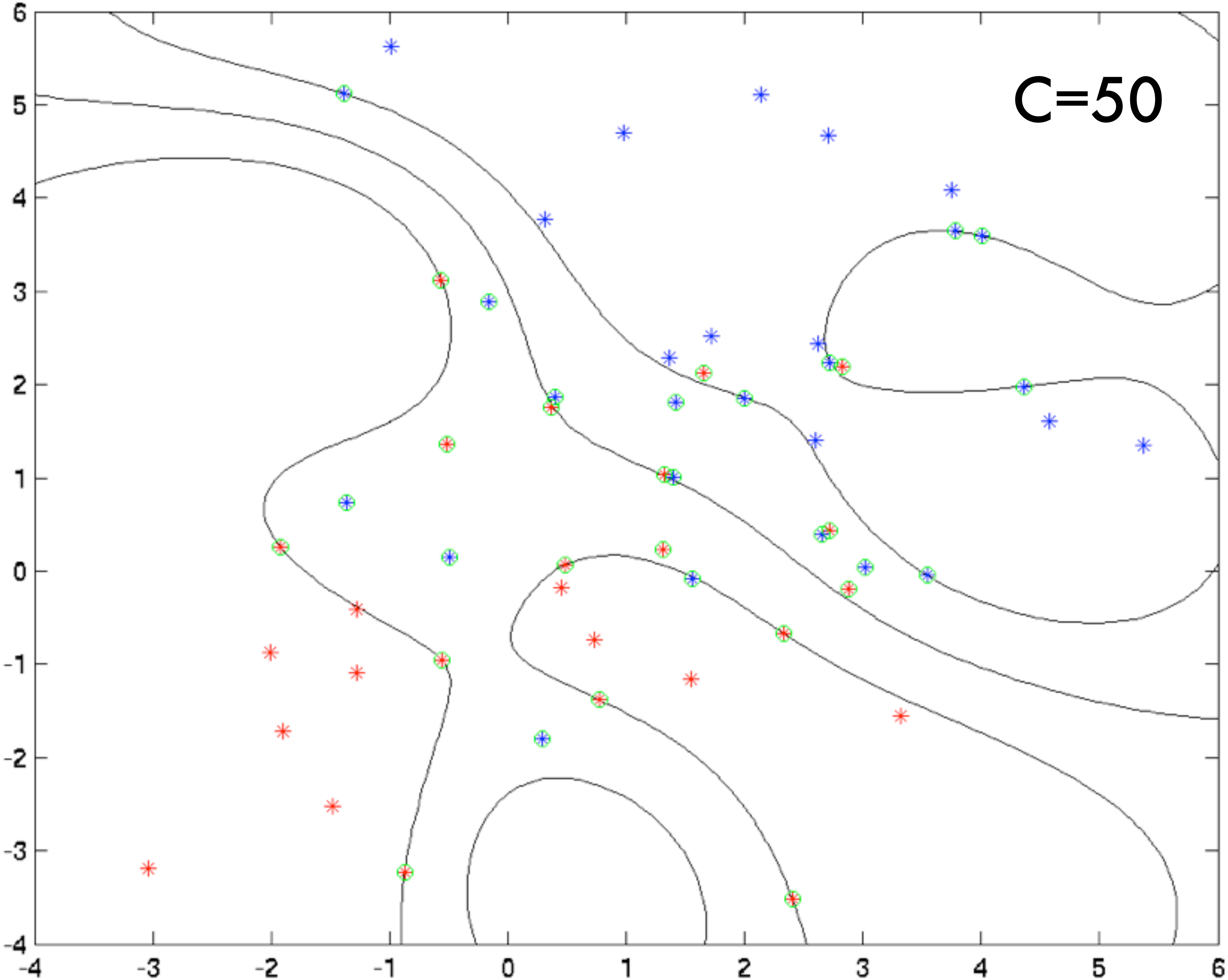
6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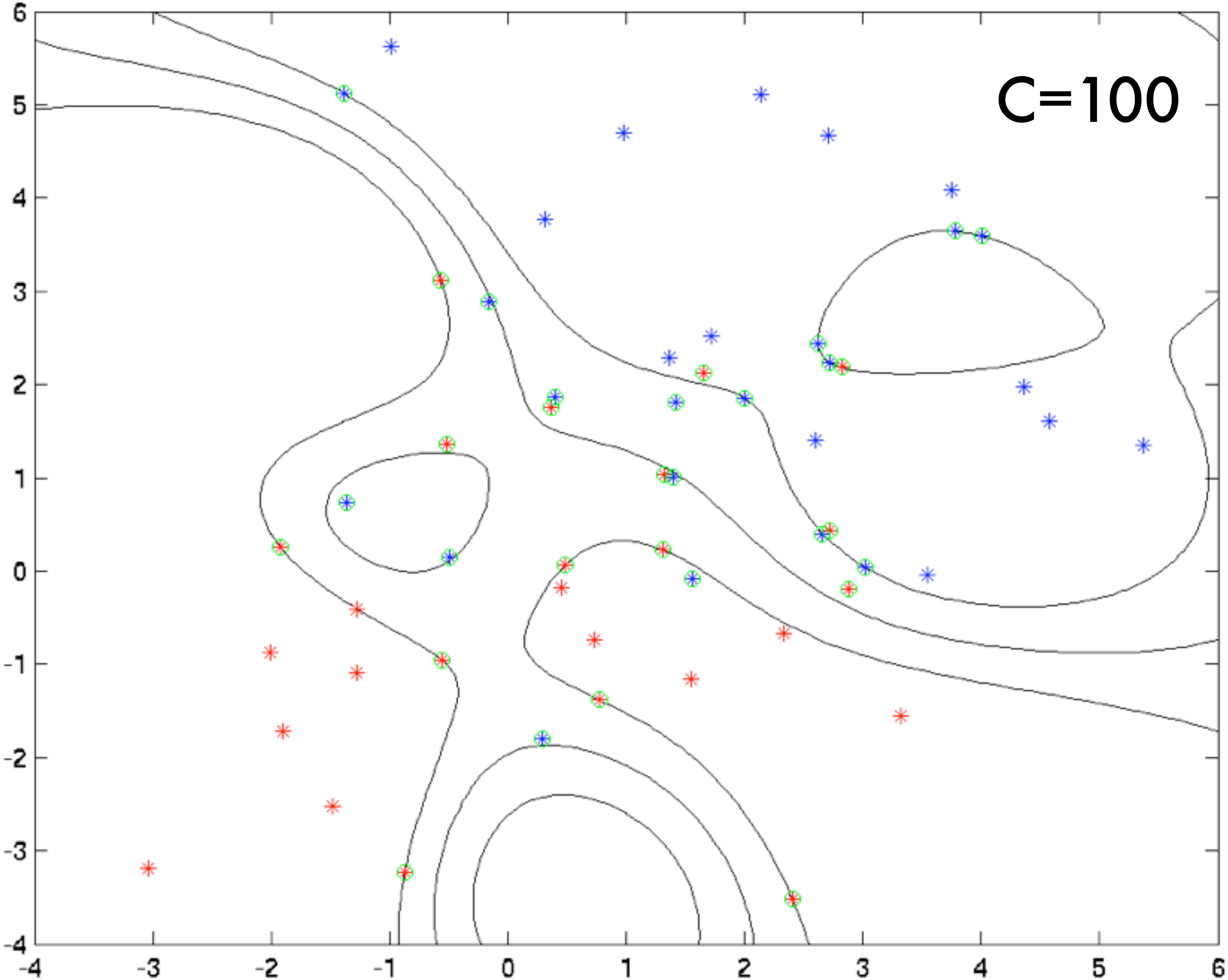
