Photo by Arthur Gretton, CMU Machine Learning Protestors at G20

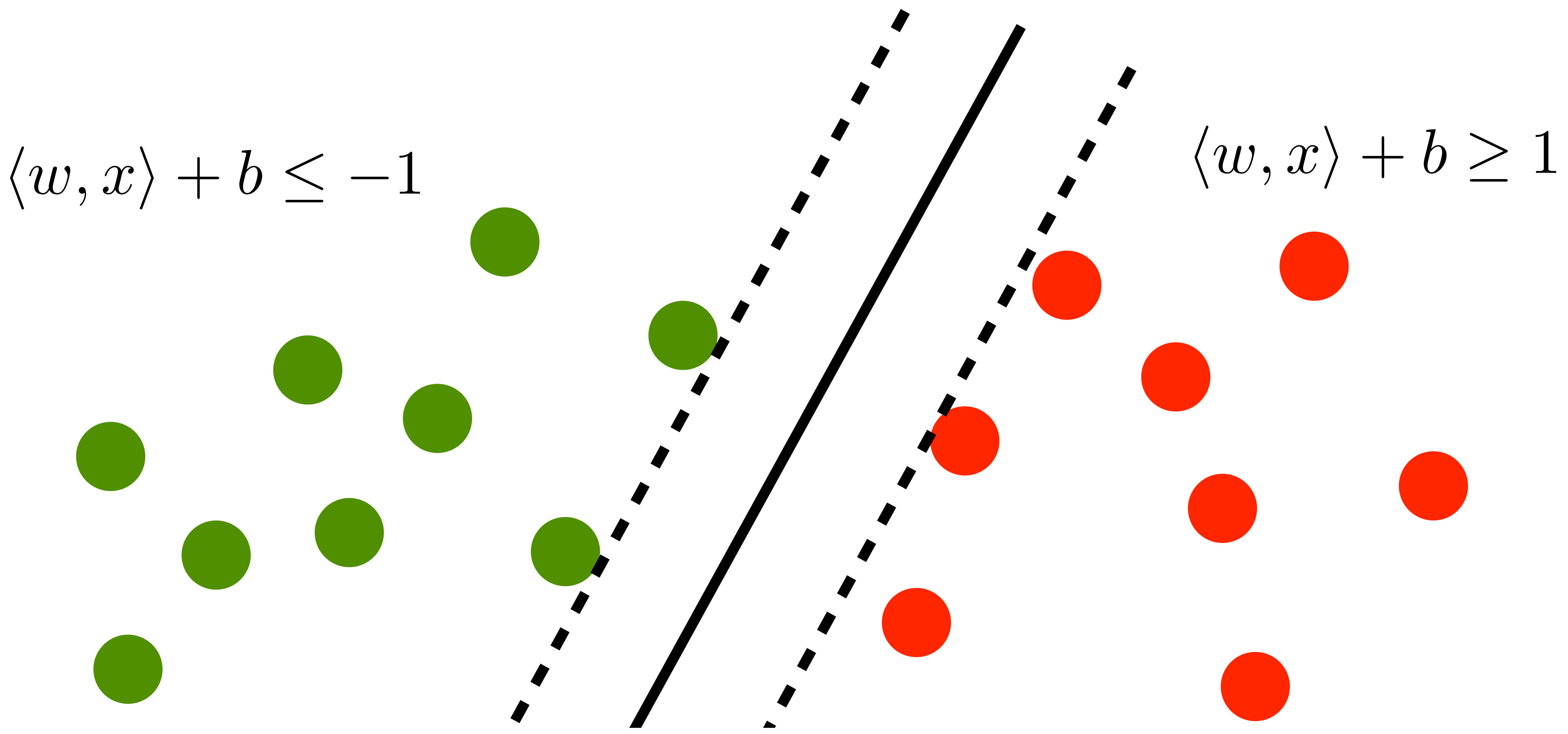
# BBM406 Fundamentals of Machine Learning

## Lecture 16: Soft Margin Classification Multi-class SVMs Kernels

HACETTEPE UNIVERSITY COMPUTER VISION LAB

Aykut Erdem // Hacettepe University // Fall 2019

# Last time… **Support Vector Machines**


$\langle w, x\rangle + b \le -1$
$\langle w, x\rangle + b \ge 1$

linear function

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

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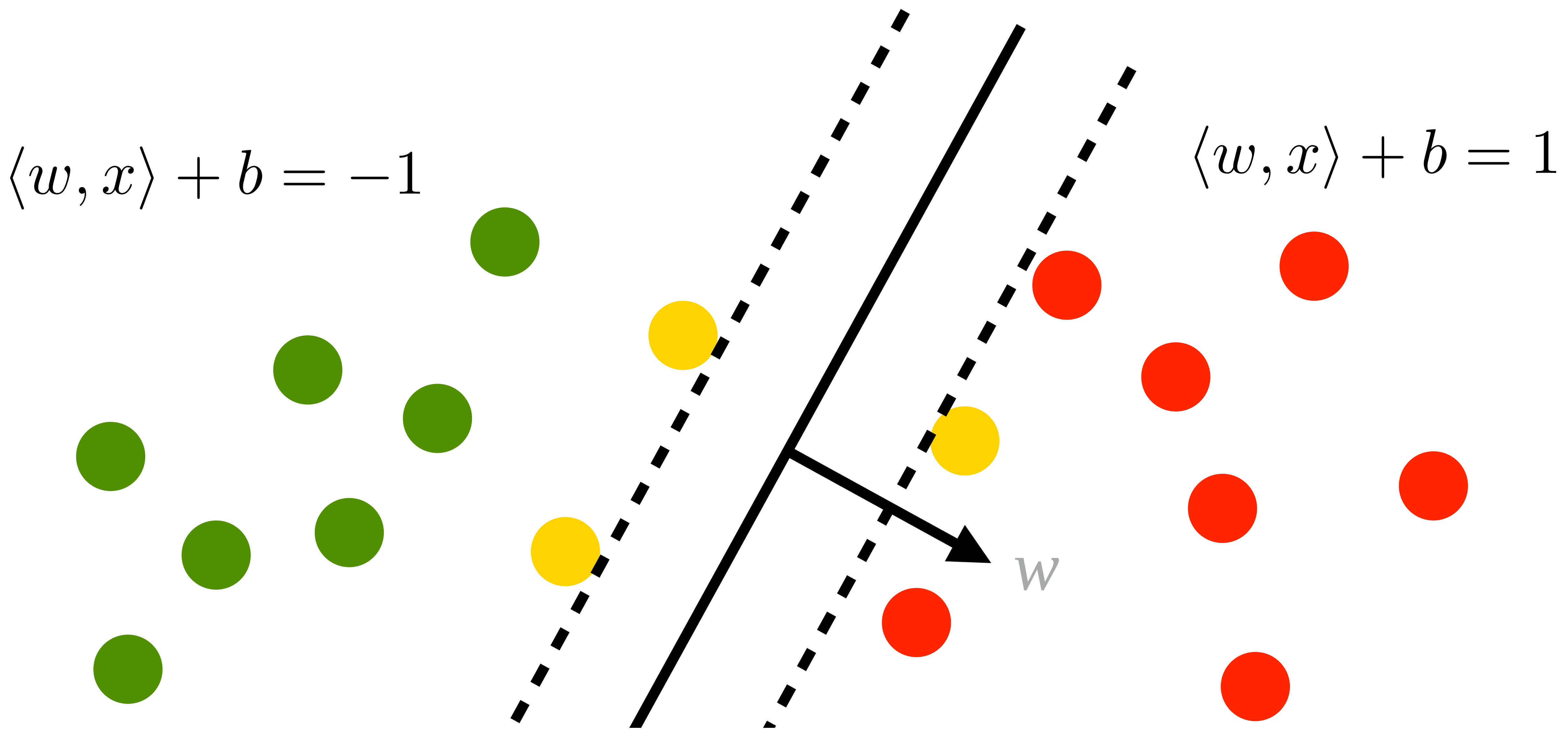
# Last time... **Support Vector Machines**



optimization problem

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

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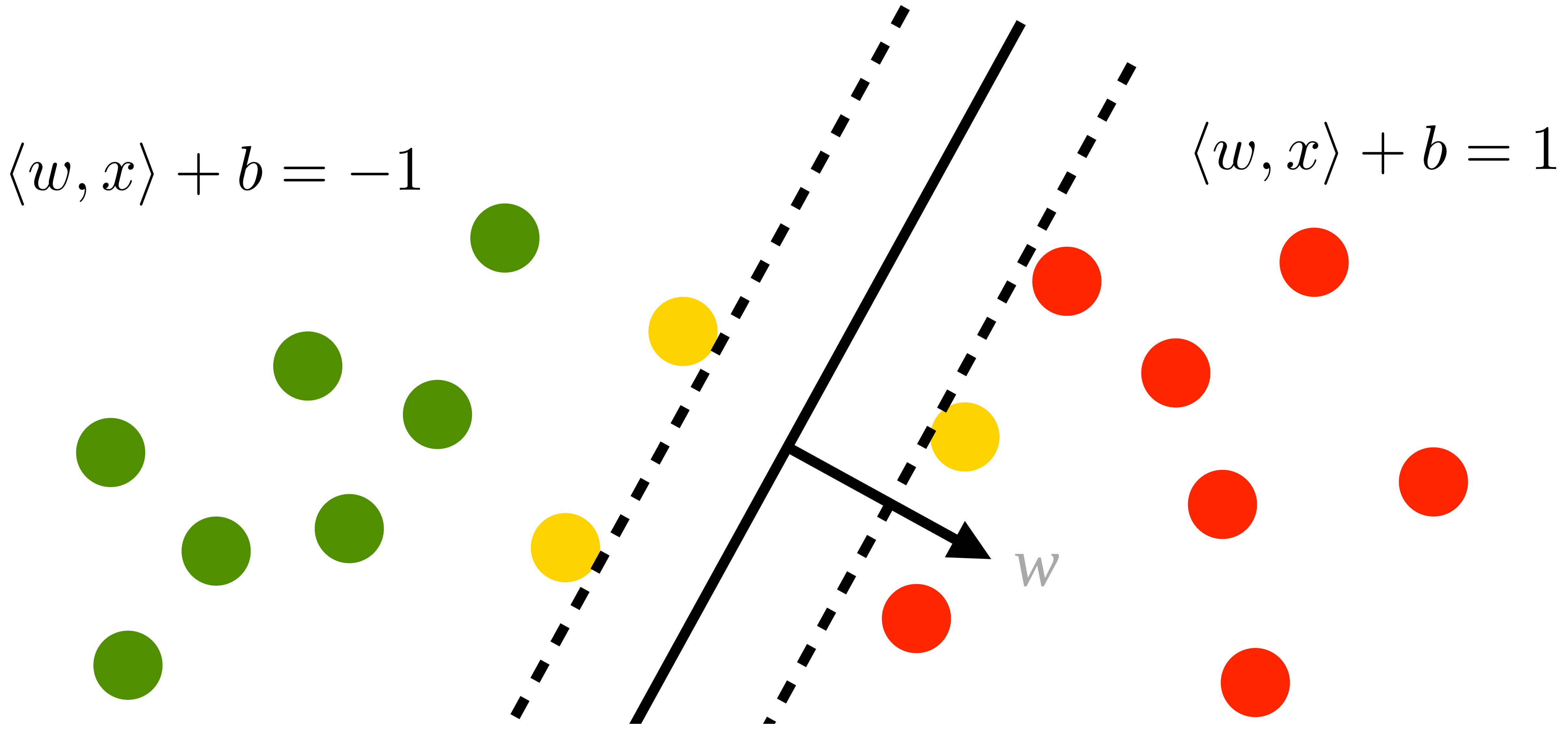
# Last time... **Support Vector Machines**


$\langle w, x \rangle + b = -1$
$\langle w, x \rangle + b = 1$
$w$

optimization problem

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

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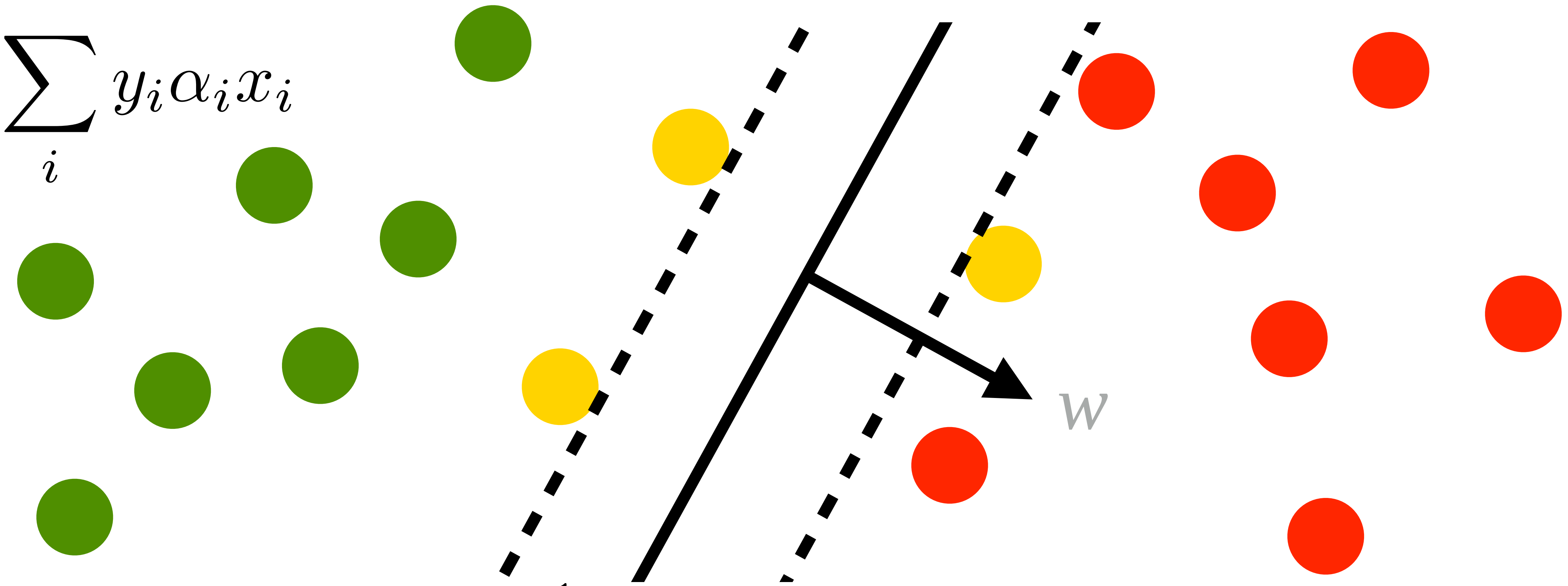
# Last time... **Support Vector Machines**

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

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



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

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

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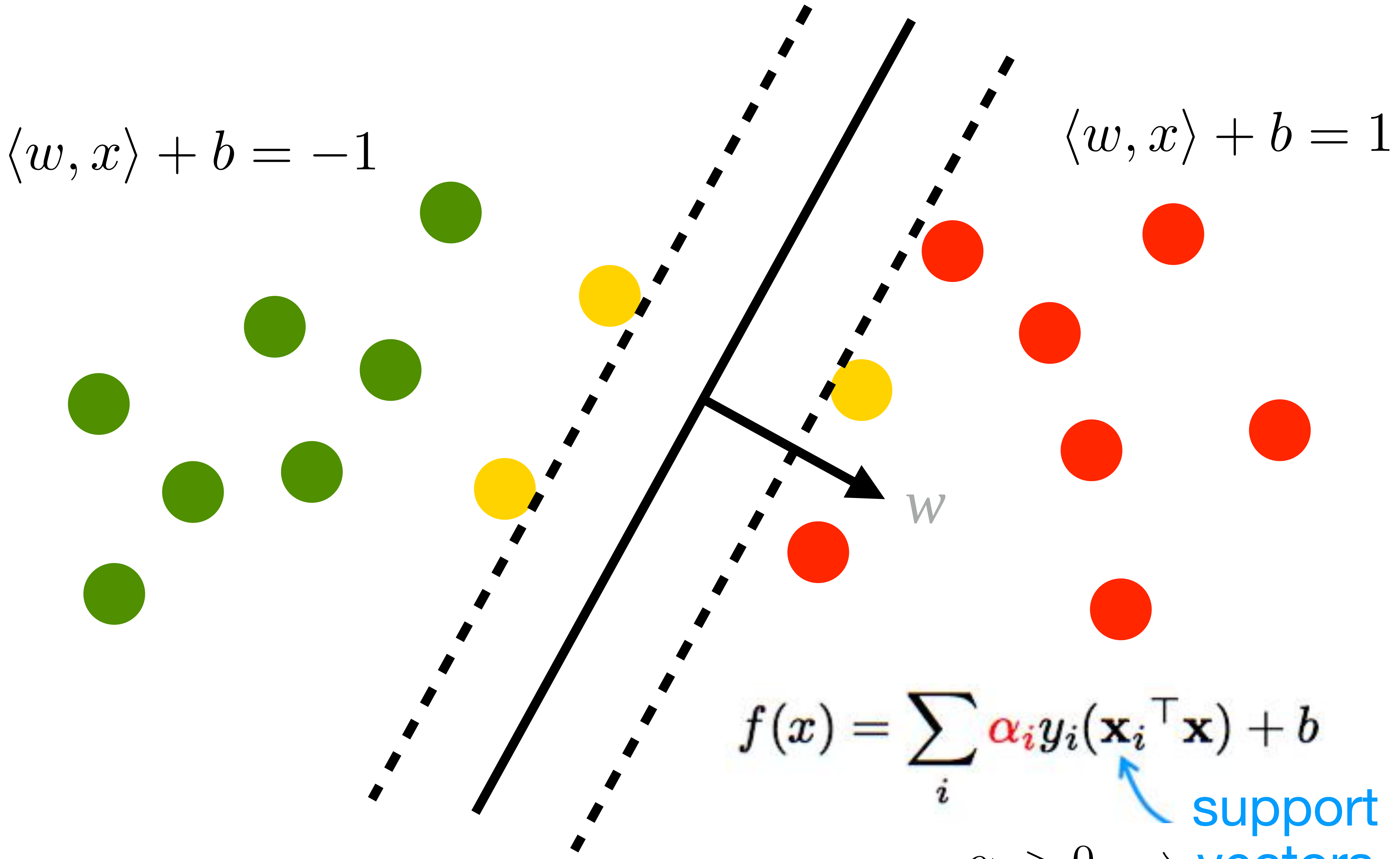
# Last time... **Large Margin Classifier**


$\langle w, x \rangle + b = -1$
$\langle w, x \rangle + b = 1$
$w$

$$f(x) = \sum_i \alpha_i y_i (\mathbf{x}_i{}^\top \mathbf{x}) + b$$

$\alpha_i > 0 \implies$ support vectors

## Today

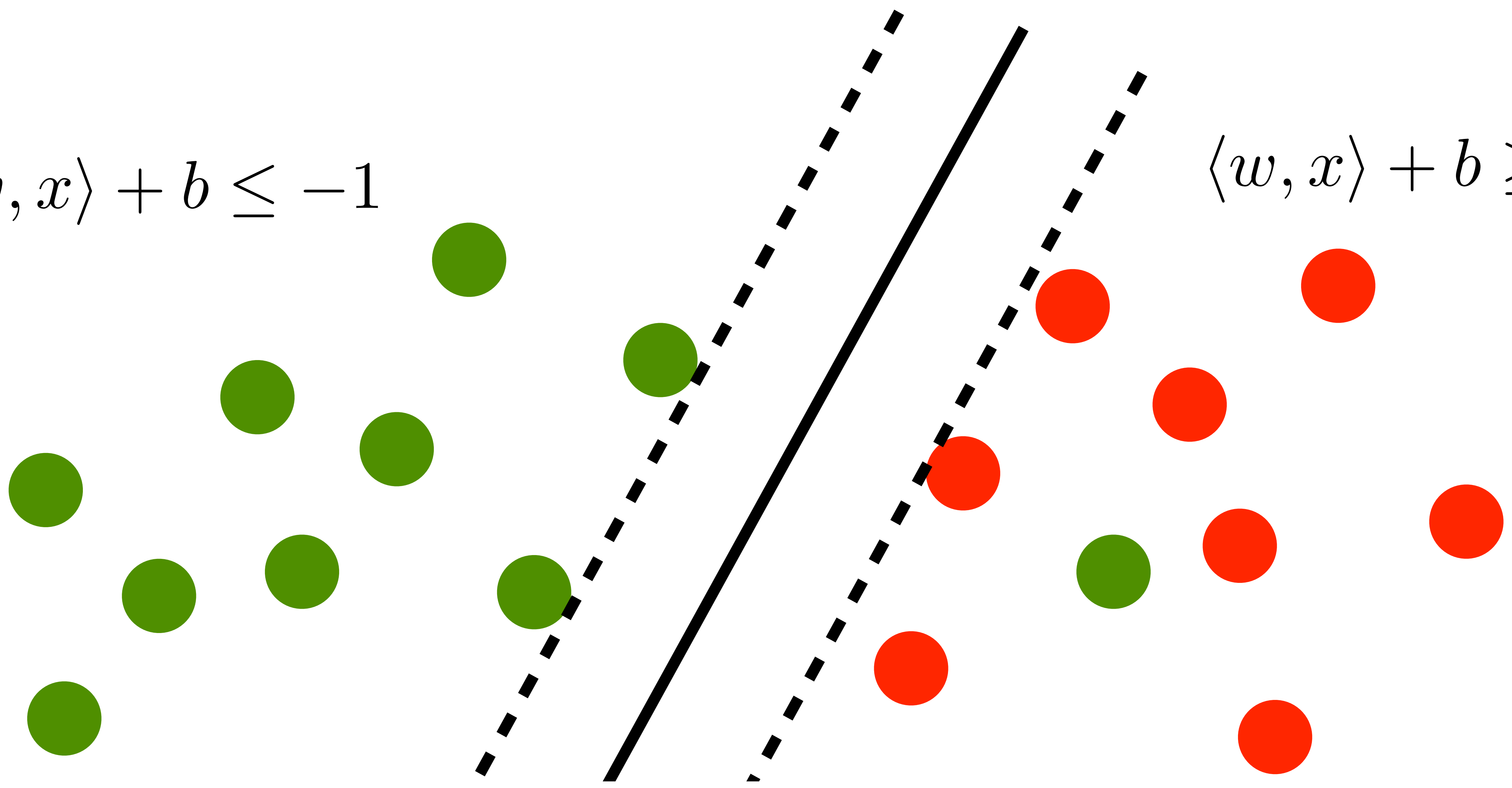
- Soft margin classification
- Multi-class classification
- Introduction to kernels

## Soft Margin Classification

# Large Margin Classifier

$\langle w, x\rangle + b \leq -1$

$\langle w, x\rangle + b \geq 1$



linear function

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

linear separator is impossible

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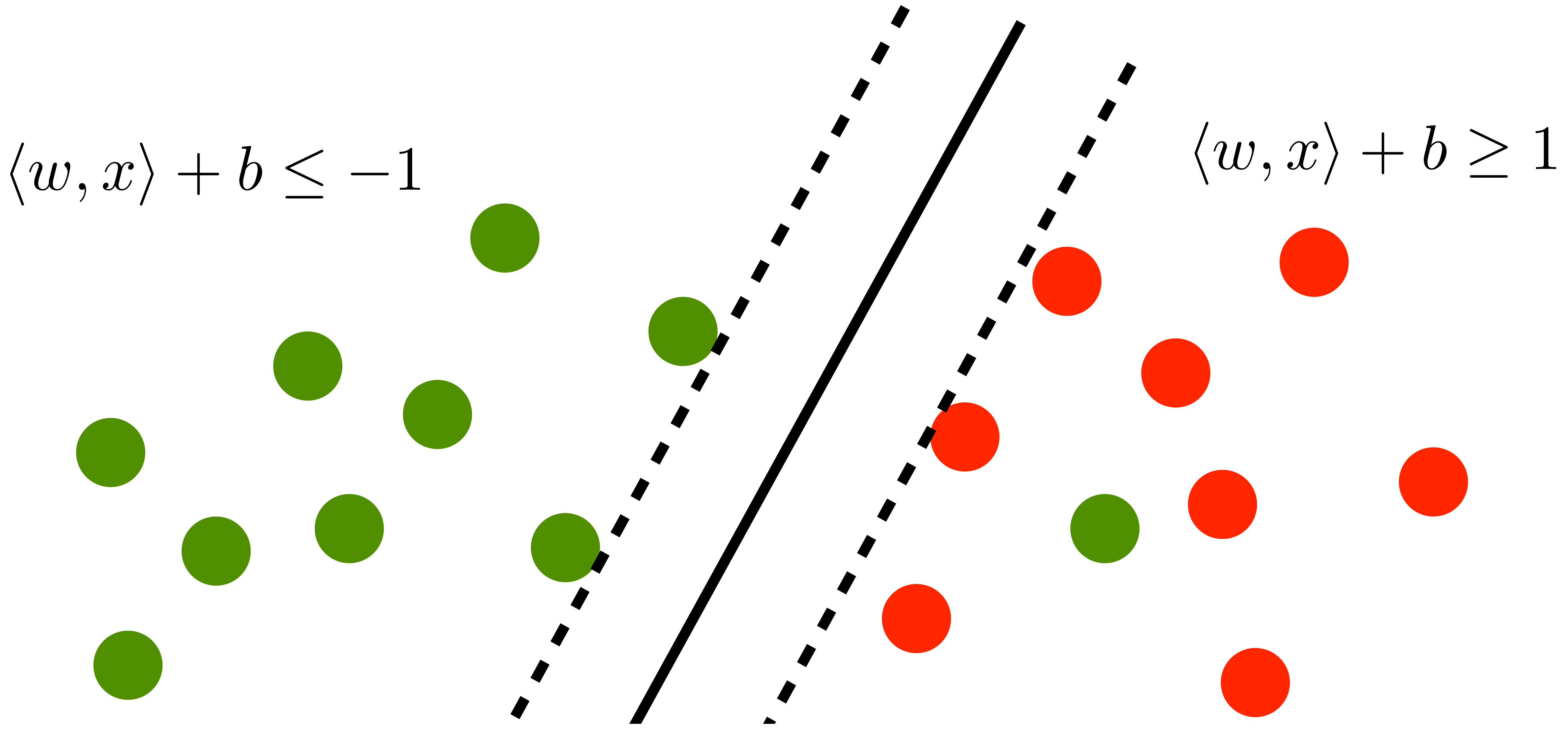
# Large Margin Classifier


$\langle w, x\rangle + b \leq -1$
$\langle w, x\rangle + b \geq 1$

minimum error separator is impossible

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

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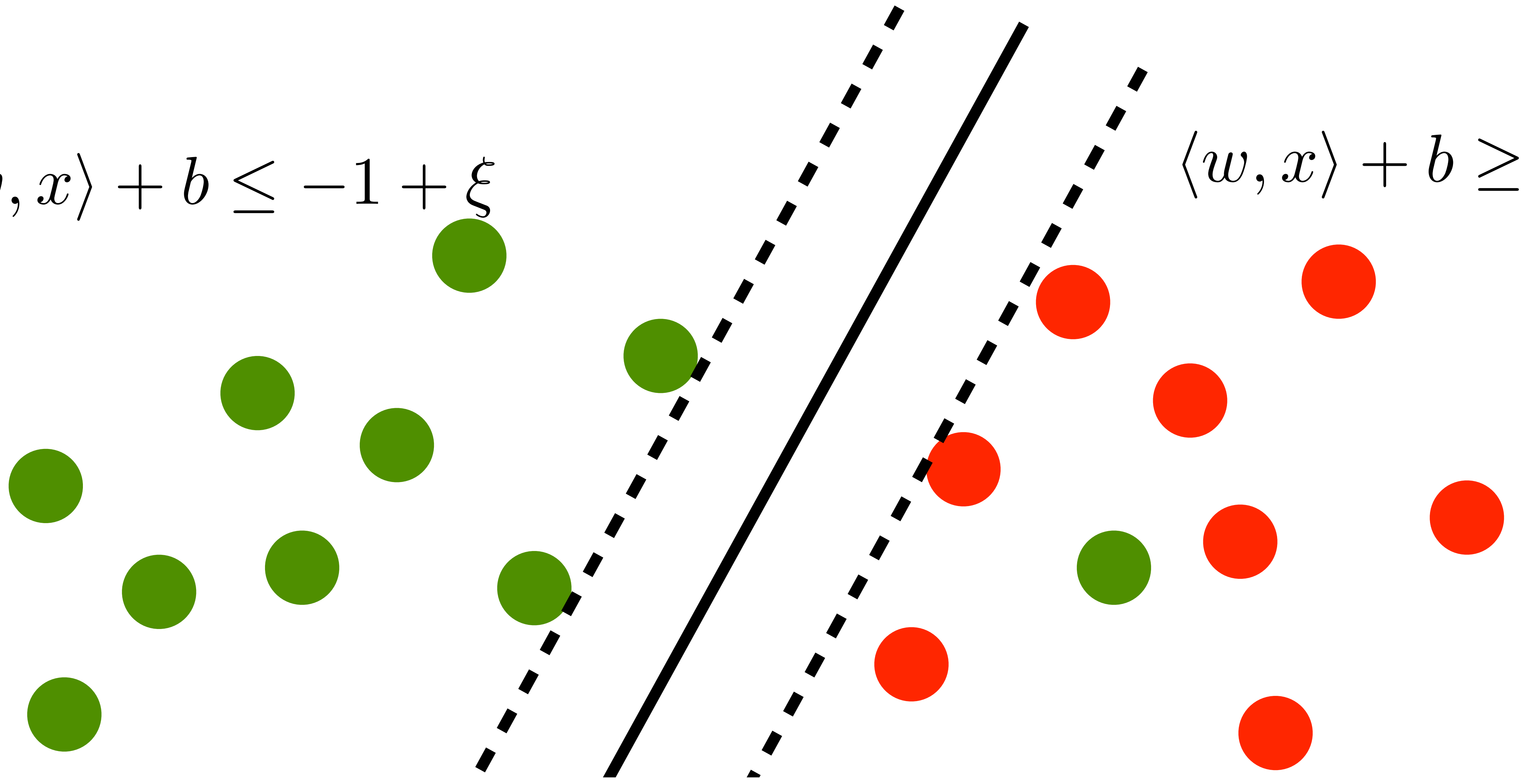
# Adding Slack Variables

$\langle w, x \rangle + b \leq -1 + \xi$

$\langle w, x \rangle + b \geq 1 - \xi$



minimize amount of slack

Convex optimization problem

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# 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)

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# Adding Slack Variables

- Hard margin problem

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

- With slack variables

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

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

Problem is always feasible. Proof:
$w = 0 \text{ and } b = 0 \text{ and } \xi_i = 1$ (also yields upper bound)

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# Dual Problem

- Primal optimization problem

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

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

- Lagrange function

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

Optimality in $w, b, \xi$ is at saddle point with $\alpha, \eta$

- Derivatives in $w, b, \xi$ need to vanish

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# 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

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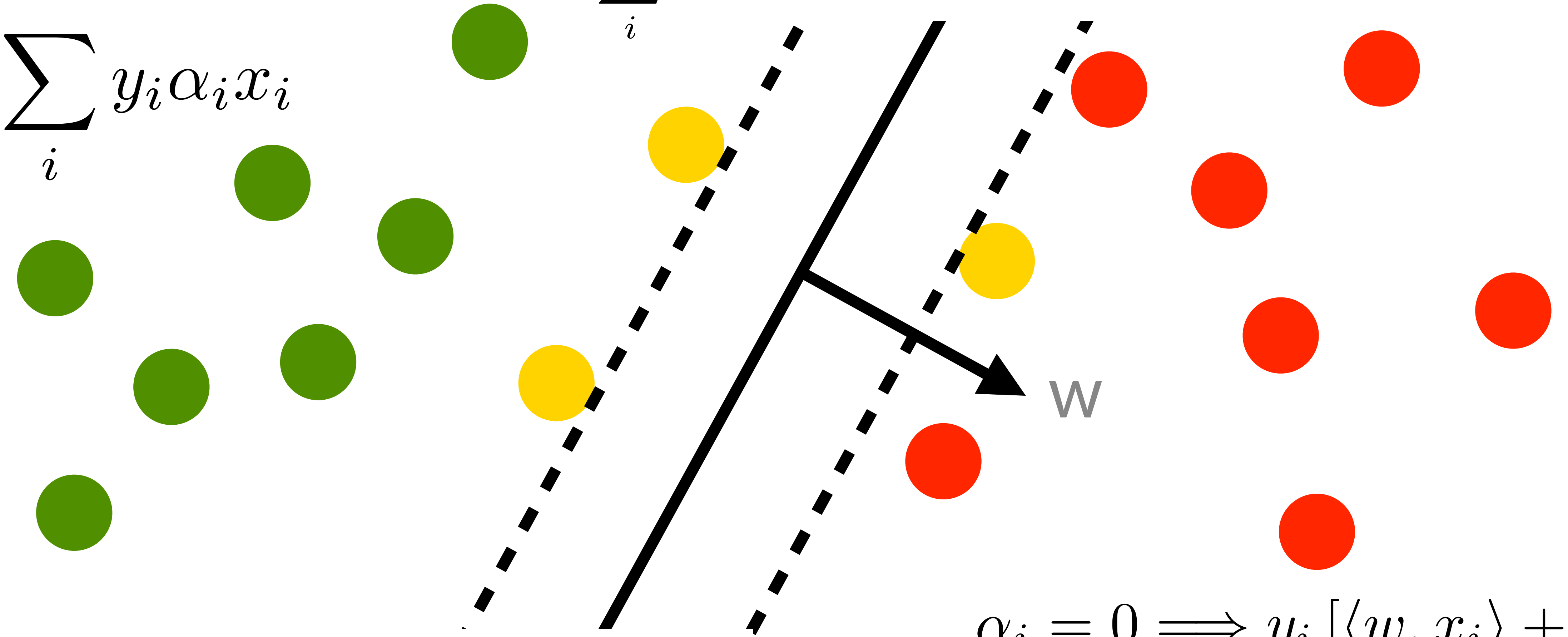
# Karush Kuhn Tucker Conditions

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

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

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



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

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

$$\eta_i\xi_i = 0$$

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

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

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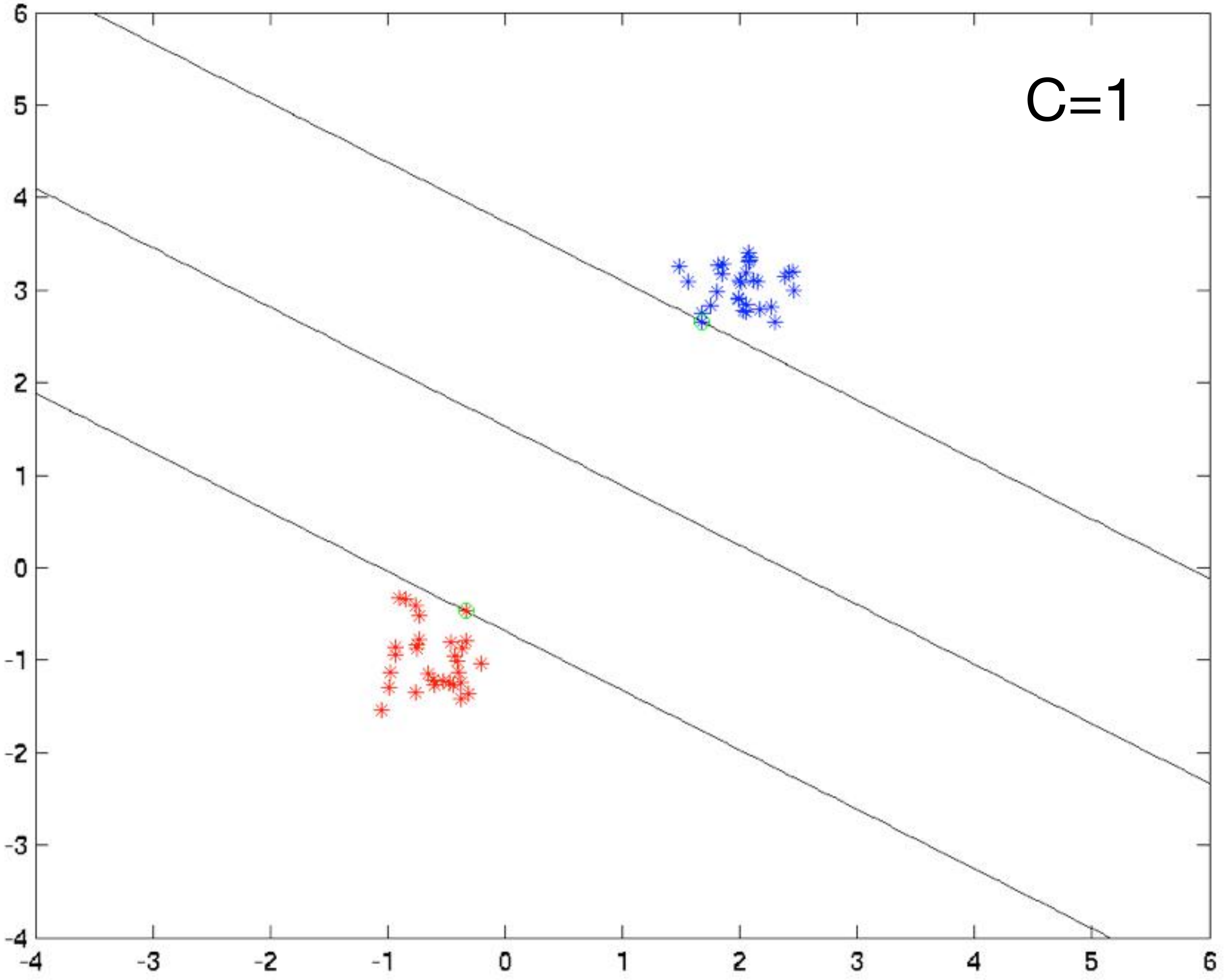

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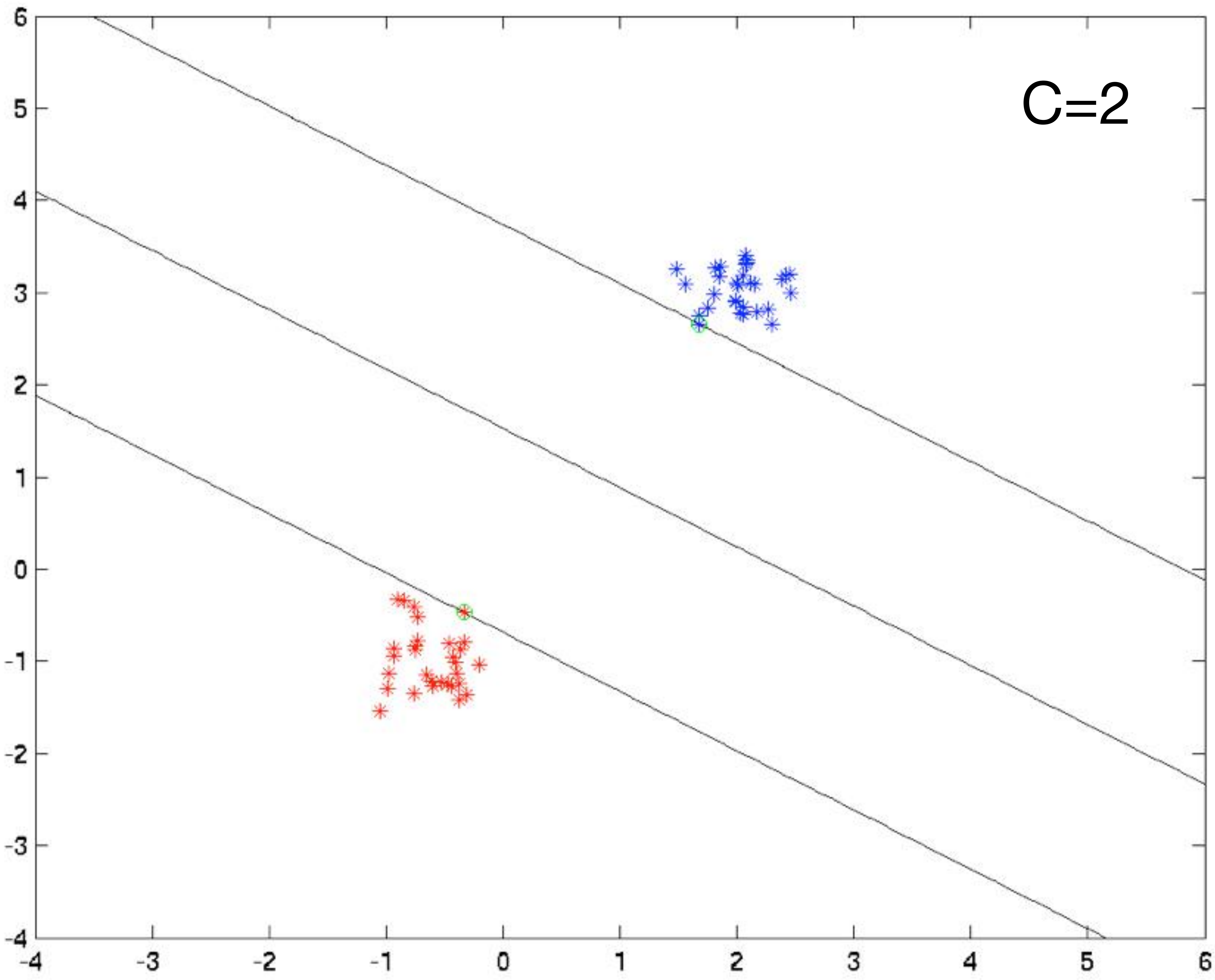

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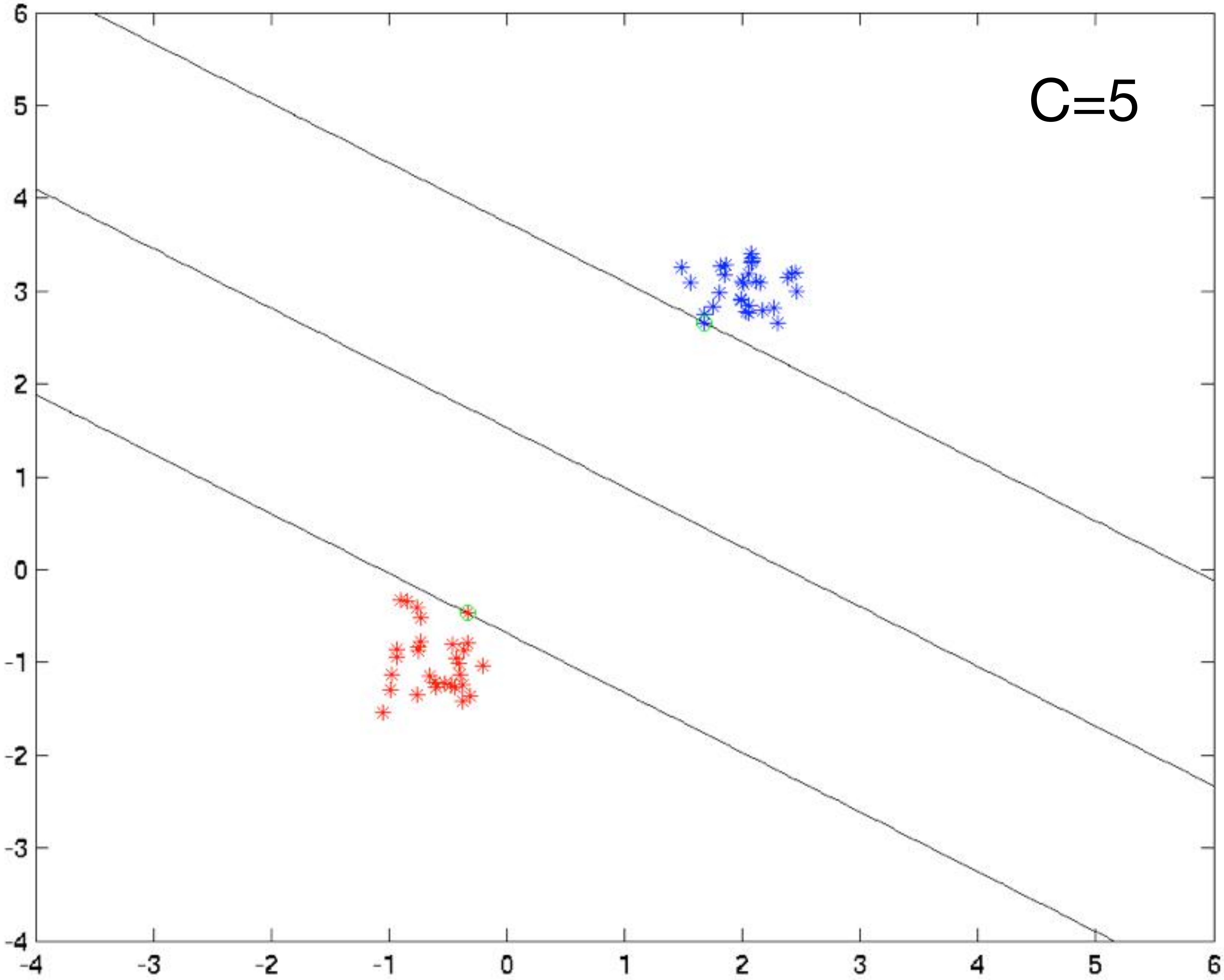