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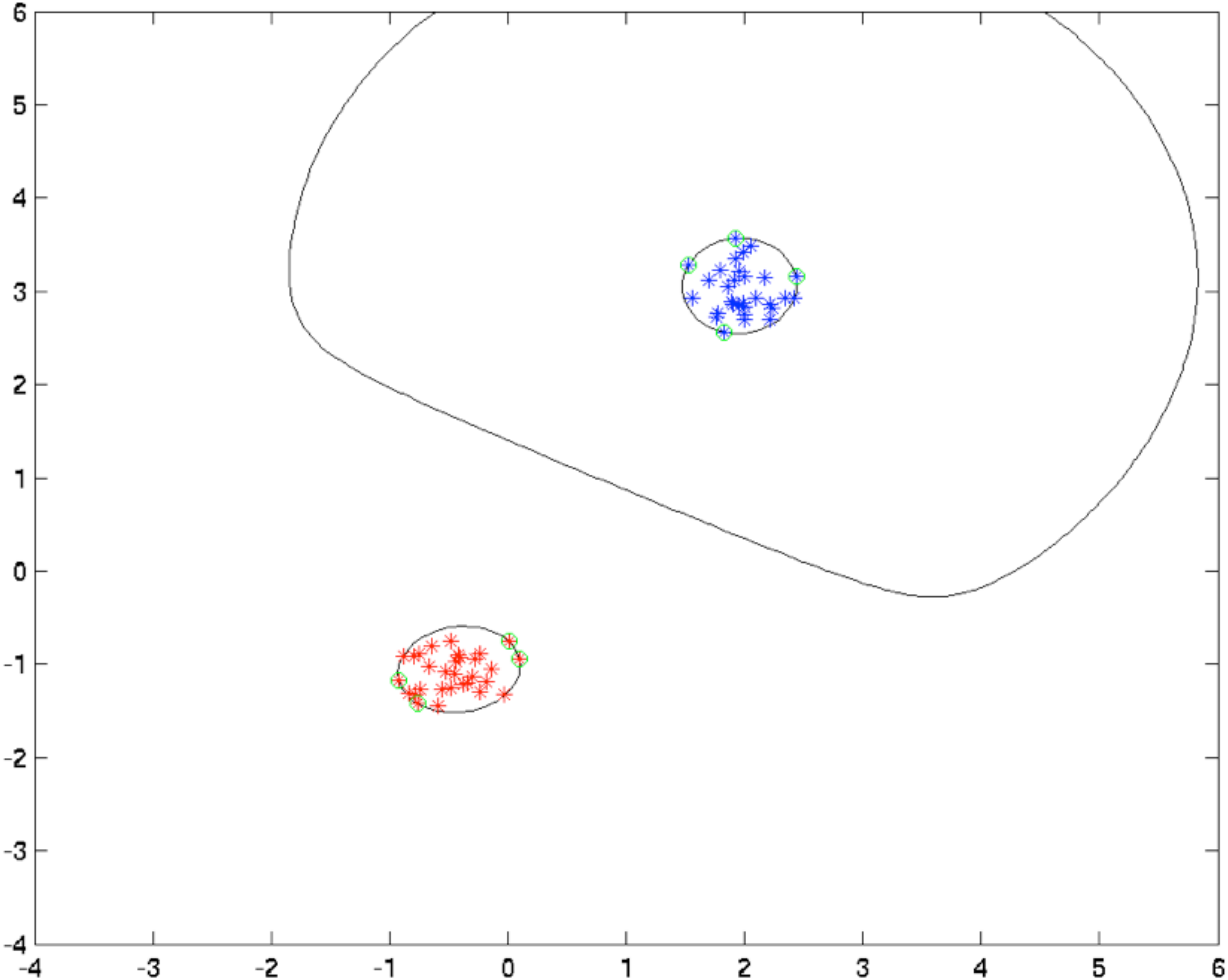
4
5
6