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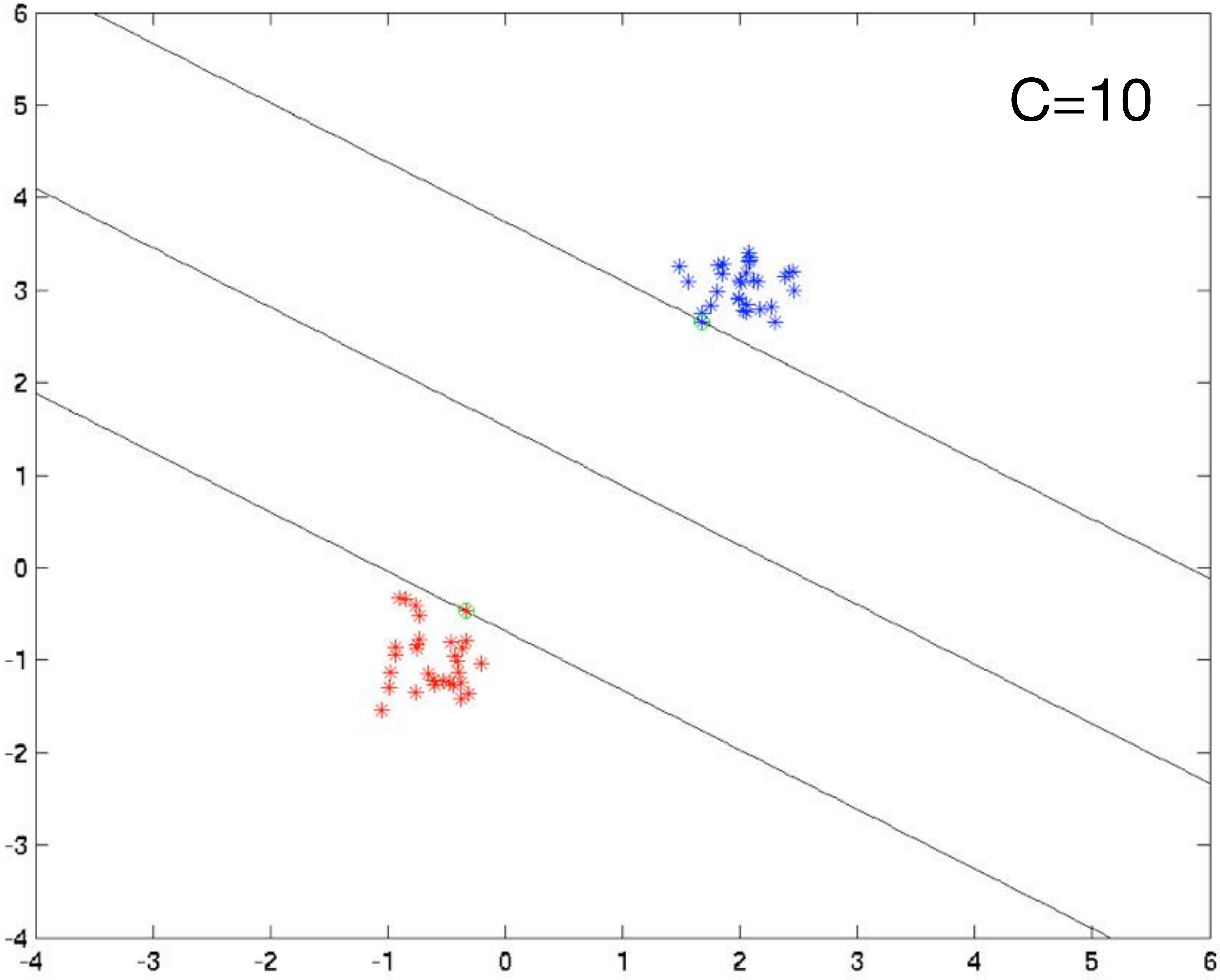

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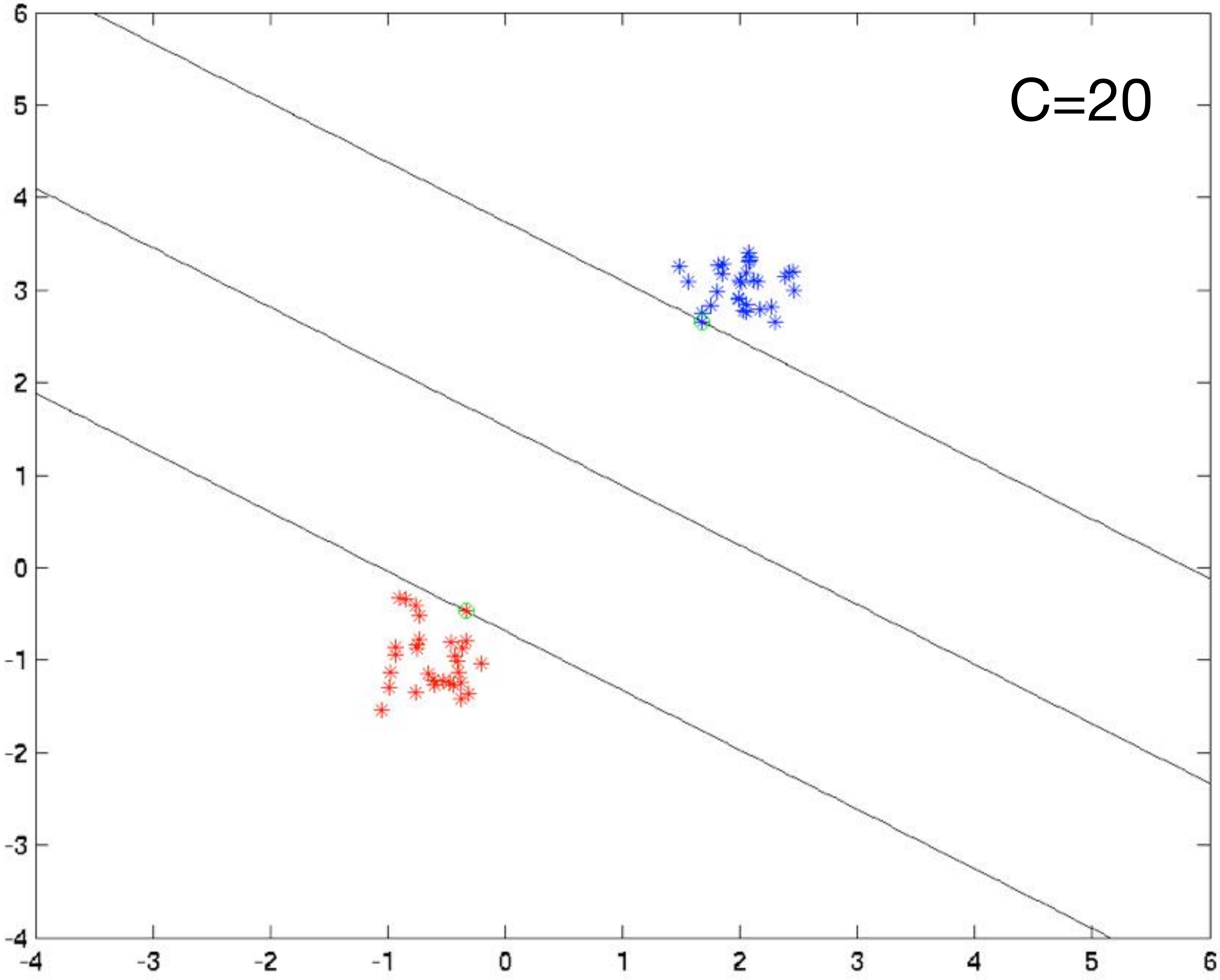

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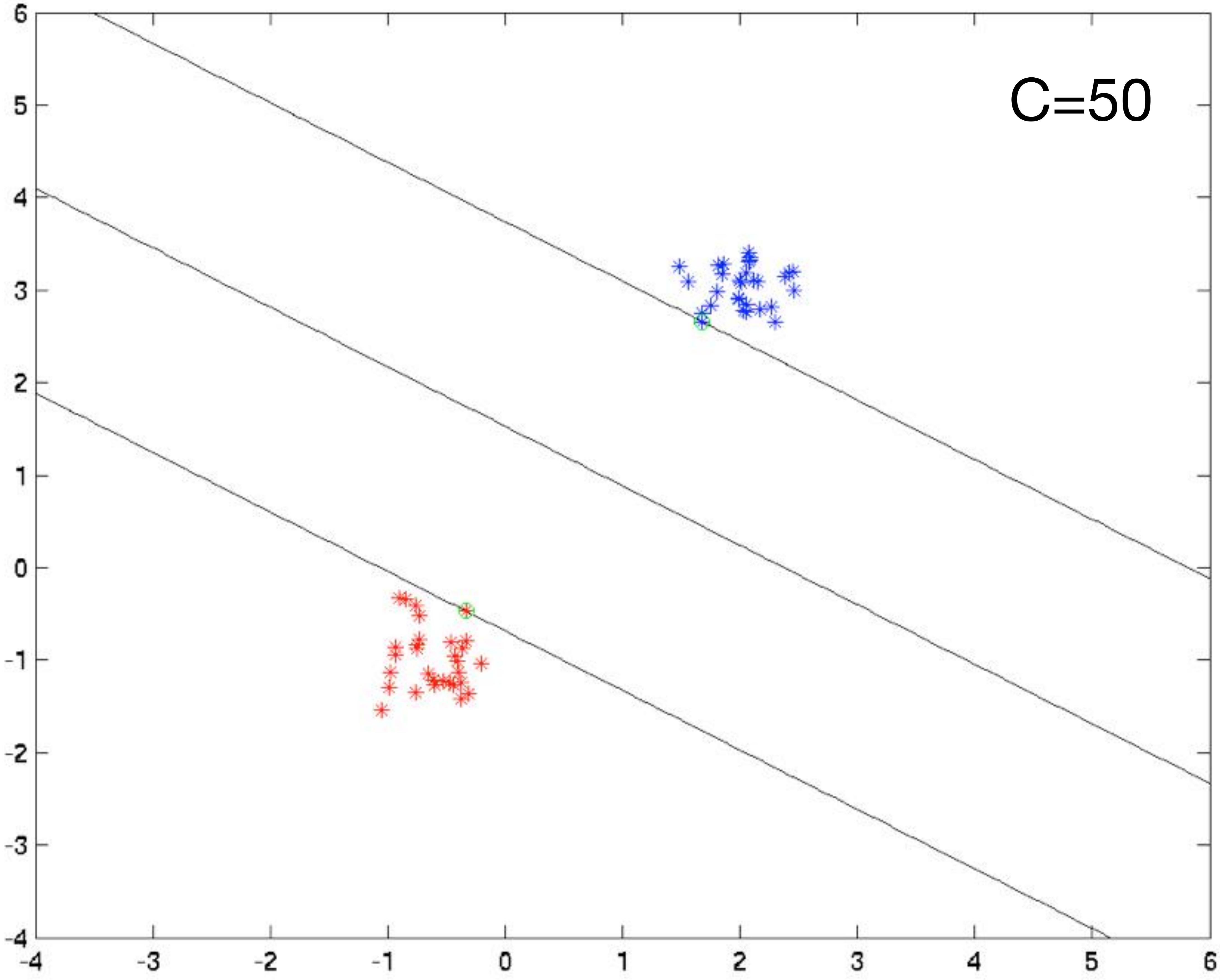

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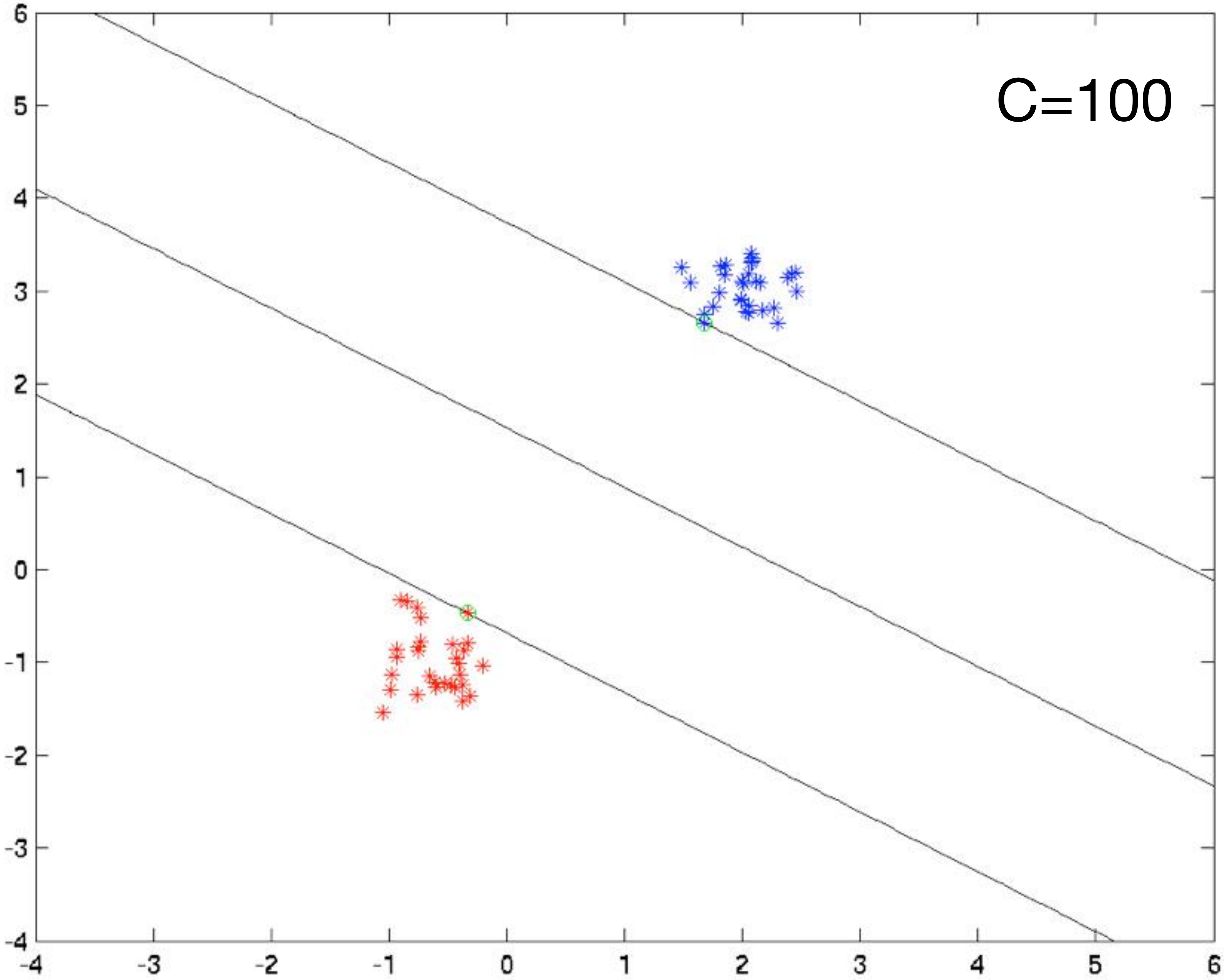

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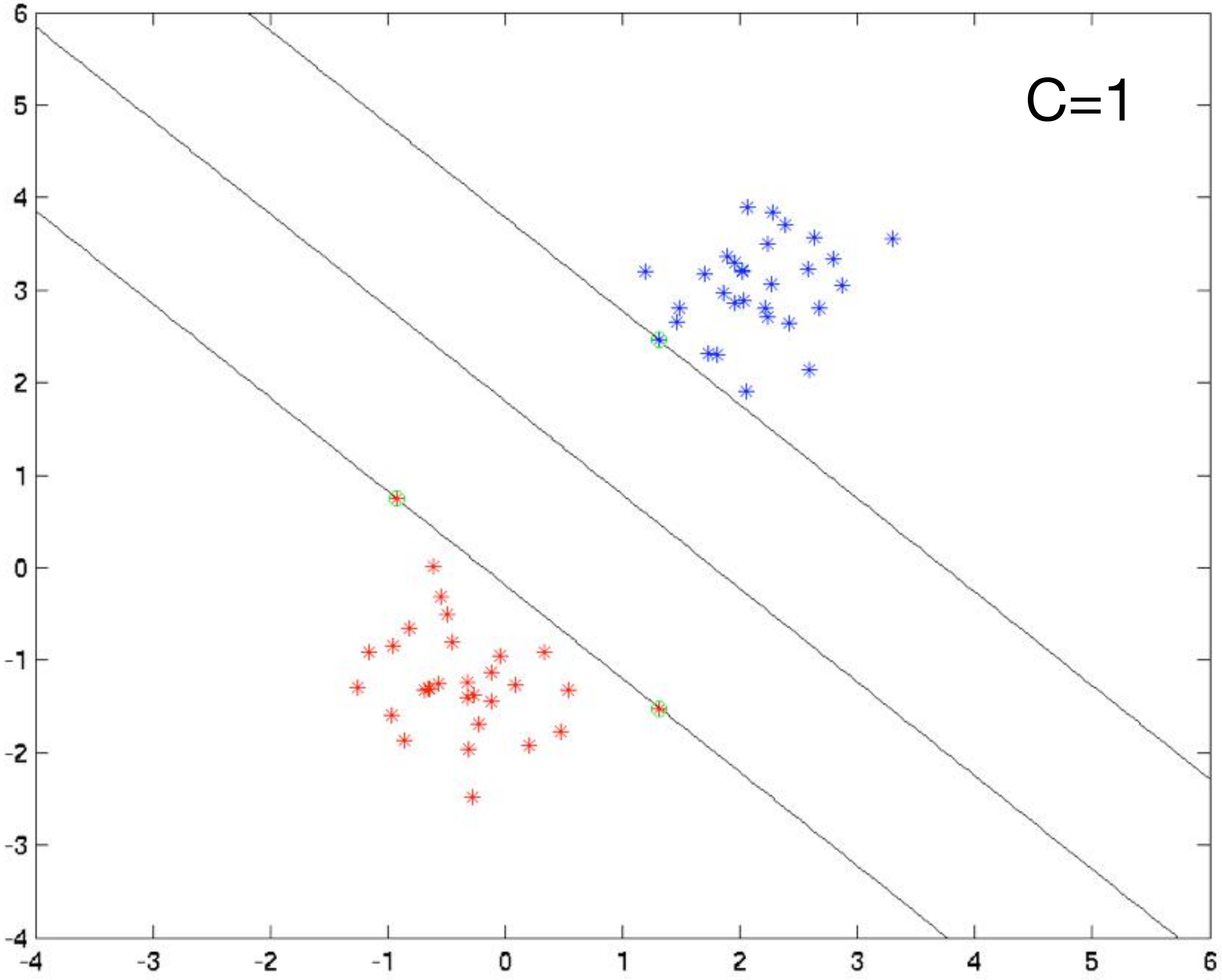

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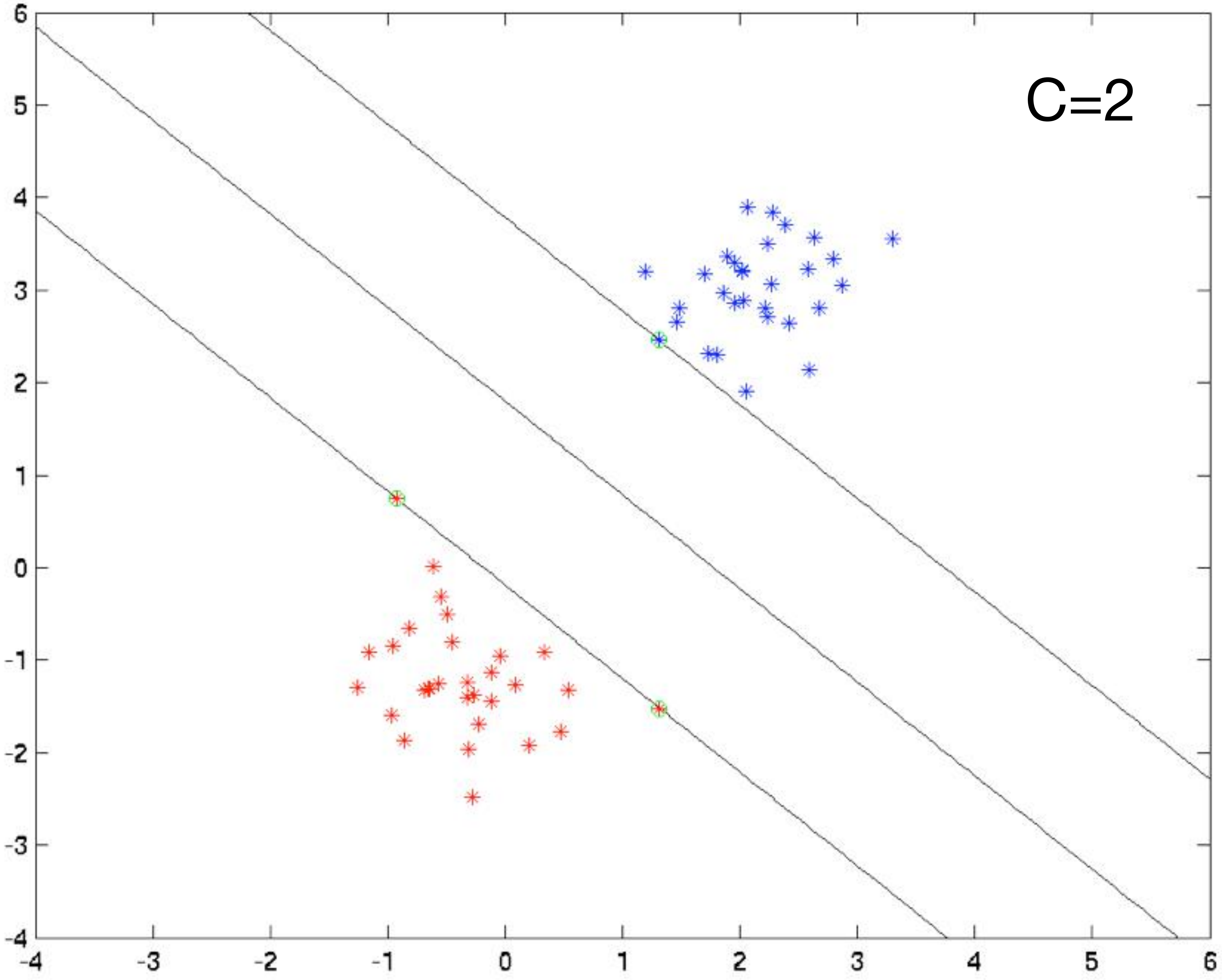