And now with a narrower kernel



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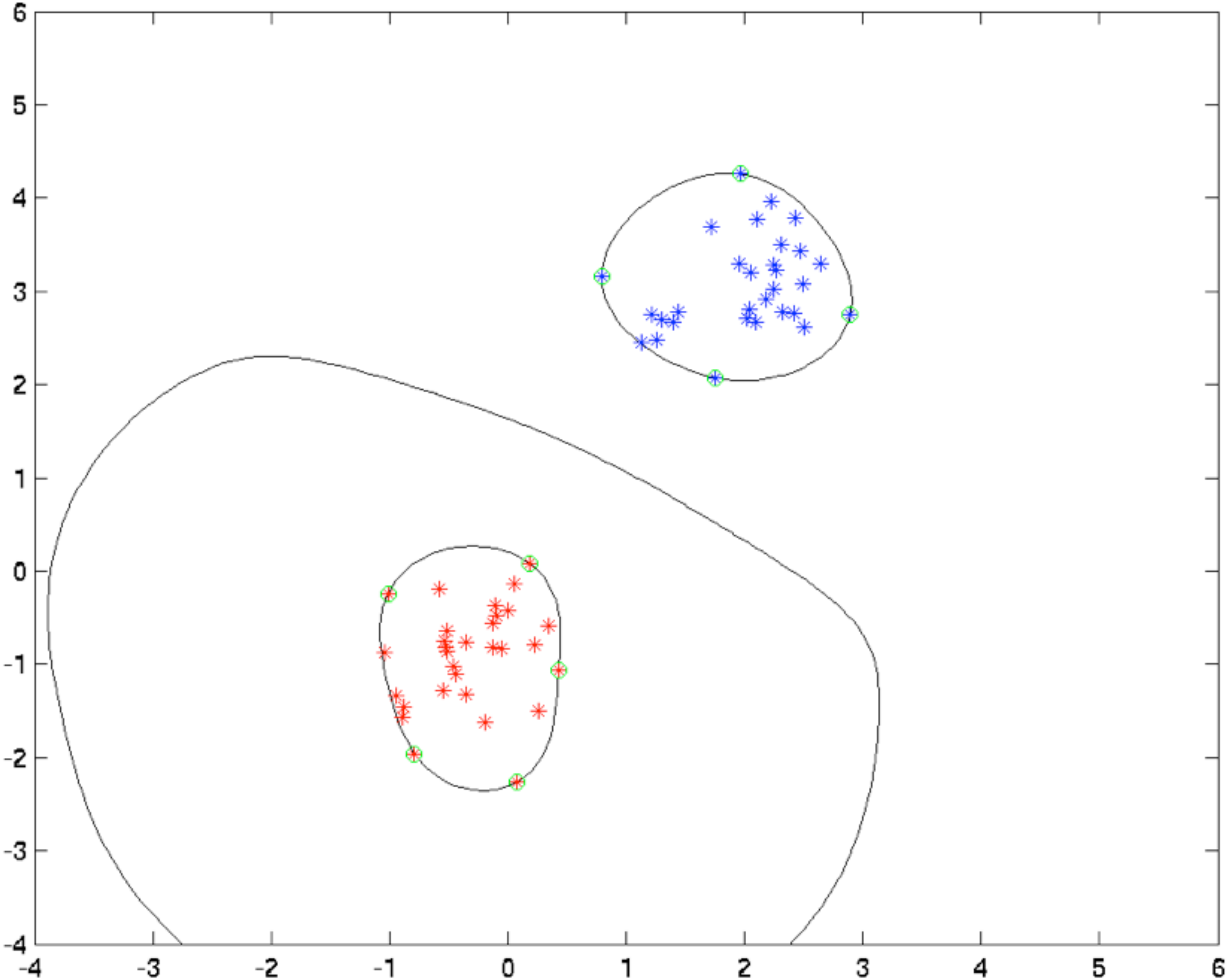

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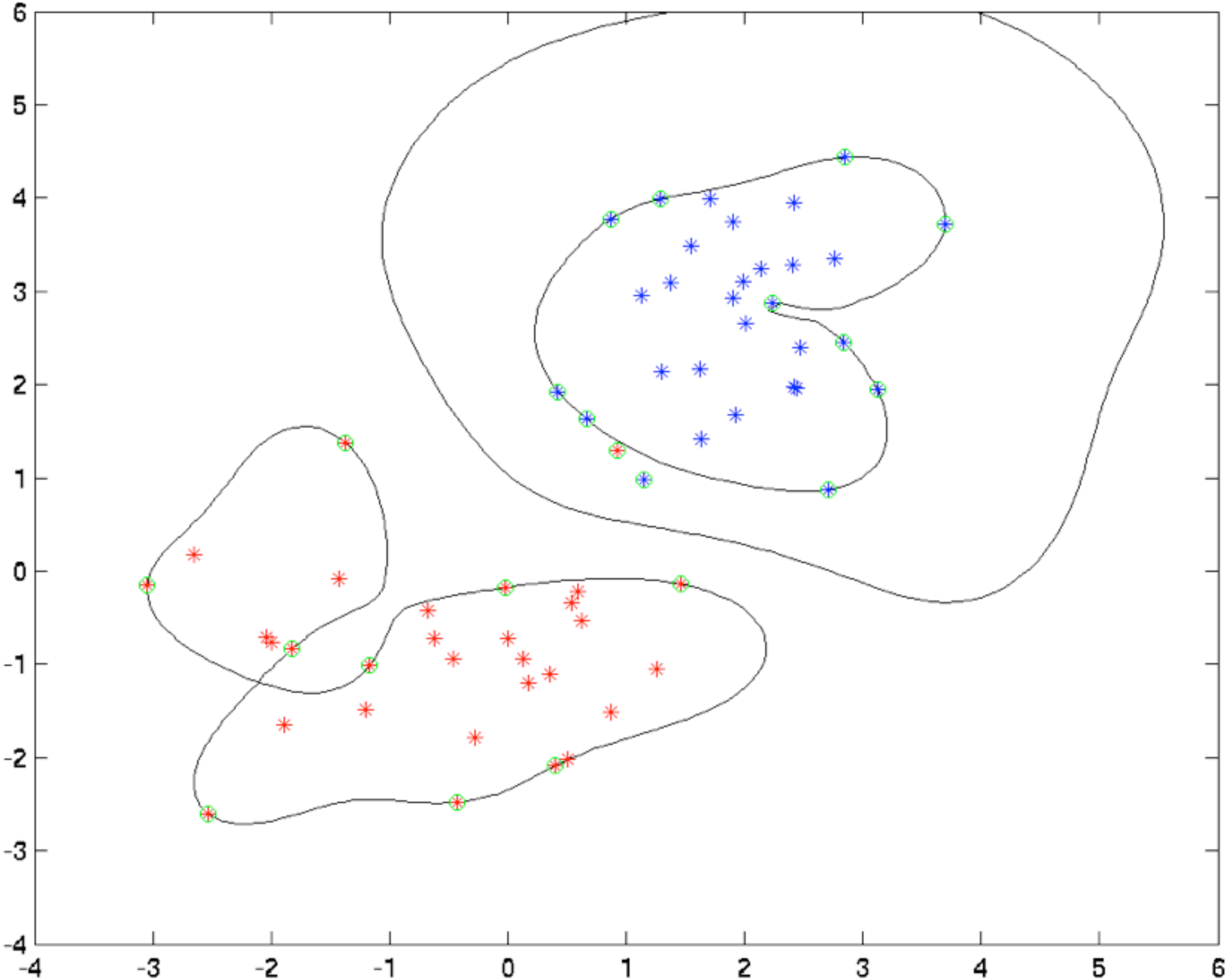