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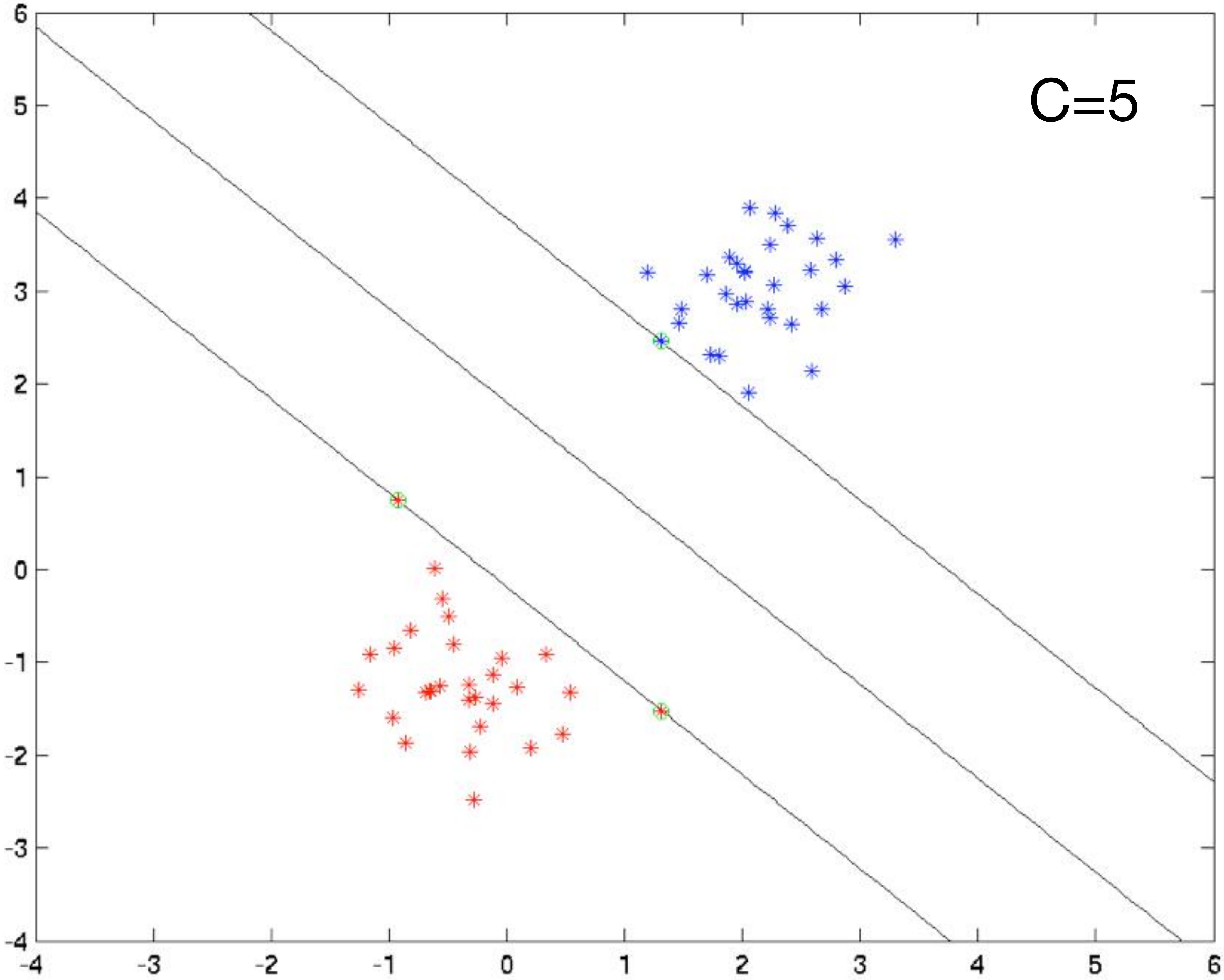

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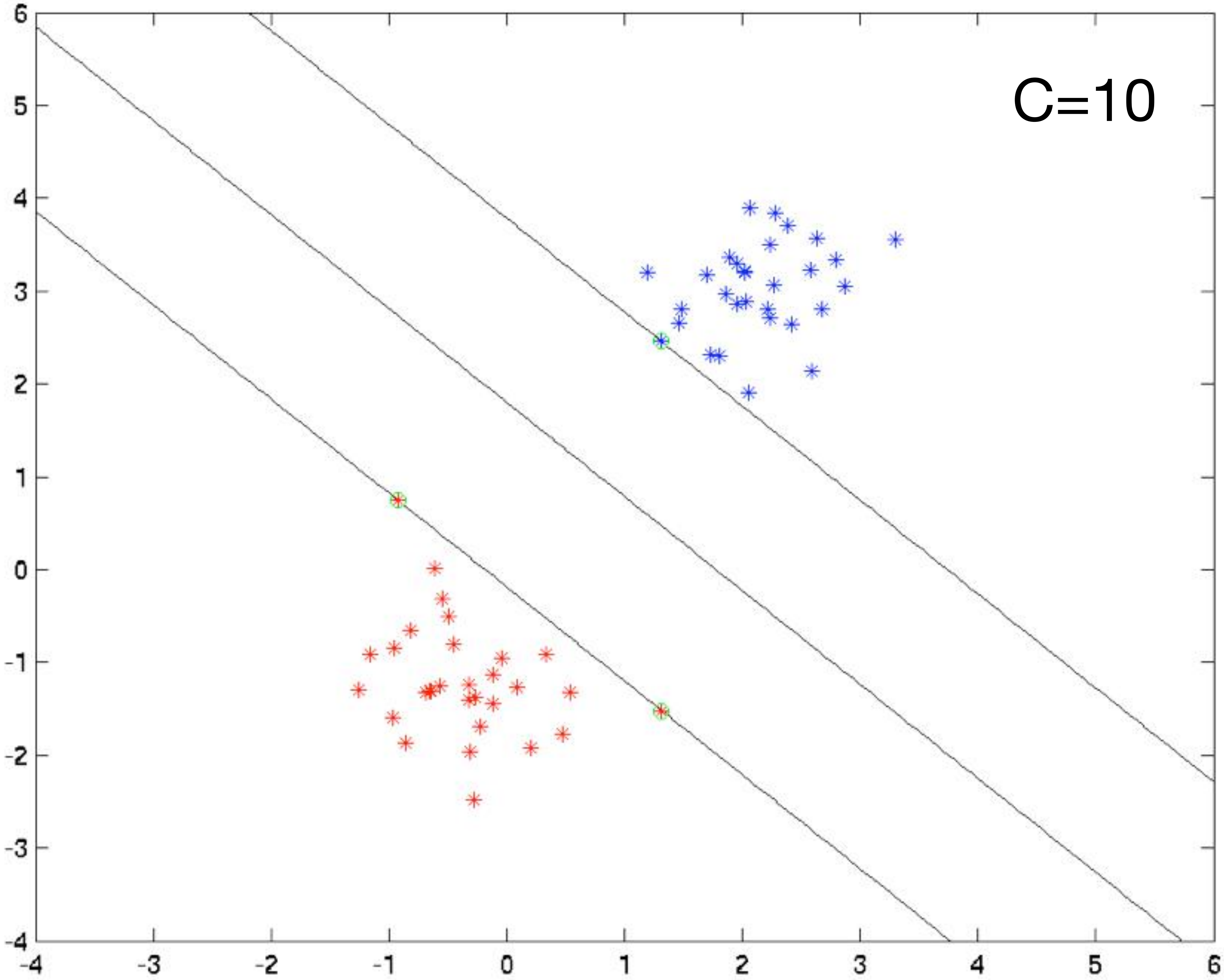

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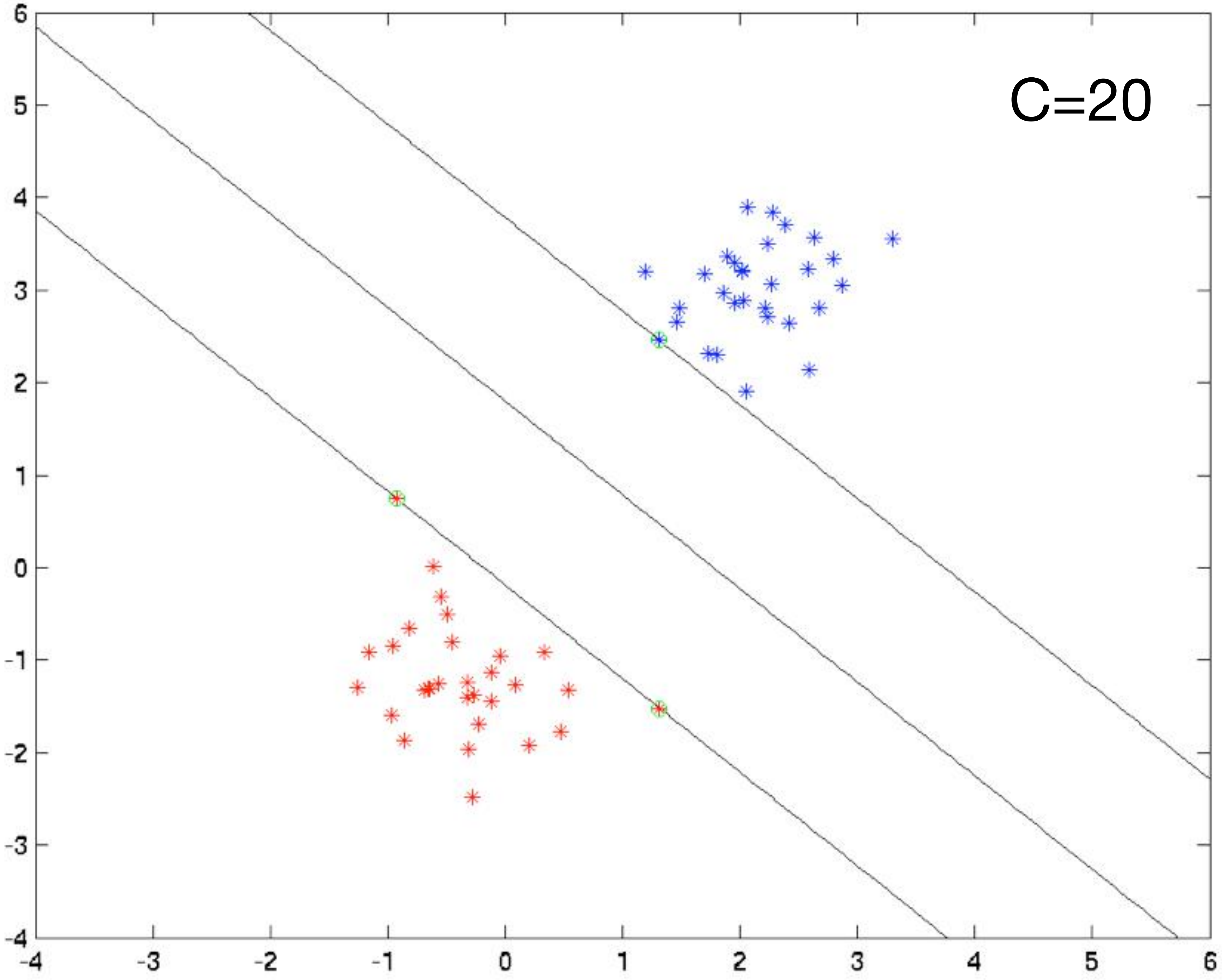

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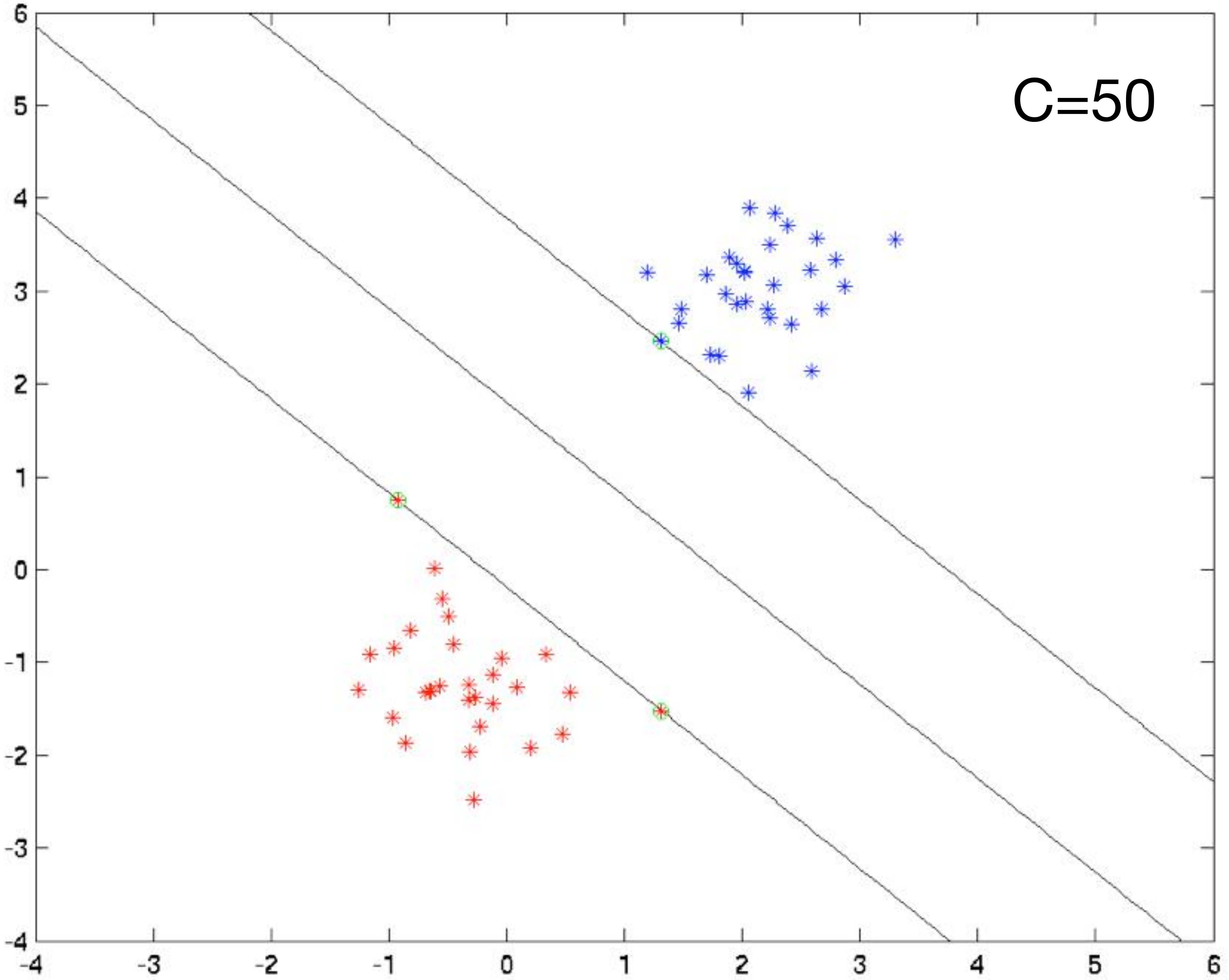

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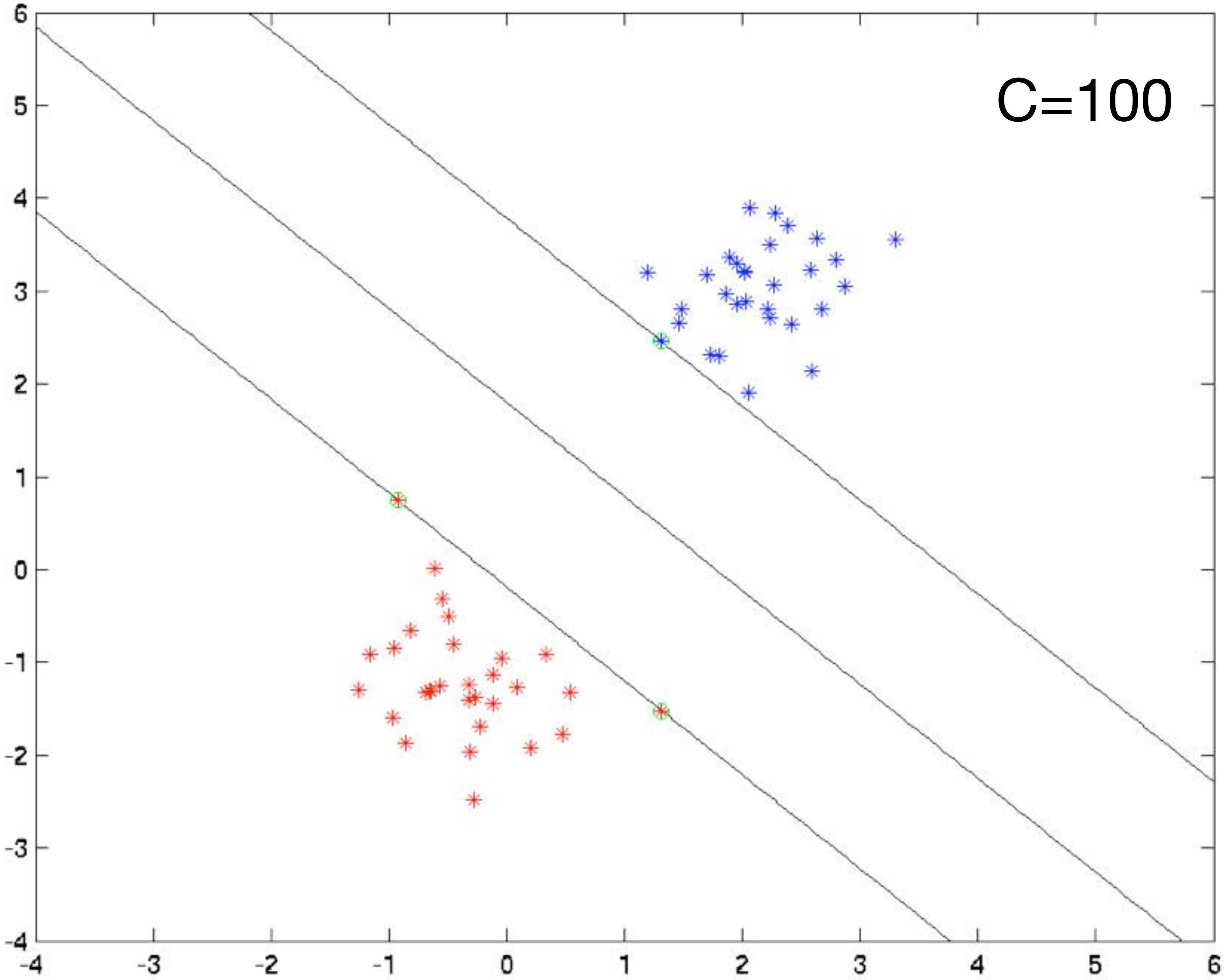

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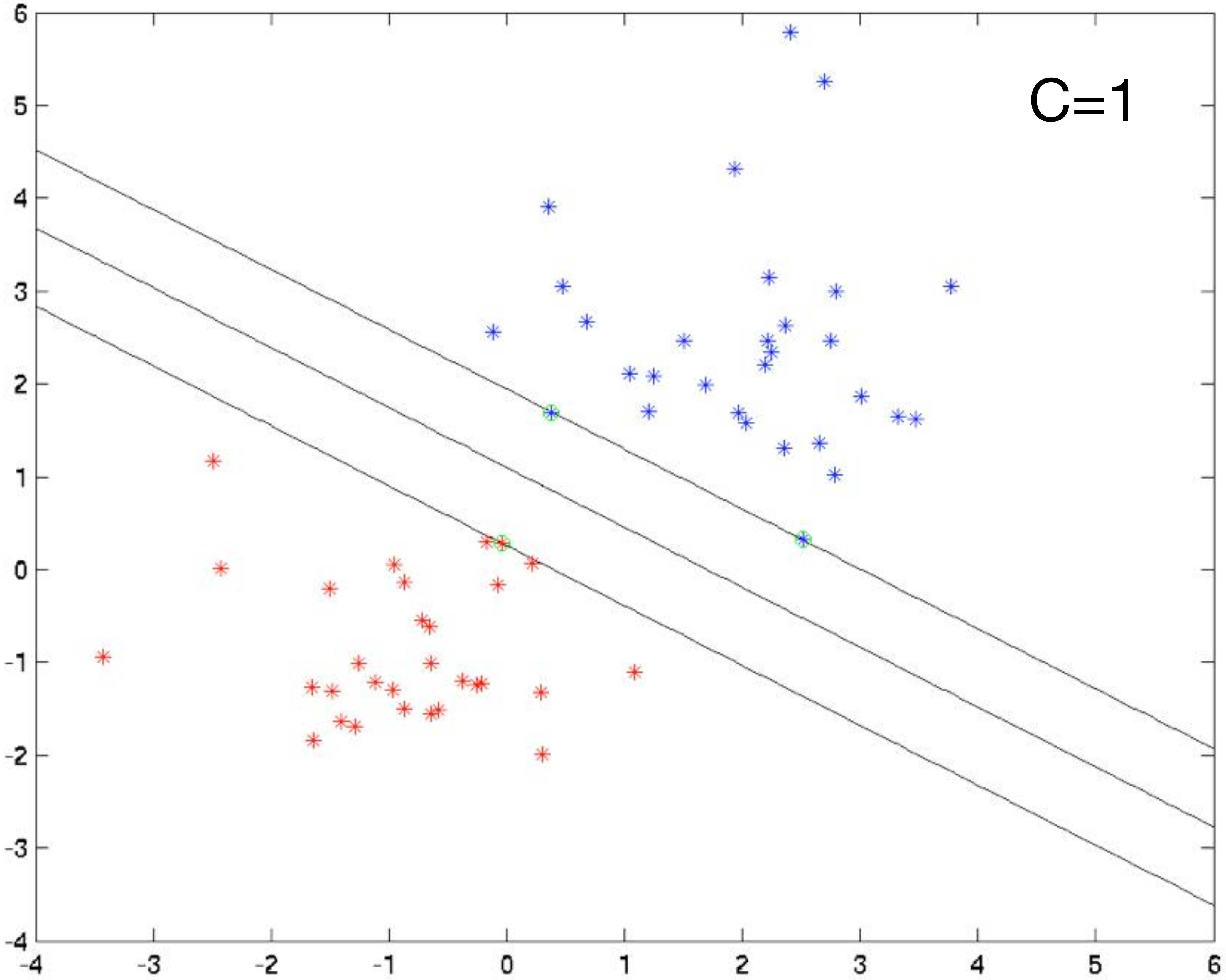