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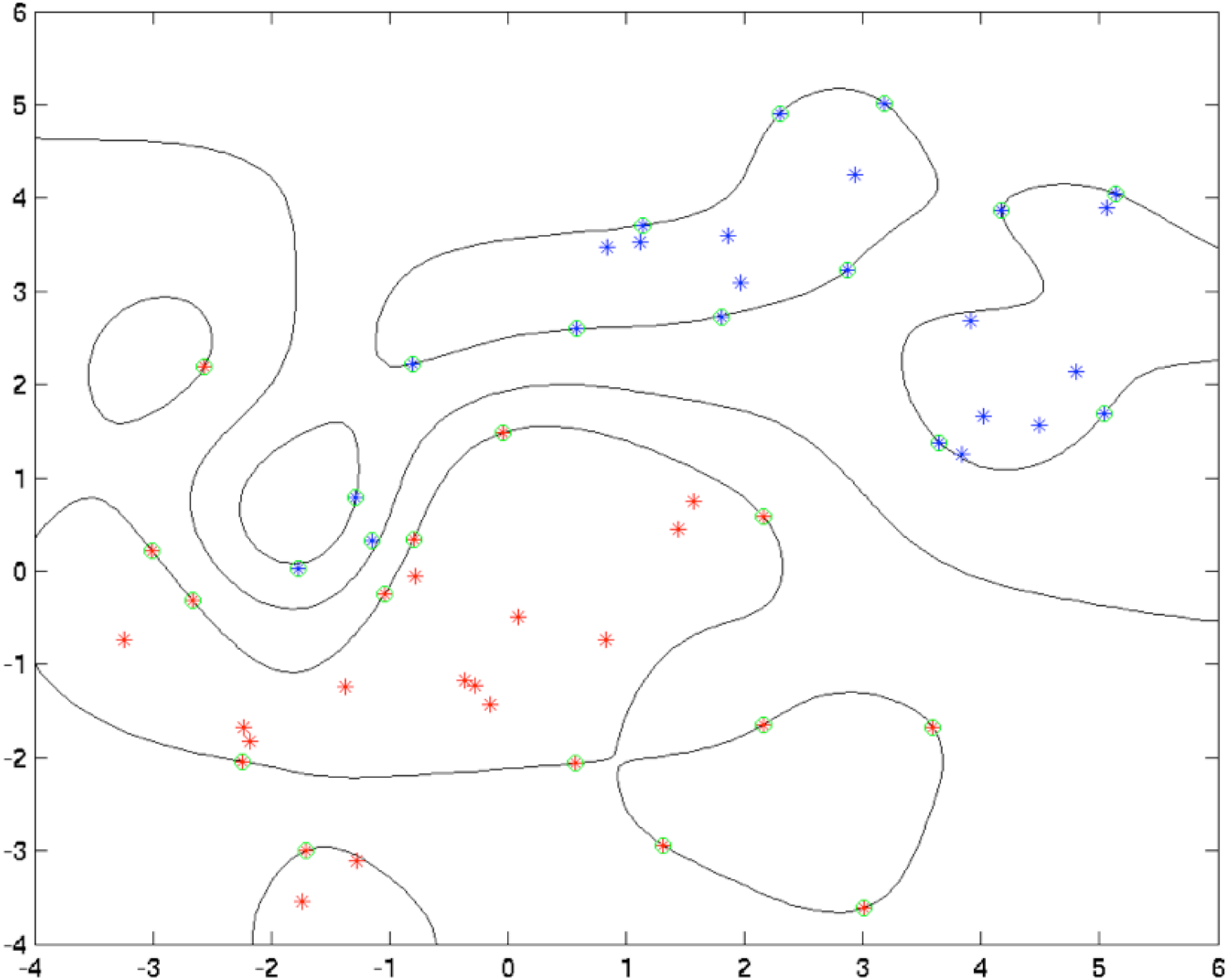

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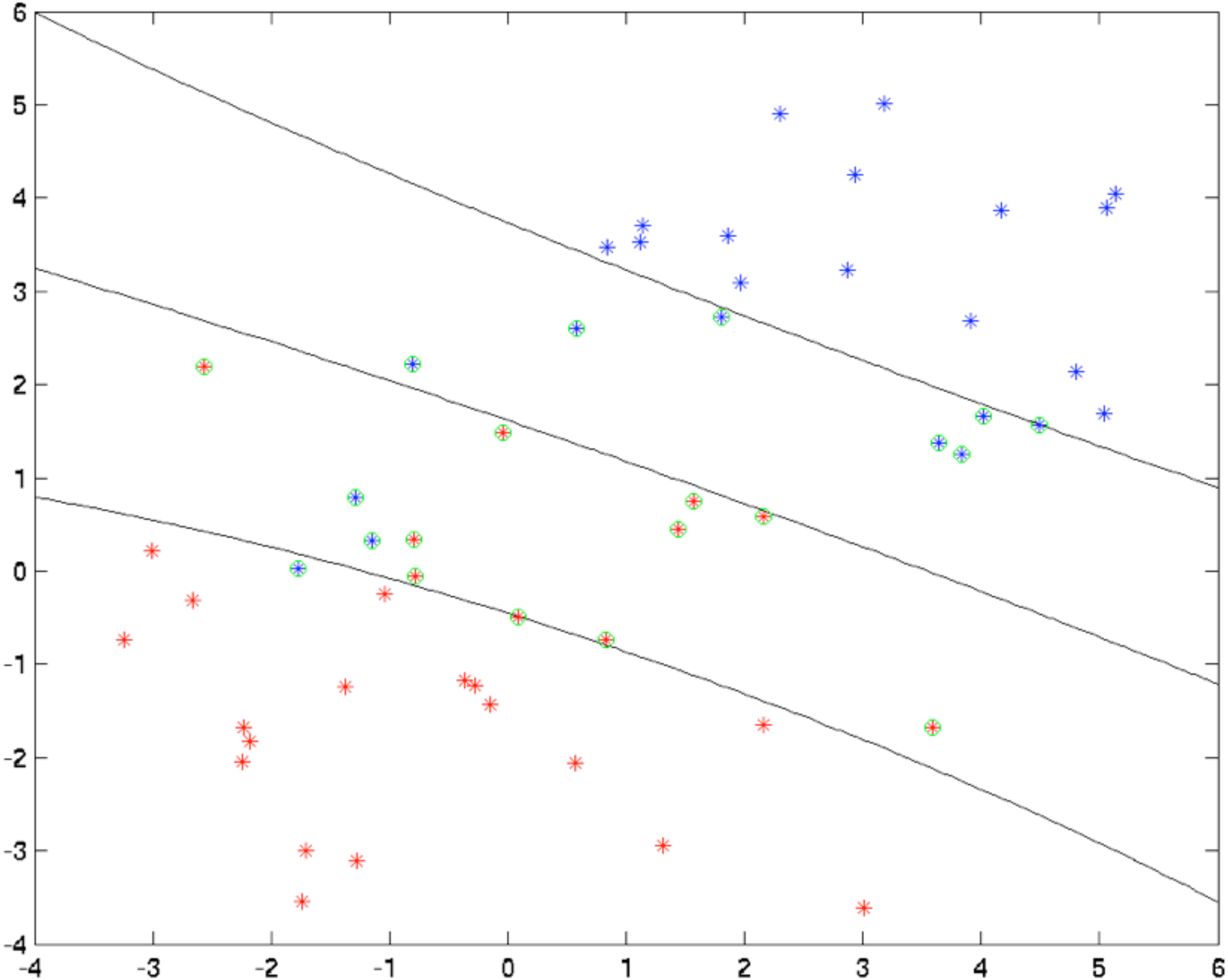
3
4
5
6

And now with a very wide kernel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-4
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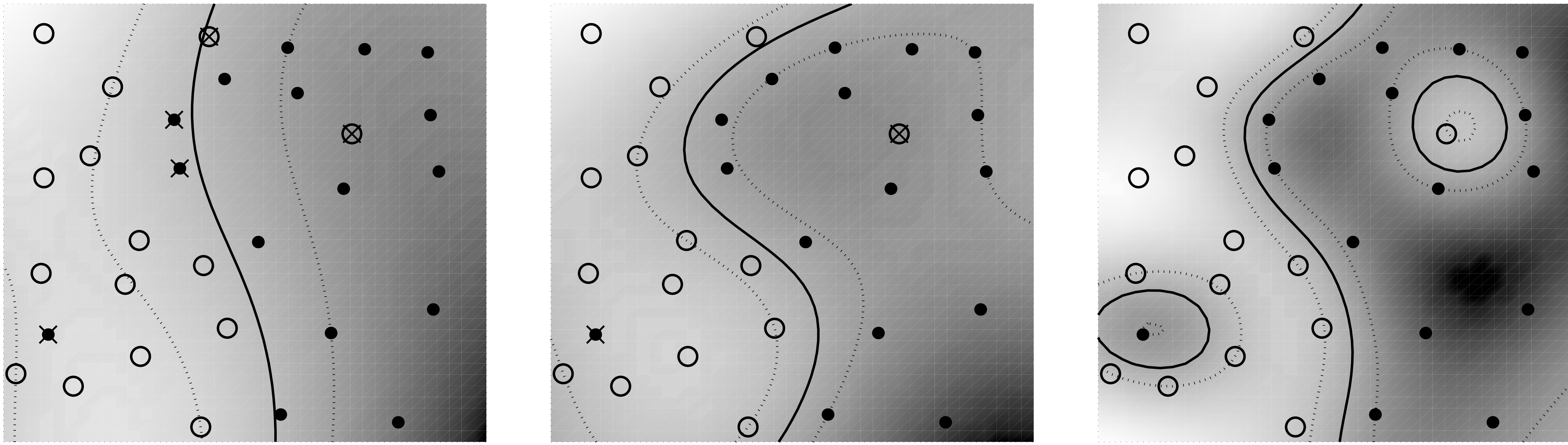
-2
-1
0
1
2
3
4
5
6