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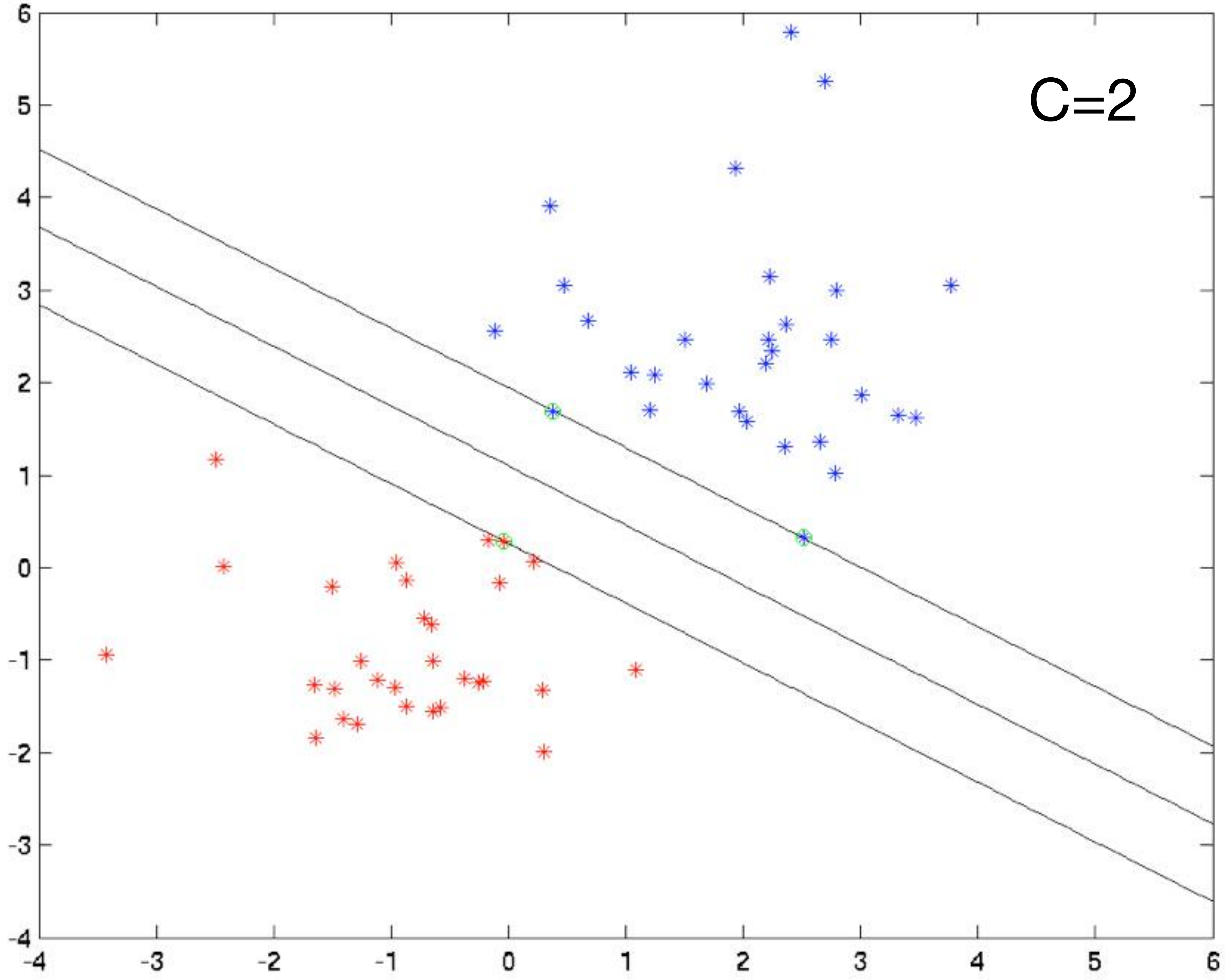

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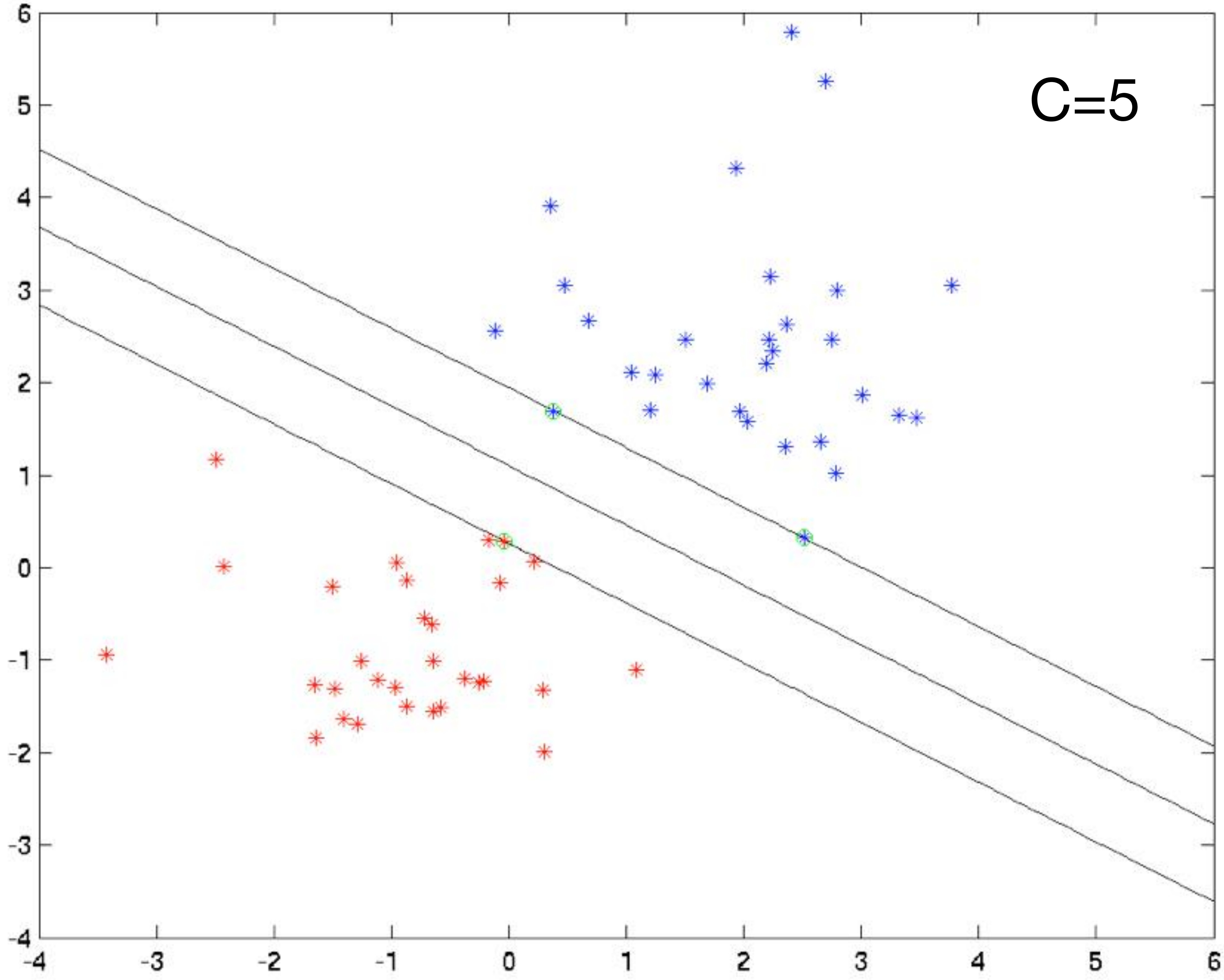

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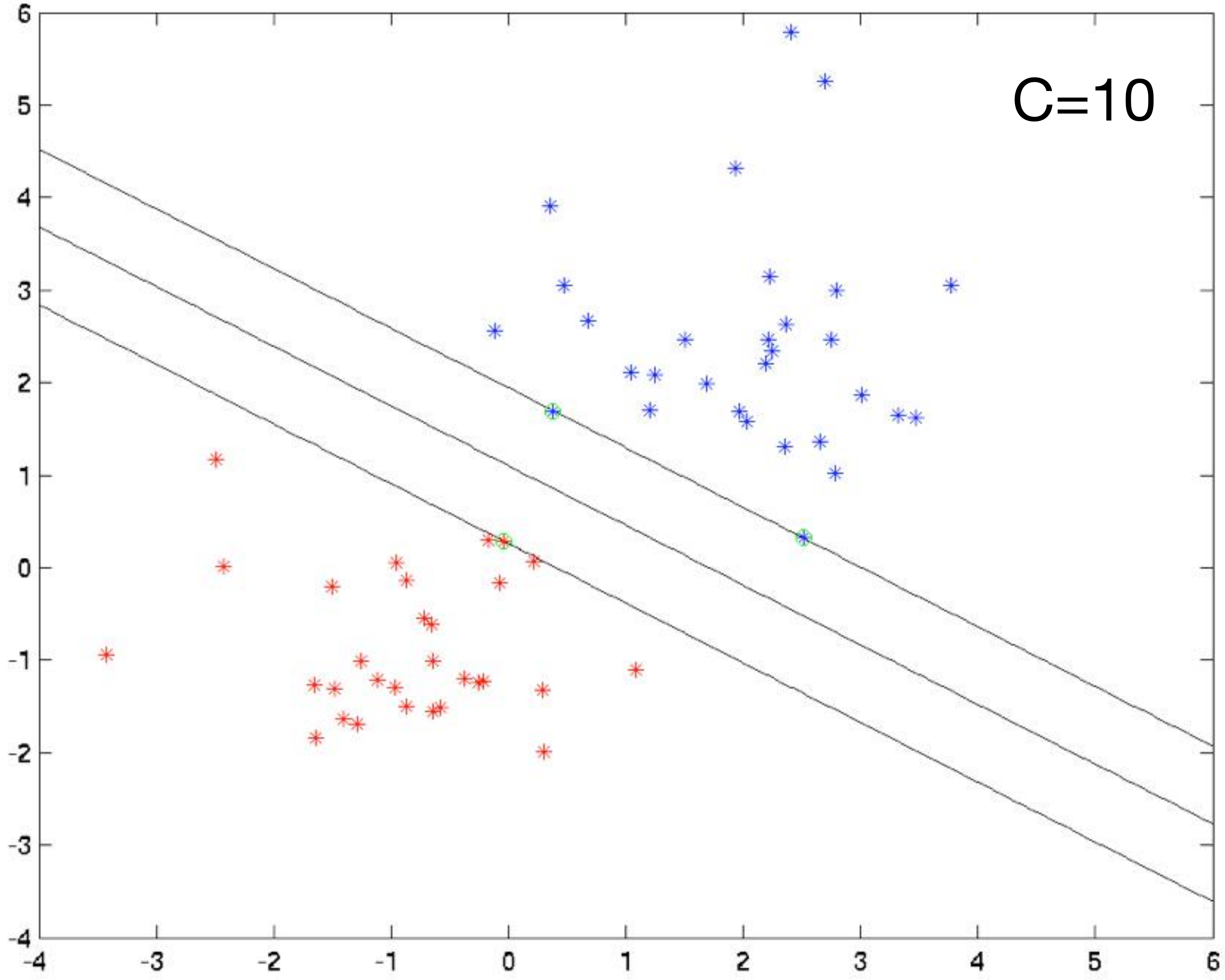

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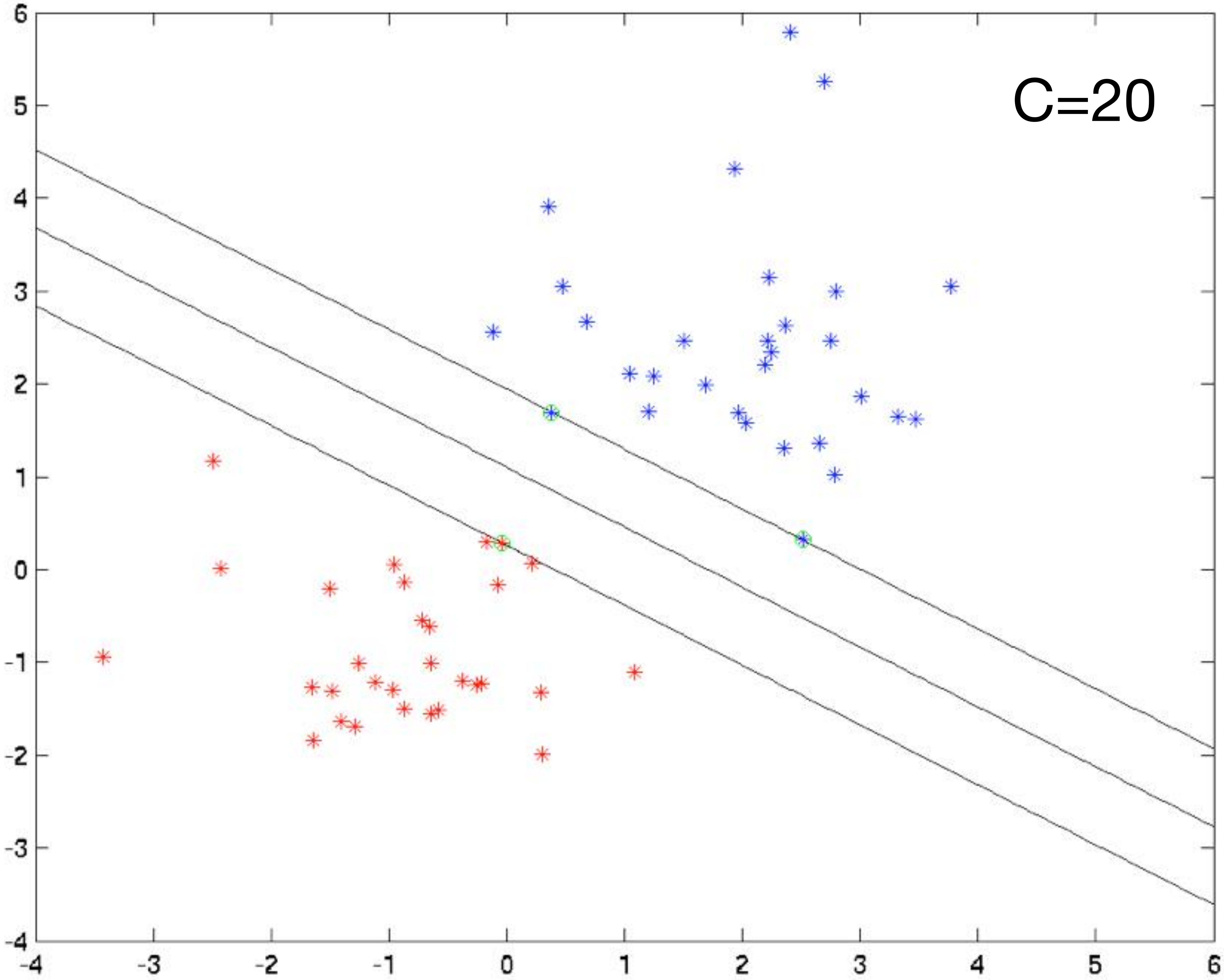

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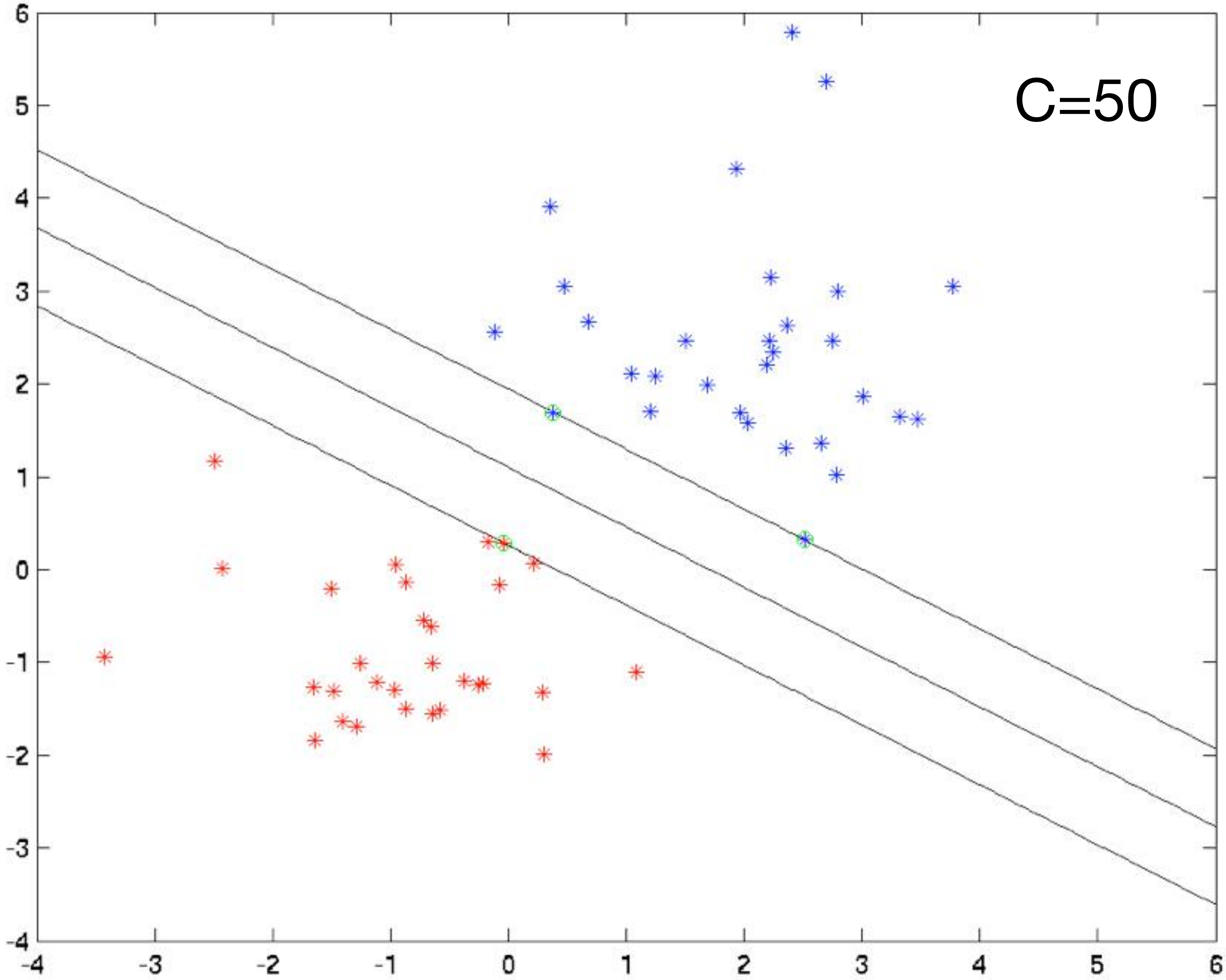

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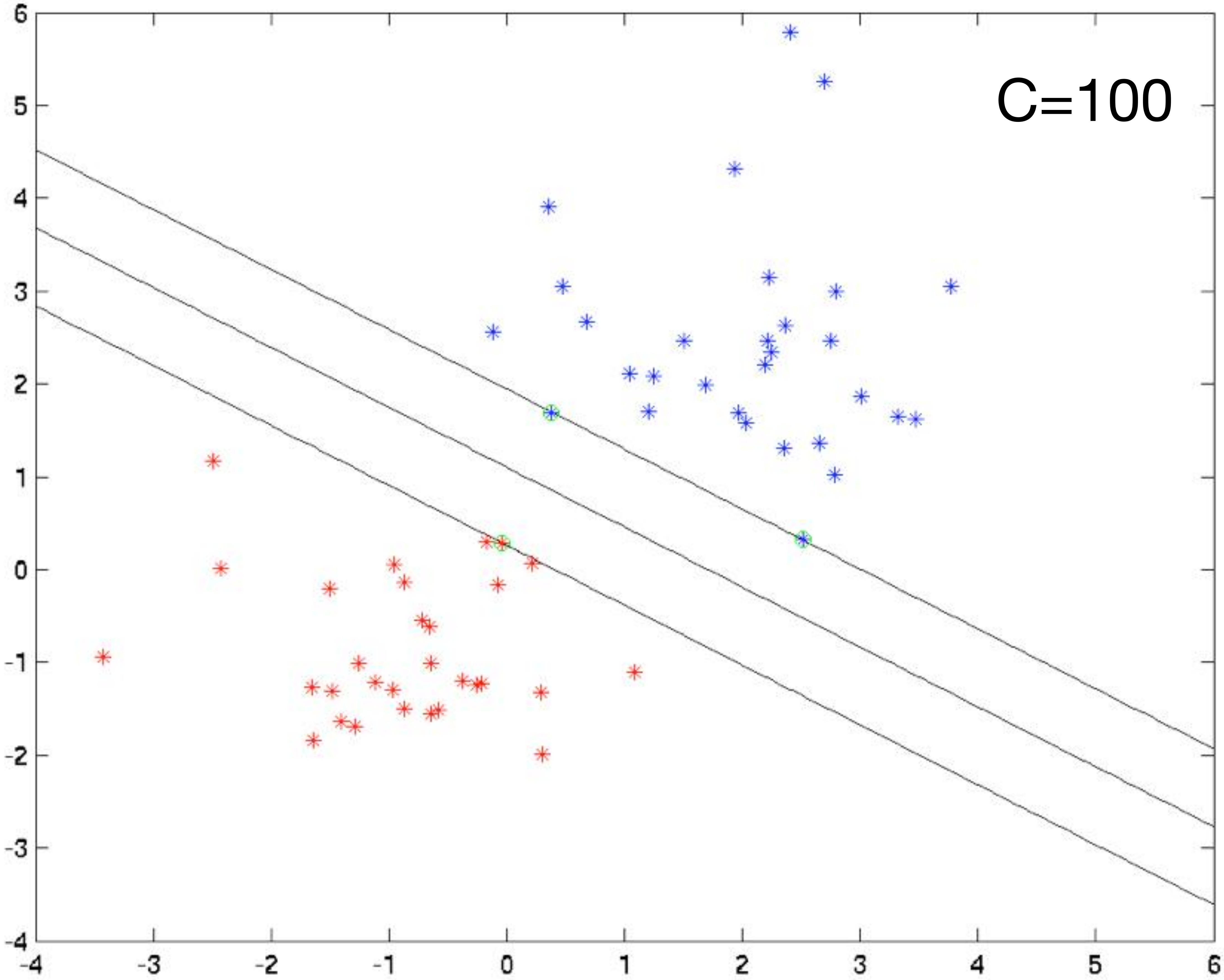