Nonlinear separation



- Increasing C allows for more nonlinearities
- Decreases number of errors
- SV boundary need not be contiguous
- Kernel width adjusts function class

Risk and Loss

Loss function point of view

- Constrained quadratic program

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

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

- Risk minimization setting

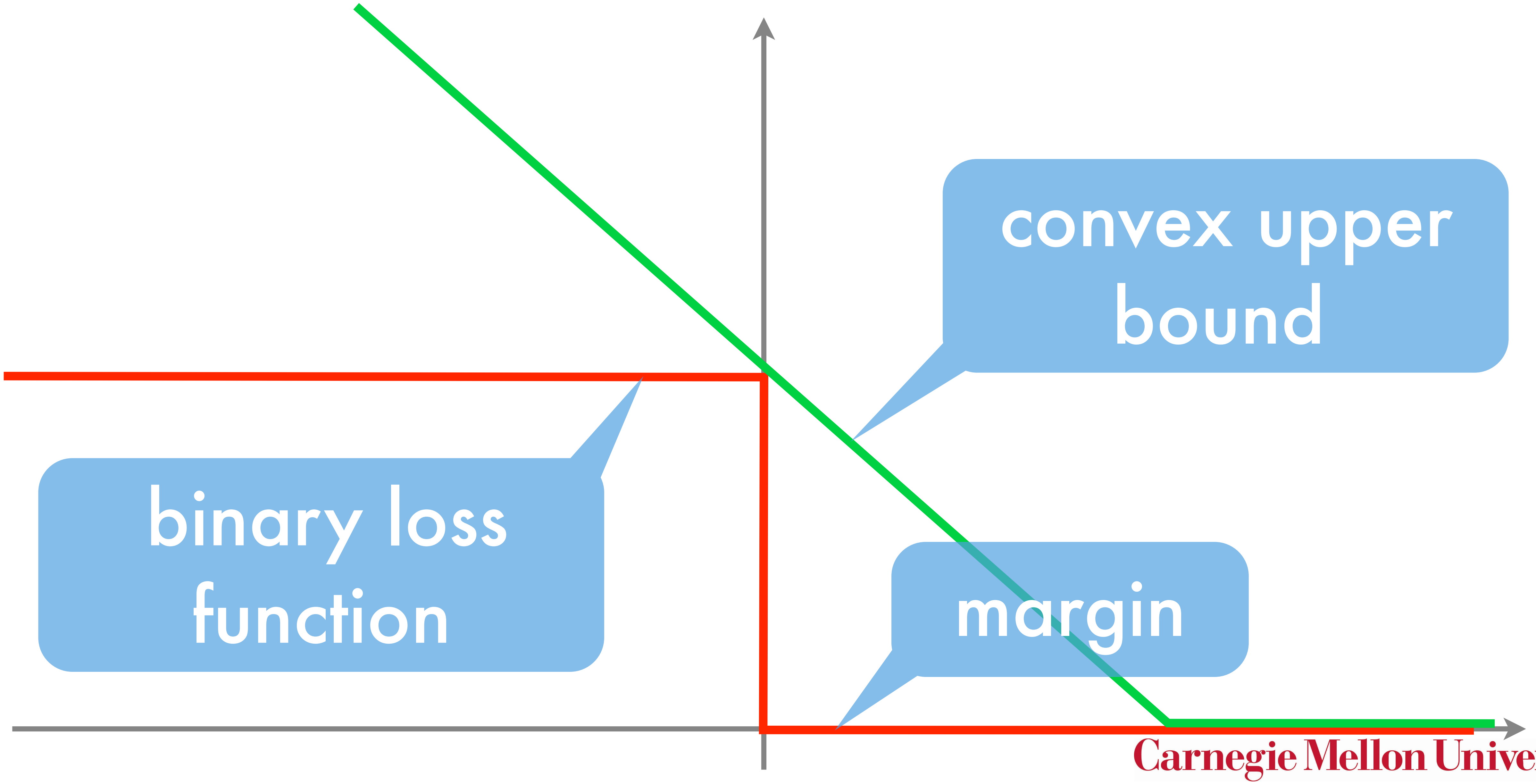
$$\underset{w,b}{\text{minimize}} \ \frac{1}{2}\|w\|^2 + C\sum_i \max\left[0, 1 - y_i\left[\langle w, x_i\rangle + b\right]\right]$$