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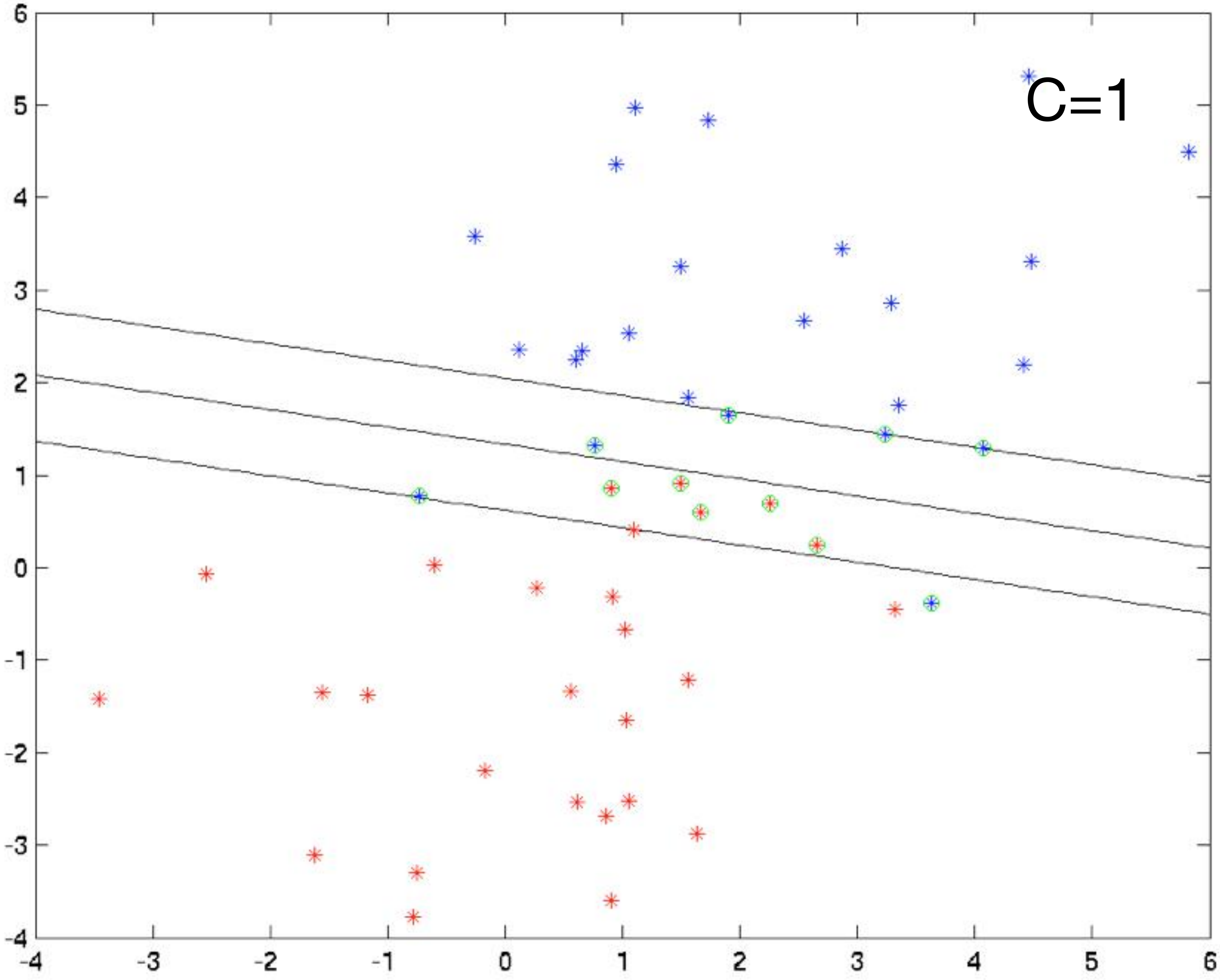

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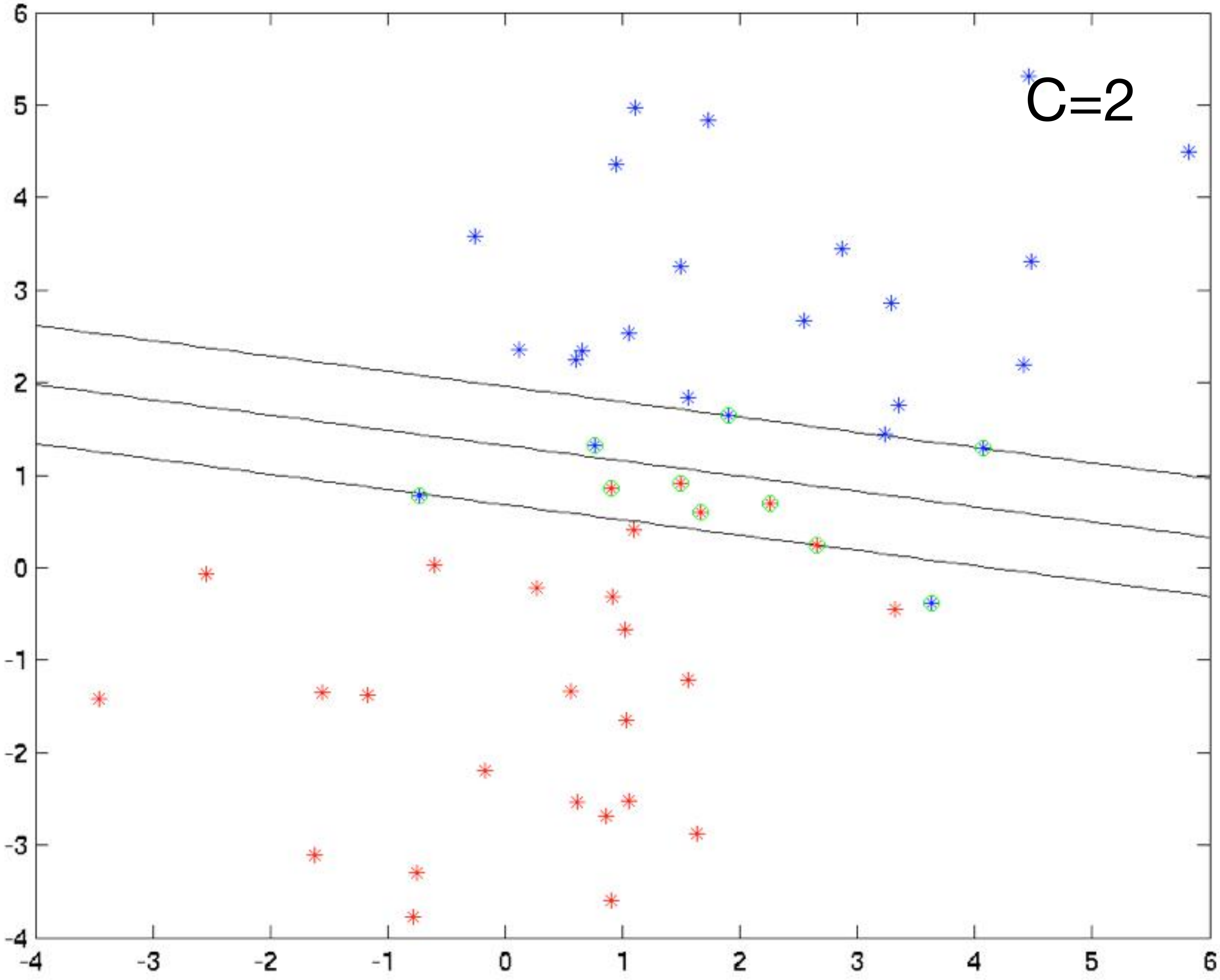

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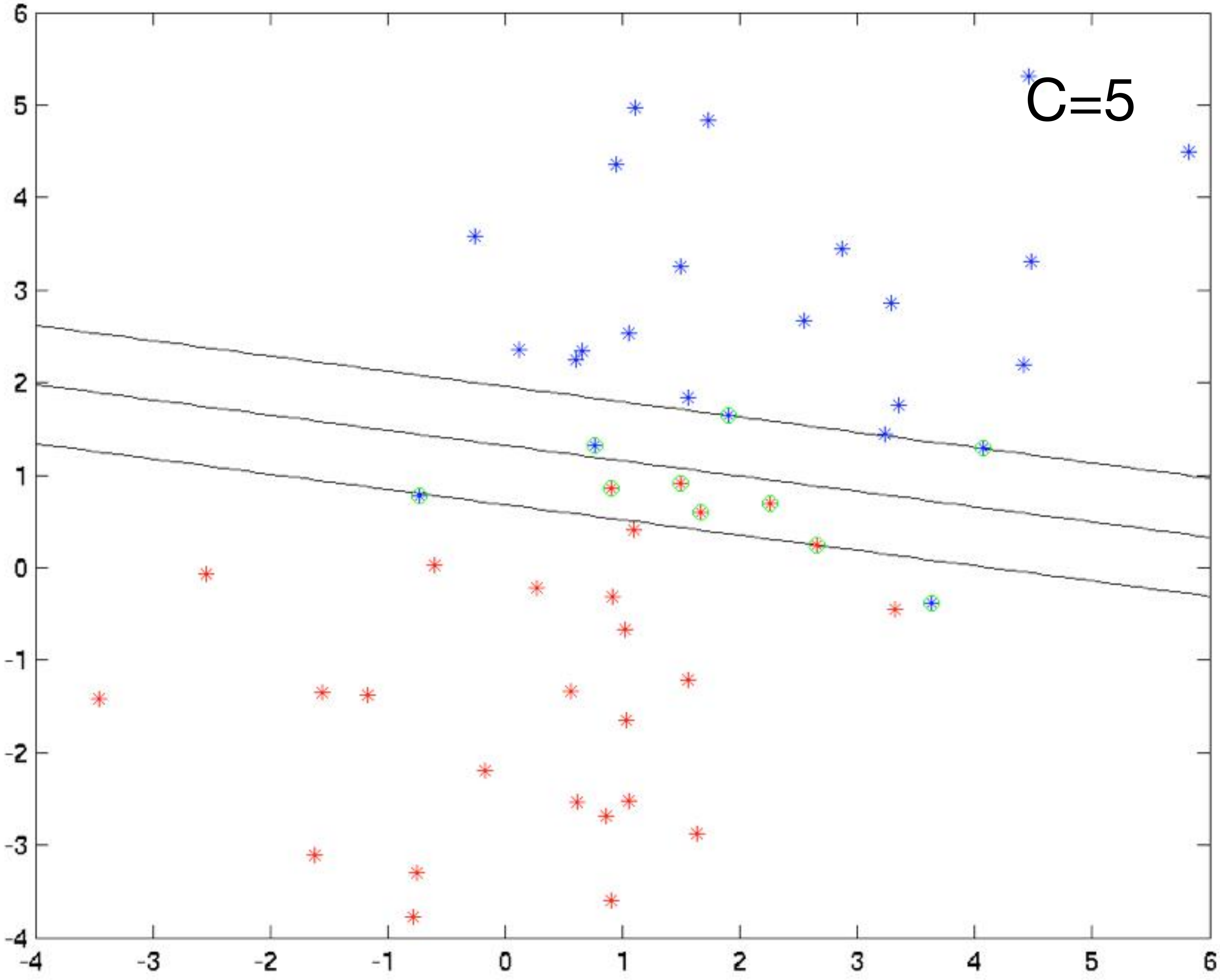

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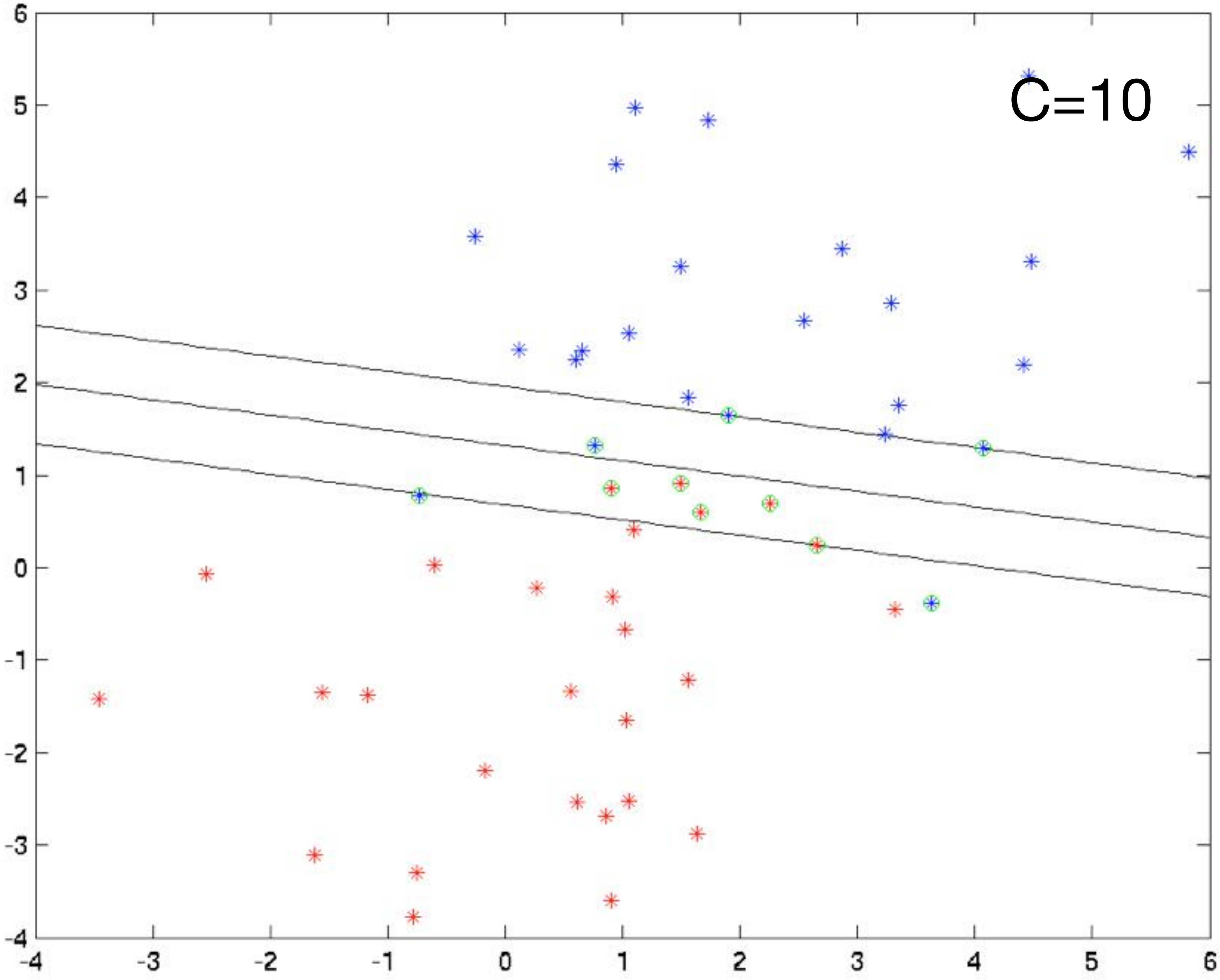

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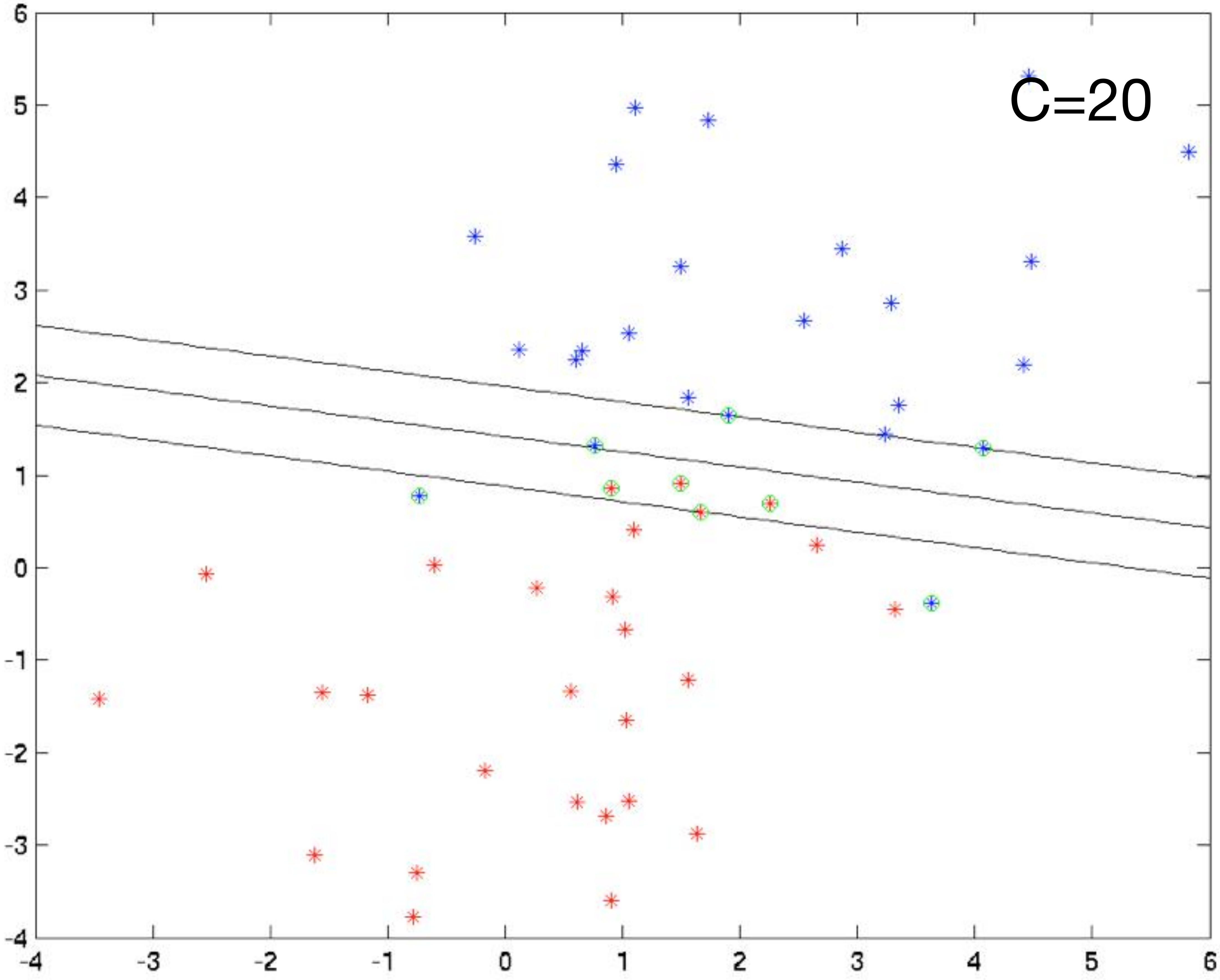

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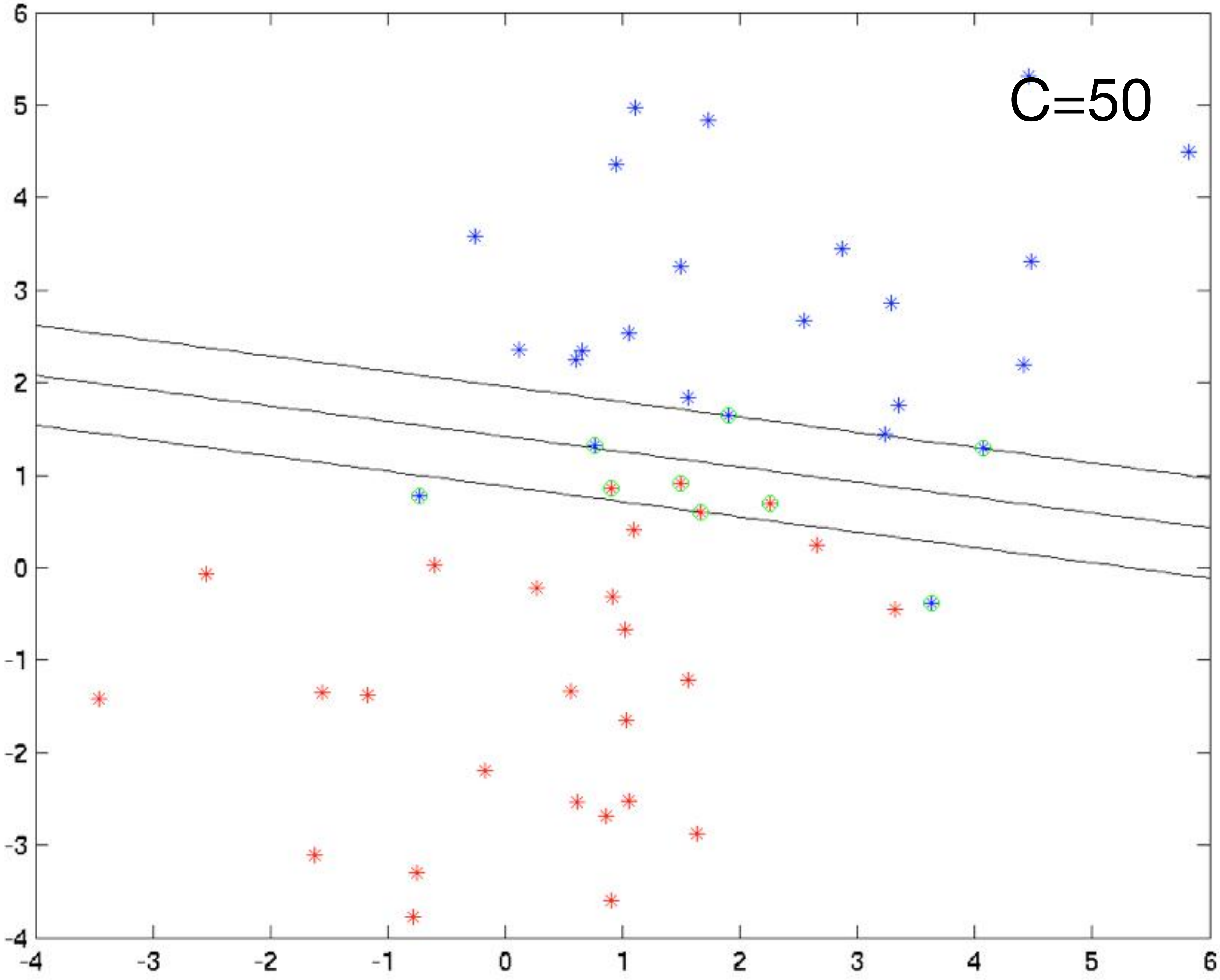

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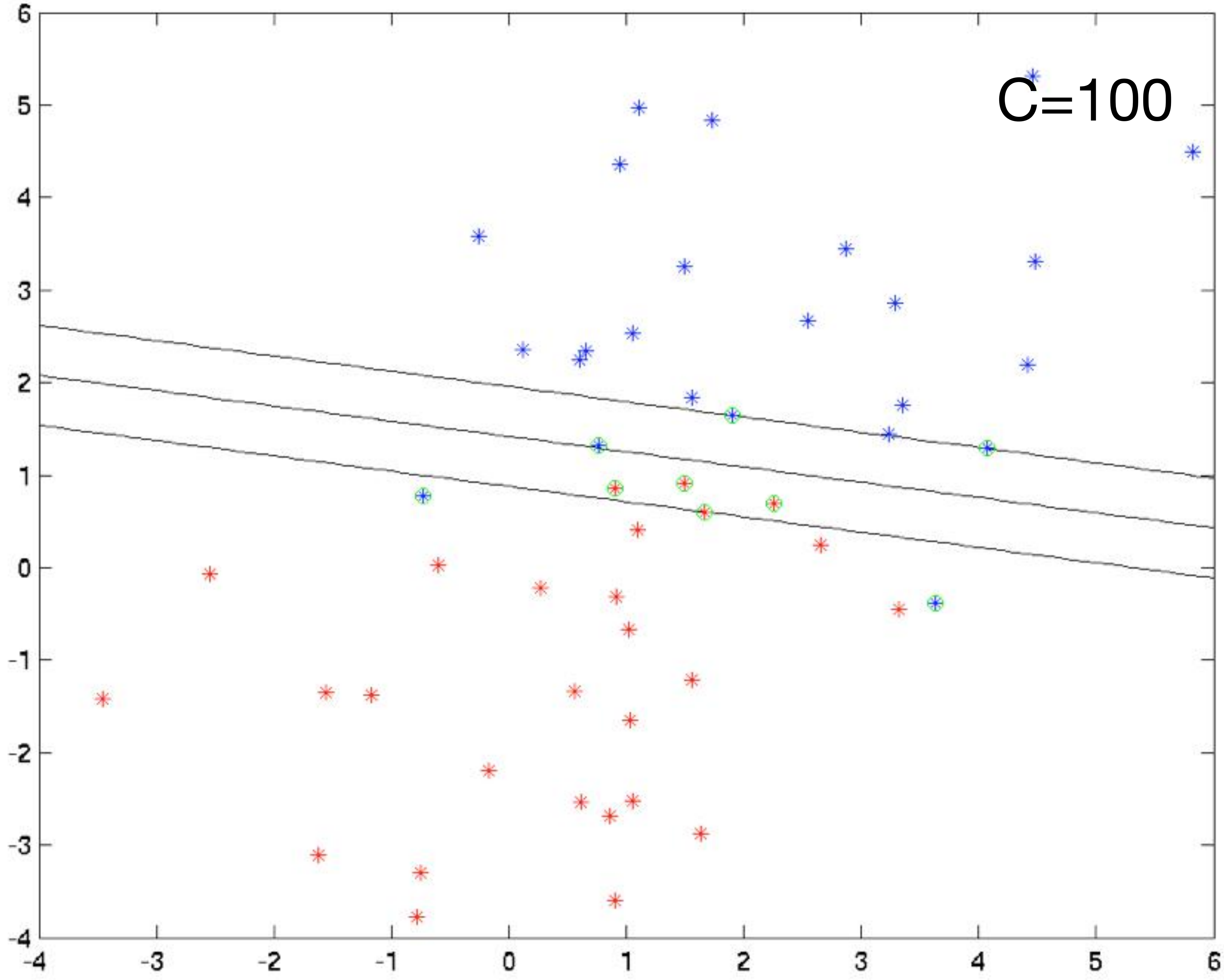

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# Solving the optimization problem

- 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).

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## Multi-class classification

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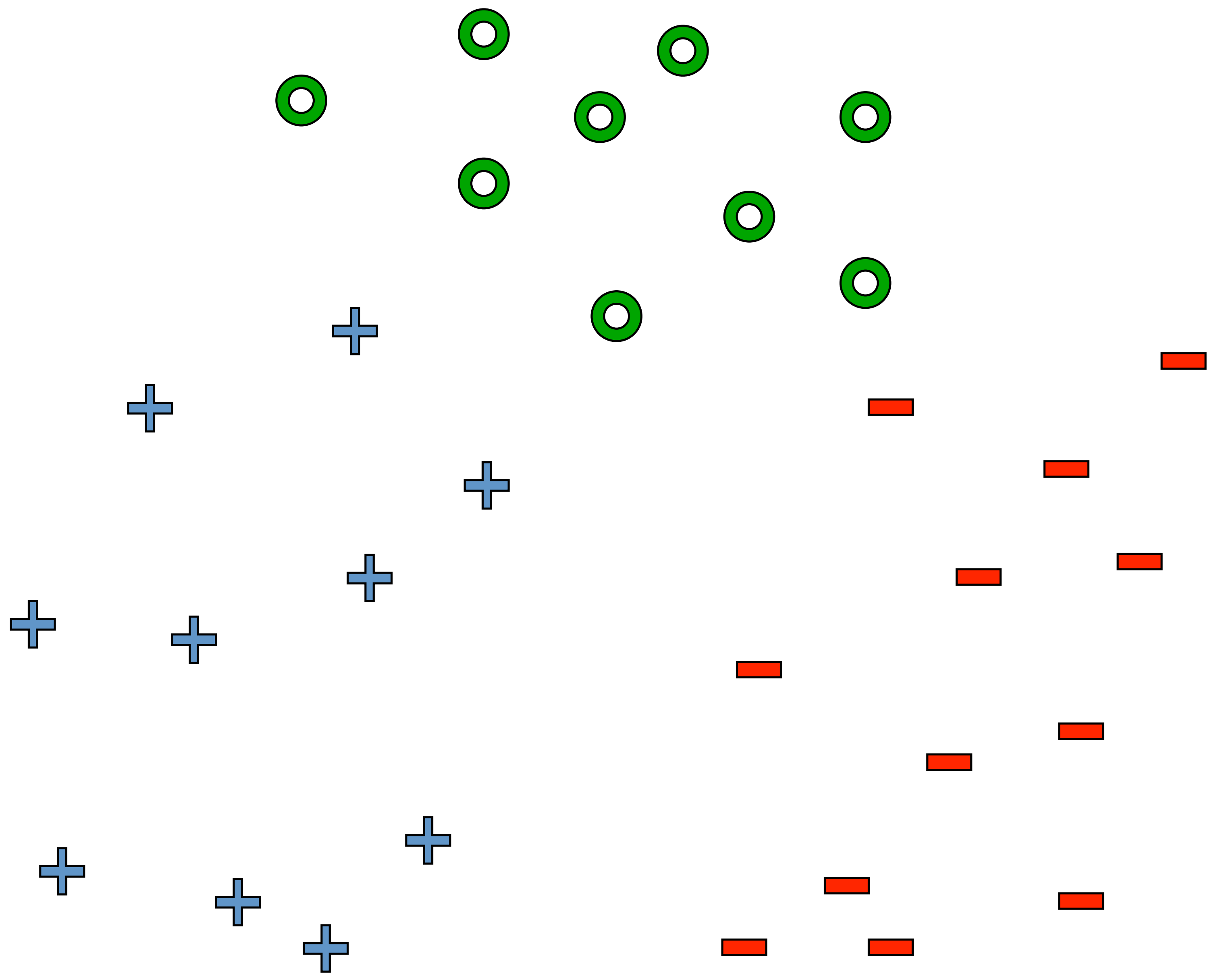
# Multi-class classification



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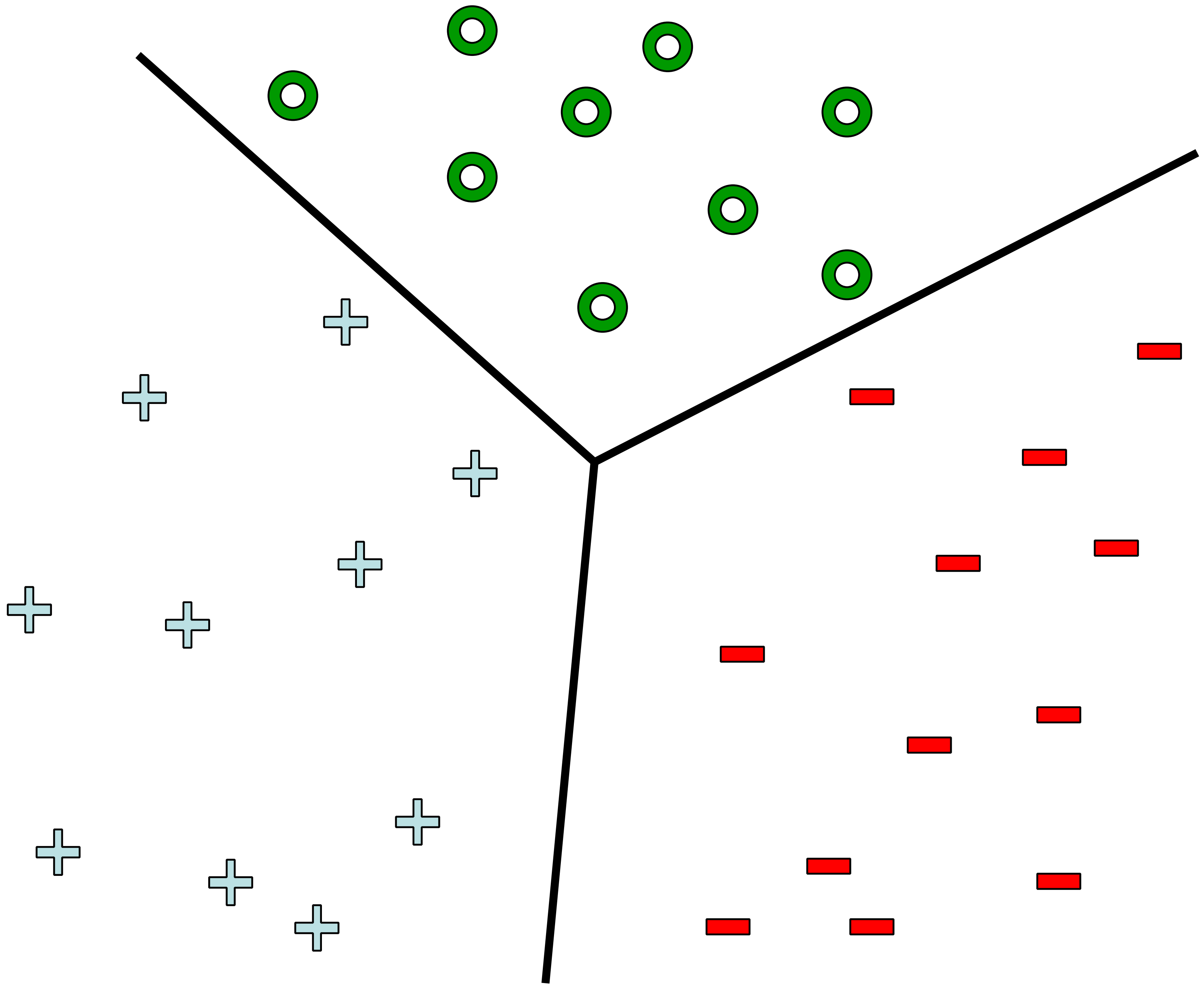
# Multi-class classification



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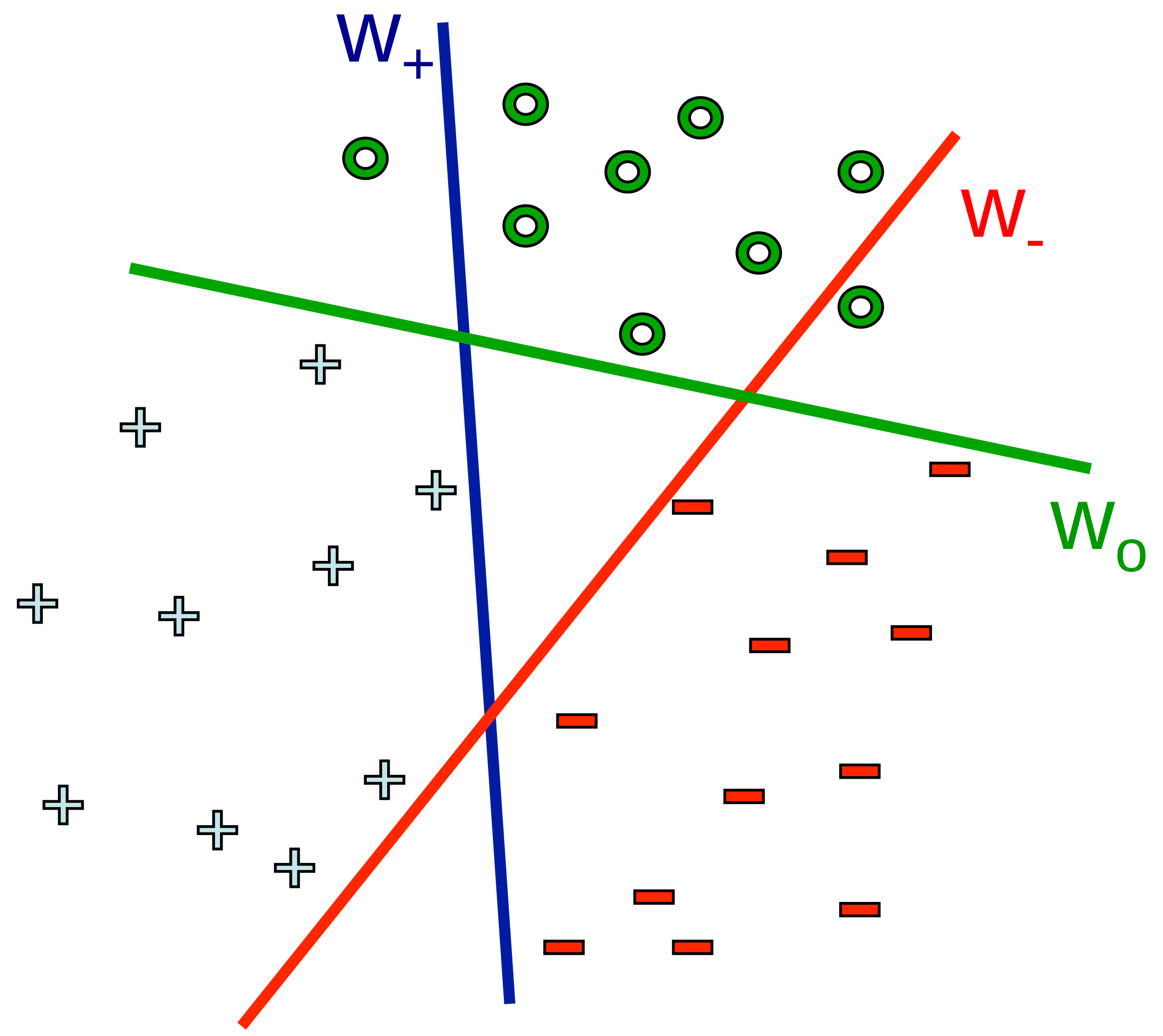
# One versus all classification



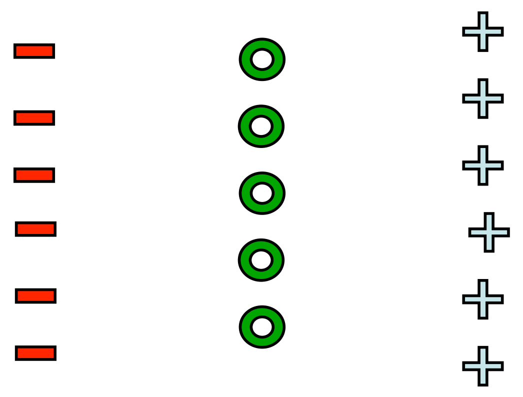
- Learn 3 classifiers:
  - - vs. {o,+}, weights $w_-$
  - + vs. {o,-}, weights $w_+$
  - o vs. {+,-}, weights $w_o$

- Predict label using:

$$\hat{y} \leftarrow \arg\max_k \; w_k \cdot x + b_k$$

- Any problems?

- Could we learn this dataset?



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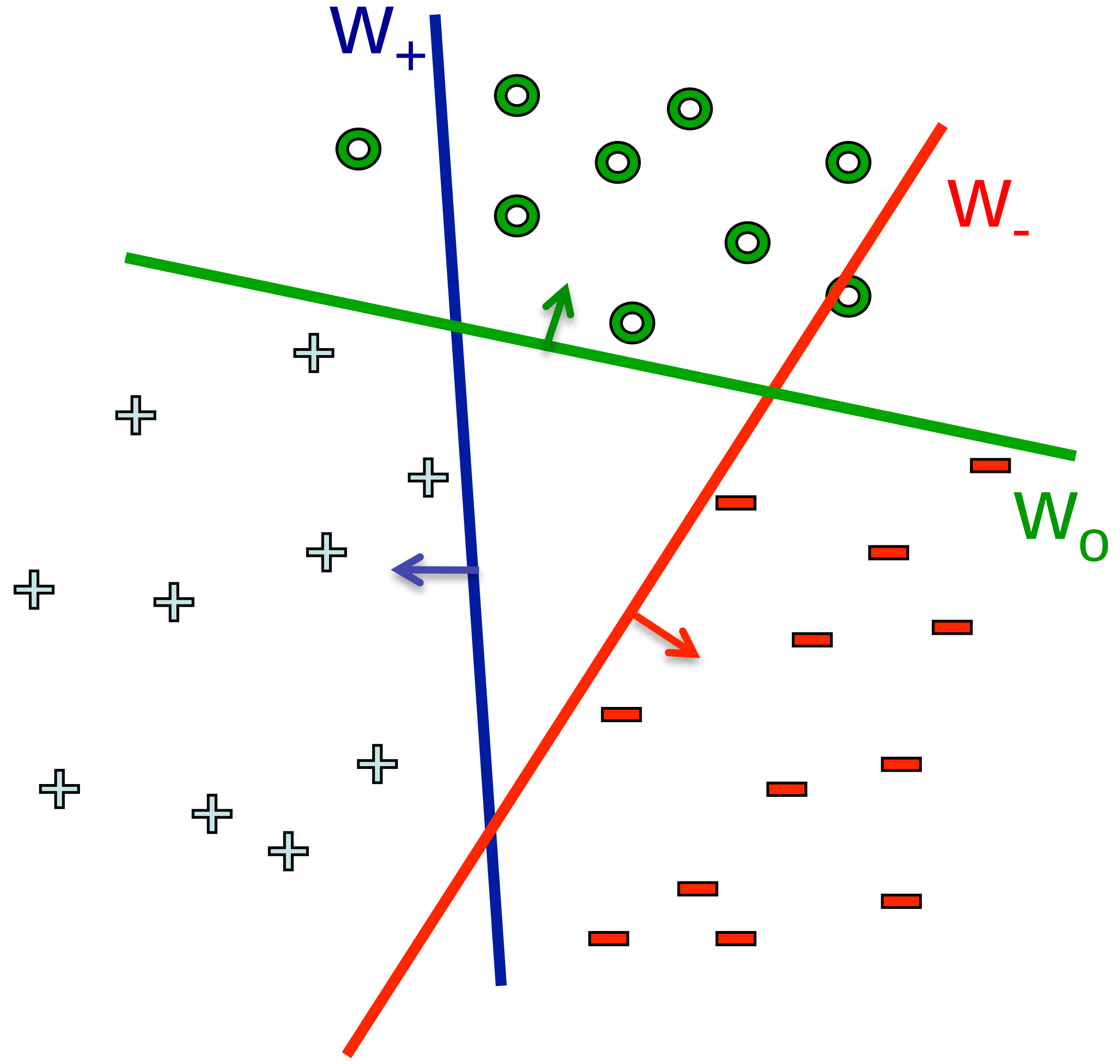
# Multi-class SVM

- Simultaneously learn 3 sets of weights:
- How do we guarantee the correct labels?
- Need new constraints!