empirical risk

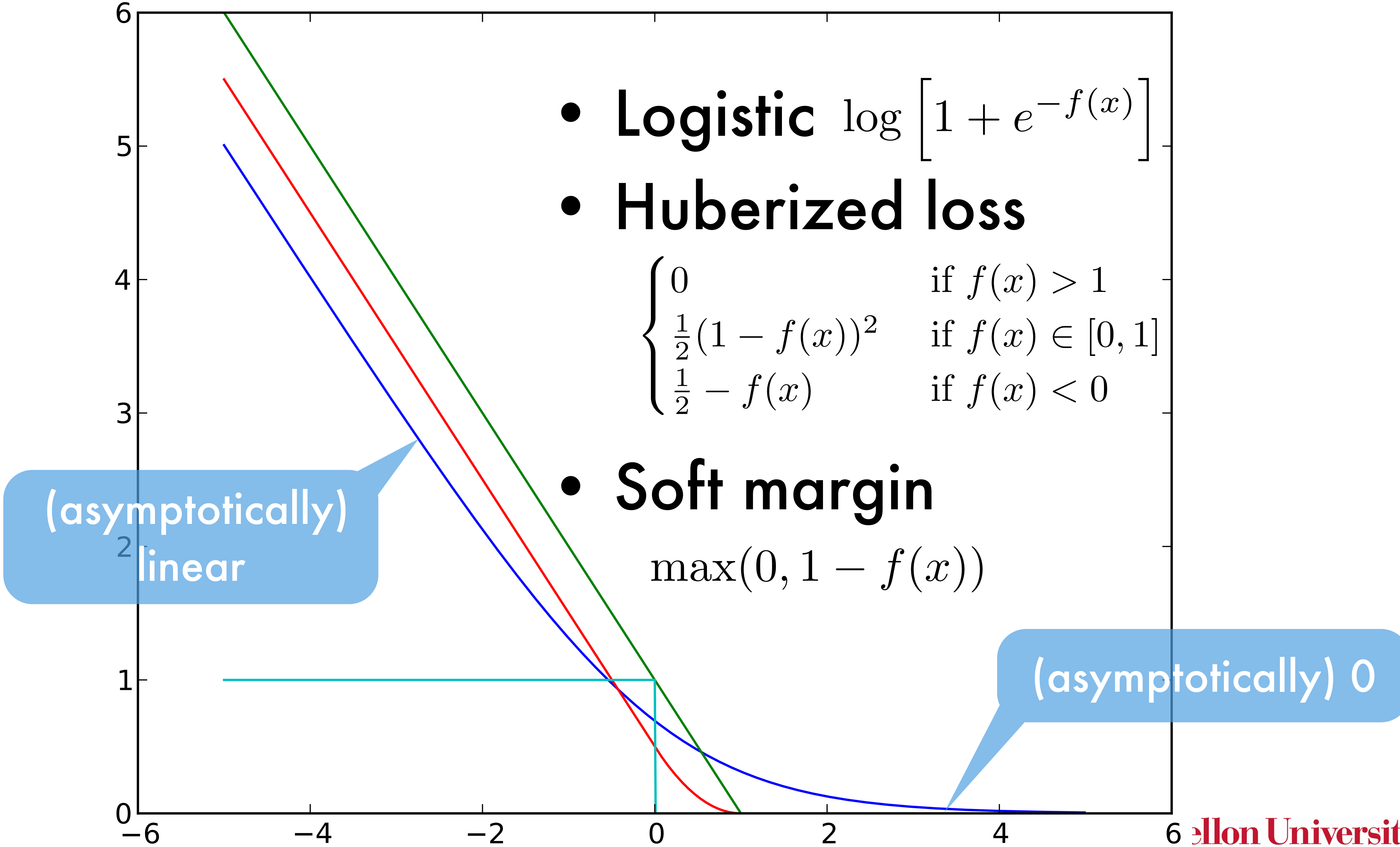
Follows from finding minimal slack variable for given (w,b) pair.

Soft margin as proxy for binary

- Soft margin loss $\max(0, 1 - yf(x))$
- Binary loss $\{yf(x) < 0\}$



More loss functions



- **Logistic** $\log\left[1 + e^{-f(x)}\right]$
- **Huberized loss**

$$\begin{cases} 0 & \text{if } f(x) > 1 \\ \frac{1}{2}(1 - f(x))^2 & \text{if } f(x) \in [0, 1] \\ \frac{1}{2} - f(x) & \text{if } f(x) < 0 \end{cases}$$

- **Soft margin**

$$\max(0, 1 - f(x))$$

Risk minimization view

- Find function f minimizing classification error

$$R[f] := \mathbf{E}_{x,y \sim p(x,y)} \left[\{ y f(x) > 0 \} \right]$$

- Compute empirical average

$$R_{\text{emp}}[f] := \frac{1}{m} \sum_{i=1}^{m} \{ y_i f(x_i) > 0 \}$$

  - Minimization is nonconvex
  - Overfitting as we minimize empirical error
- Compute convex upper bound on the loss
- Add regularization for capacity control

regularization

$$R_{\text{reg}}[f] := \frac{1}{m} \sum_{i=1}^{m} \max(0, 1 - y_i f(x_i)) + \lambda \Omega[f]$$

how to control λ

Summary

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