The "score" of the correct class must be better than the "score" of wrong classes:

$$w^{(y_j)} \cdot x_j + b^{(y_j)} > w^{(y)} \cdot x_j + b^{(y)} \qquad \forall j,\ y \neq y_j$$

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# Multi-class SVM

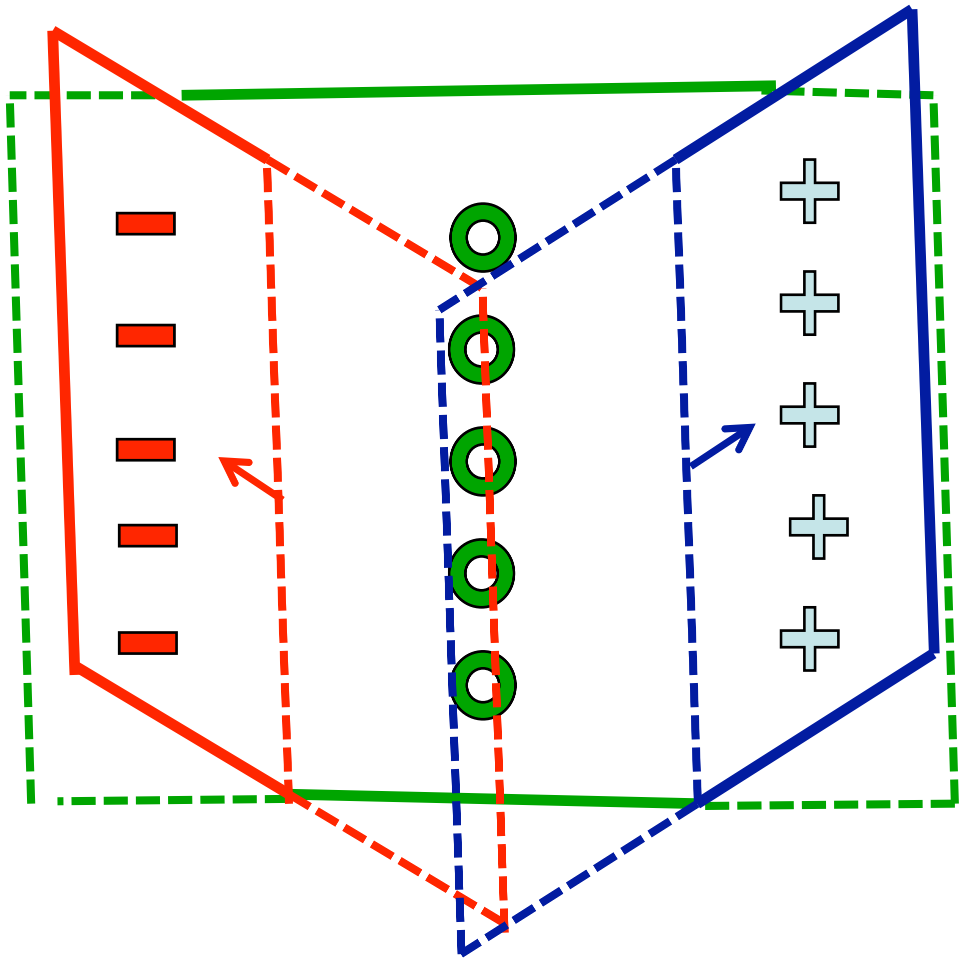
- As for the SVM, we introduce slack variables and maximize margin:

$$\begin{aligned} &\text{minimize}_{\mathbf{w},b} \quad \textstyle\sum_y \mathbf{w}^{(y)}.\mathbf{w}^{(y)} + C\sum_j \xi_j \\ &\mathbf{w}^{(y_j)}.\mathbf{x}_j + b^{(y_j)} \geq \mathbf{w}^{(y')}.\mathbf{x}_j + b^{(y')} + 1 - \xi_j, \ \forall y' \neq y_j, \ \forall j \\ &\hfill \xi_j \geq 0, \ \forall j \end{aligned}$$

To predict, we use:

$$\hat{y} \leftarrow \arg\max_k \ w_k \cdot x + b_k$$

Now can we learn it? →



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# Kernels

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# Non-linear features

- Regression
  We got nonlinear functions by preprocessing
- Perceptron
  - Map data into feature space $x \to \phi(x)$
  - Solve problem in this space
  - Query replace $\langle x, x' \rangle$ by $\langle \phi(x), \phi(x') \rangle$ for code
- Feature Perceptron
  - Solution in span of $\phi(x_i)$

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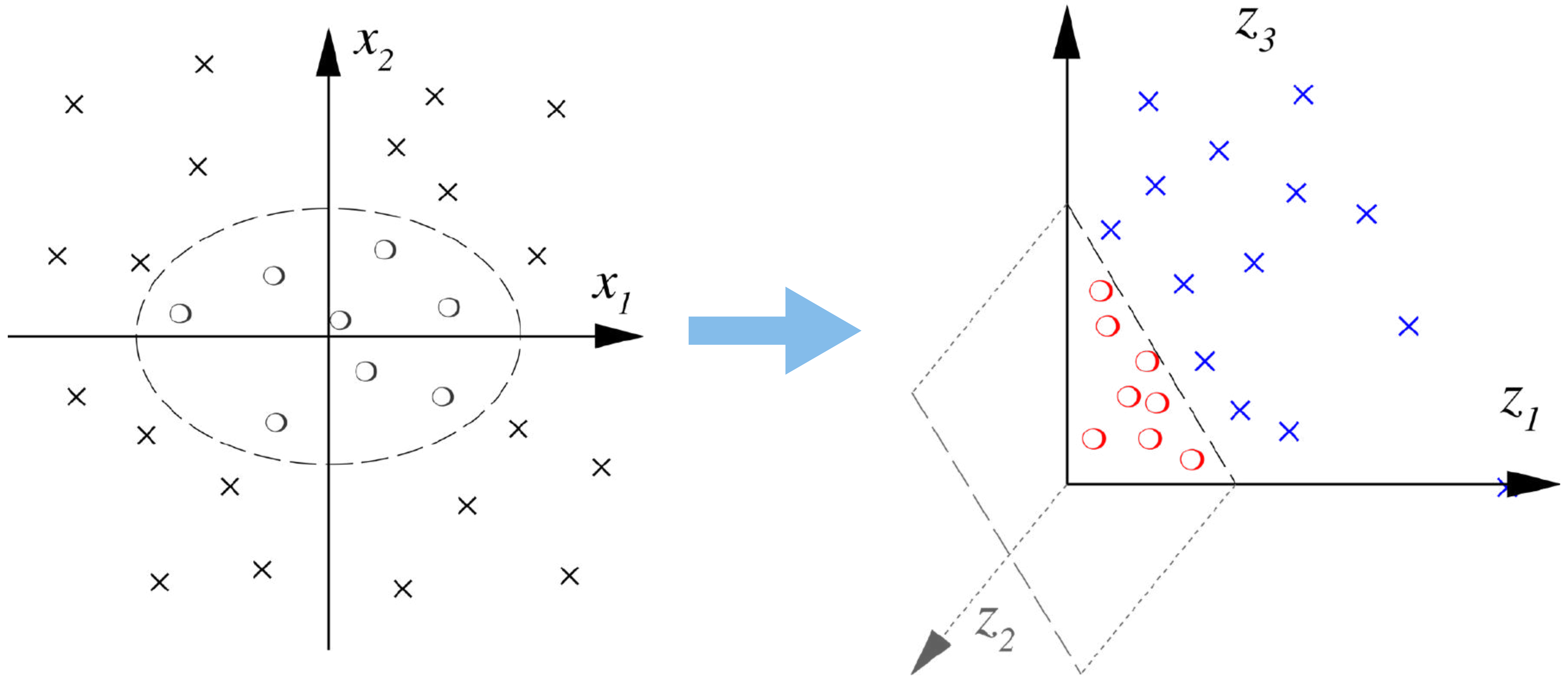
# Non-linear features



- Separating surfaces are Circles, hyperbolae, parabolae

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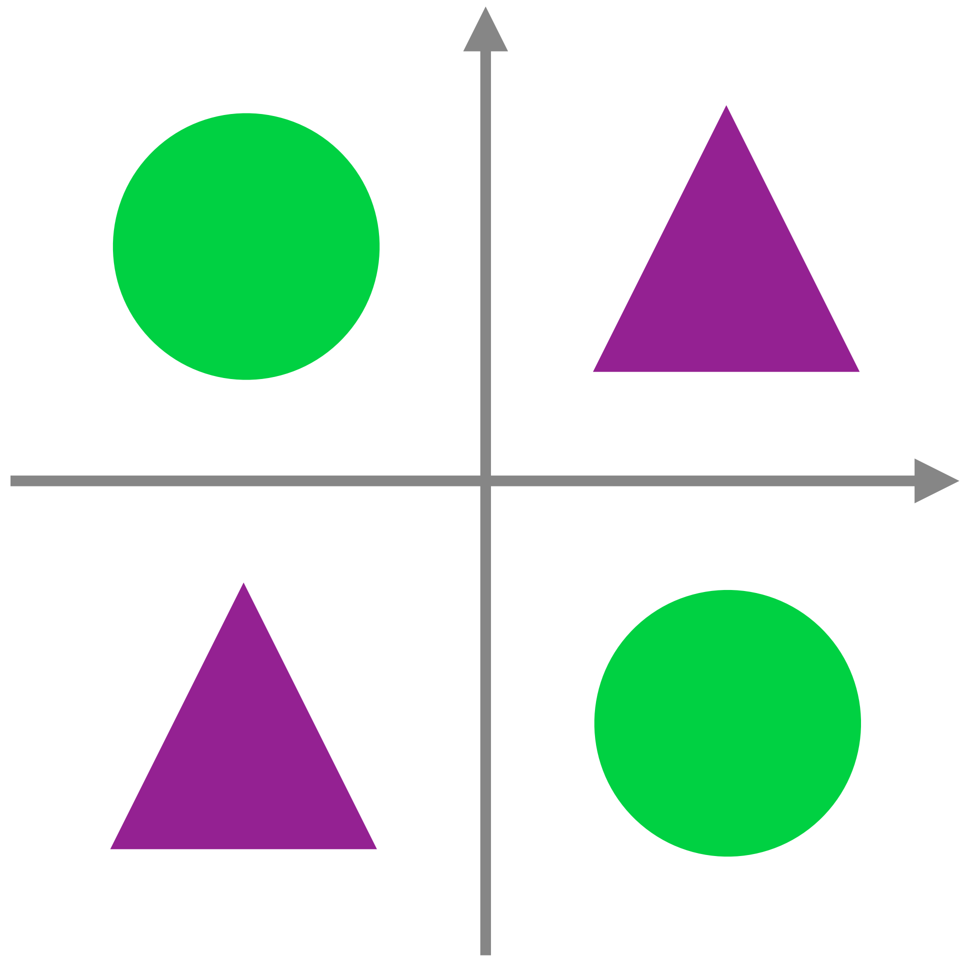
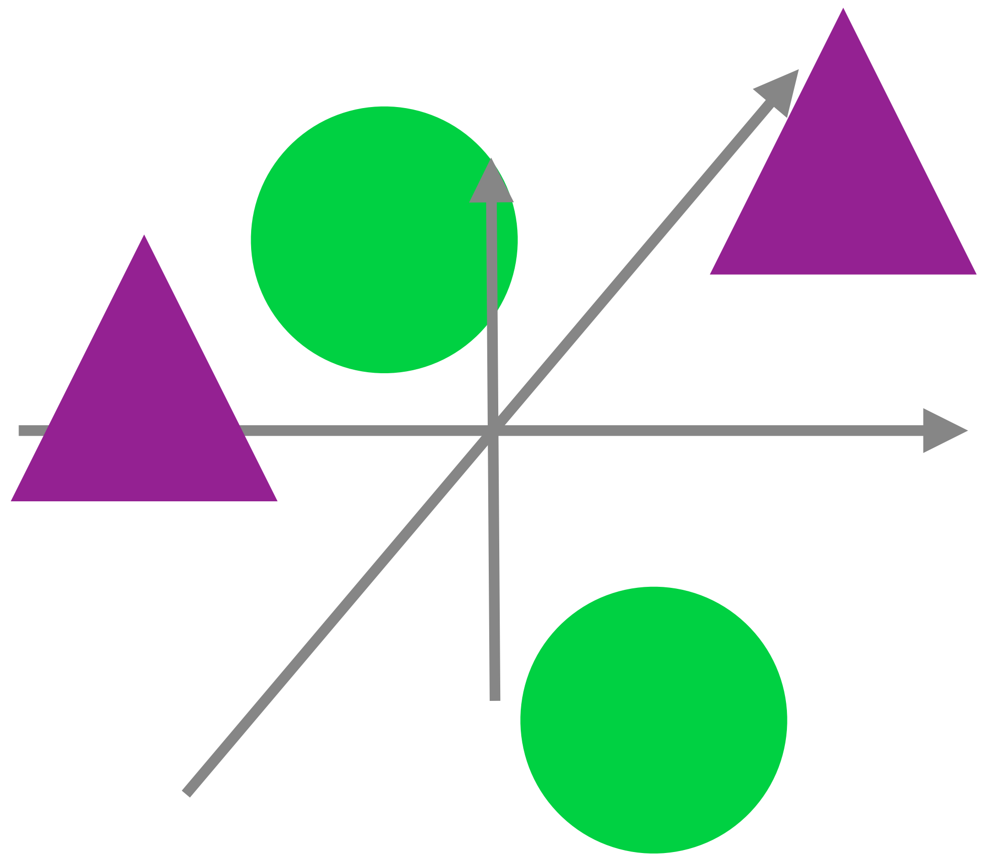
# Solving XOR


$(x_1, x_2)$


$(x_1, x_2, x_1 x_2)$

- XOR not linearly separable
- Mapping into 3 dimensions makes it easily solvable

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# Quadratic Features

## Quadratic Features in $\mathbb{R}^2$

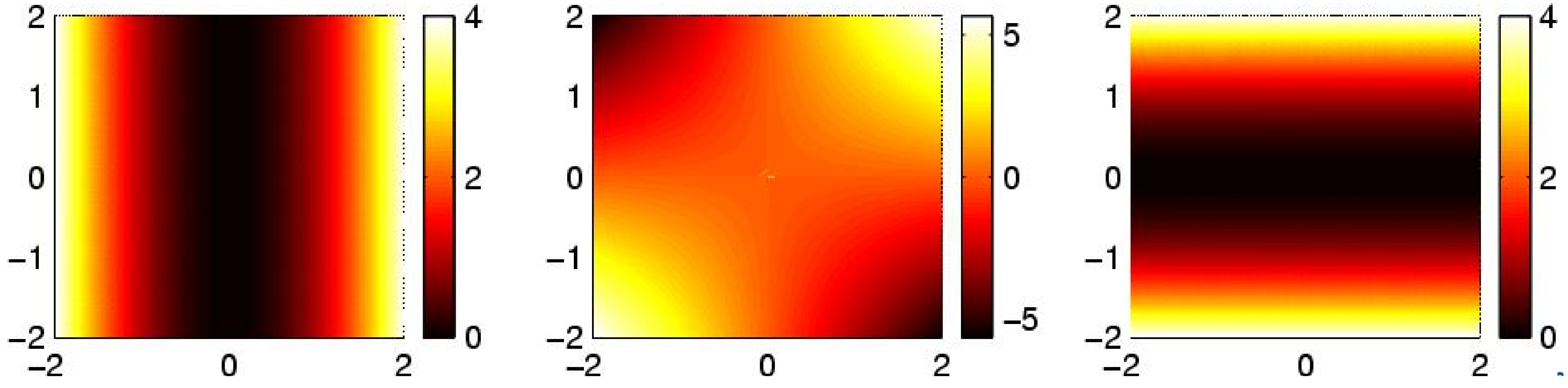
$$\Phi(x) := \left(x_1^2, \sqrt{2}x_1x_2, x_2^2\right)$$

## Dot Product

$$\begin{aligned}\langle \Phi(x), \Phi(x')\rangle &= \left\langle \left(x_1^2, \sqrt{2}x_1x_2, x_2^2\right), \left({x'_1}^2, \sqrt{2}x'_1x'_2, {x'_2}^2\right)\right\rangle \\ &= \langle x, x'\rangle^2.\end{aligned}$$

## Insight

Trick works for any polynomials of order via $\langle x, x'\rangle^d$.



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## SVM with a polynomial Kernel visualization

Created by:
Udi Aharoni

# Computational Efficiency

**Problem**

- Extracting features can sometimes be very costly.
- Example: second order features in 1000 dimensions. This leads to $5 \cdot 10^5$ numbers. For higher order polynomial features much worse.

**Solution**

Don't compute the features, try to compute dot products implicitly. For some features this works ...

**Definition**

A kernel function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a symmetric function in its arguments for which the following property holds

$$k(x, x') = \langle \Phi(x), \Phi(x') \rangle \text{ for some feature map } \Phi.$$

If $k(x, x')$ is much cheaper to compute than $\Phi(x)$ ...

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# Recap: The Perceptron

```
**initialize** $w = 0$ and $b = 0$
**repeat**
  **if** $y_i [\langle w, x_i \rangle + b] \leq 0$ **then**
    $w \leftarrow w + y_i x_i$ and $b \leftarrow b + y_i$
  **end if**
**until** all classified correctly
```

- Nothing happens if classified correctly
- Weight vector is linear combination $w = \sum_{i \in I} y_i x_i$
- Classifier is linear combination of inner products $f(x) = \sum_{i \in I} y_i \langle x_i, x \rangle + b$

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# Recap: The Perceptron on features

```
initialize $w, b = 0$
repeat
    Pick $(x_i, y_i)$ from data
    if $y_i(w \cdot \Phi(x_i) + b) \leq 0$ then
        $w' = w + y_i \Phi(x_i)$
        $b' = b + y_i$
until $y_i(w \cdot \Phi(x_i) + b) > 0$ for all $i$
```

- Nothing happens if classified correctly
- Weight vector is linear combination $w = \sum_{i \in I} y_i \phi(x_i)$
- Classifier is linear combination of inner products $f(x) = \sum_{i \in I} y_i \langle \phi(x_i), \phi(x) \rangle + b$

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# The Kernel Perceptron

```
initialize $f = 0$
repeat
    Pick $(x_i, y_i)$ from data
    if $y_i f(x_i) \leq 0$ then
        $f(\cdot) \leftarrow f(\cdot) + y_i k(x_i, \cdot) + y_i$
until $y_i f(x_i) > 0$ for all $i$
```

- Nothing happens if classified correctly
- Weight vector is linear combination $w = \sum_{i \in I} y_i \phi(x_i)$
- Classifier is linear combination of inner products

$$f(x) = \sum_{i \in I} y_i \langle \phi(x_i), \phi(x) \rangle + b = \sum_{i \in I} y_i k(x_i, x) + b$$

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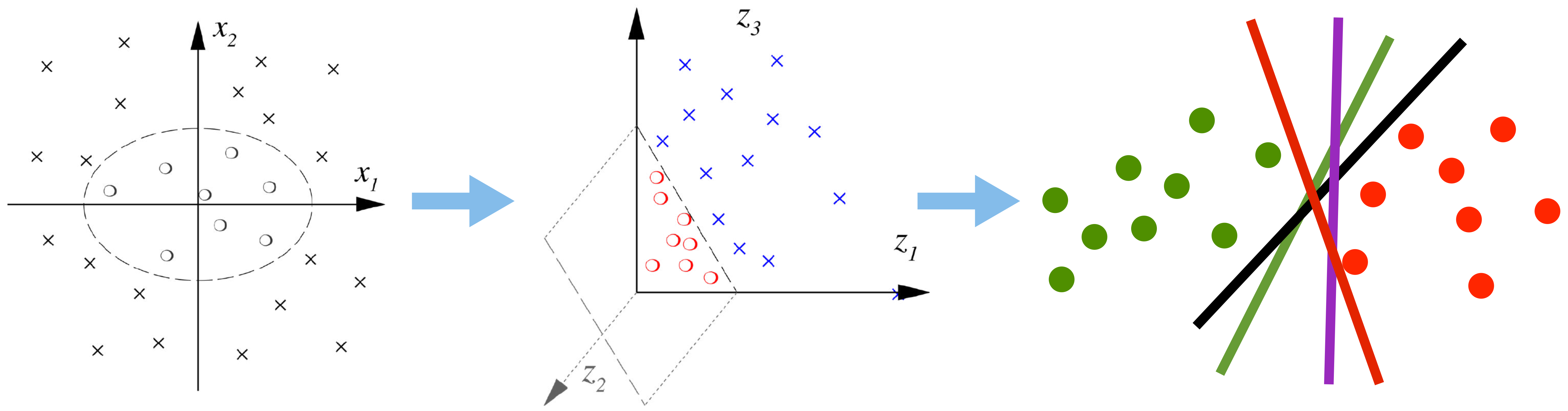
# Processing Pipeline



- Original data
- Data in feature space (implicit)
- Solve in feature space using kernels

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# Polynomial Kernels

## Idea

- We want to extend $k(x, x') = \langle x, x' \rangle^2$ to

  $$k(x, x') = (\langle x, x' \rangle + c)^d \text{ where } c > 0 \text{ and } d \in \mathbb{N}.$$

- Prove that such a kernel corresponds to a dot product.

## Proof strategy

Simple and straightforward: compute the explicit sum given by the kernel, i.e.

$$k(x, x') = (\langle x, x' \rangle + c)^d = \sum_{i=0}^{m} \binom{d}{i} (\langle x, x' \rangle)^i c^{d-i}$$

Individual terms $(\langle x, x' \rangle)^i$ are dot products for some $\Phi_i(x)$.

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## Kernel Conditions

**Computability**

We have to be able to compute $k(x, x')$ efficiently (much cheaper than dot products themselves).

**"Nice and Useful" Functions**

The features themselves have to be useful for the learning problem at hand. Quite often this means smooth functions.

**Symmetry**

Obviously $k(x, x') = k(x', x)$ due to the symmetry of the dot product $\langle \Phi(x), \Phi(x') \rangle = \langle \Phi(x'), \Phi(x) \rangle$.

**Dot Product in Feature Space**

Is there always a $\Phi$ such that $k$ really is a dot product?

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# Mercer's Theorem

## The Theorem

For any symmetric function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ which is square integrable in $\mathcal{X} \times \mathcal{X}$ and which satisfies

$$\int_{\mathcal{X}\times\mathcal{X}} k(x,x')f(x)f(x')dxdx' \geq 0 \text{ for all } f \in L_2(\mathcal{X})$$

there exist $\phi_i : \mathcal{X} \to \mathbb{R}$ and numbers $\lambda_i \geq 0$ where

$$k(x,x') = \sum_i \lambda_i \phi_i(x)\phi_i(x') \text{ for all } x, x' \in \mathcal{X}.$$

## Interpretation

Double integral is the continuous version of a vector-matrix-vector multiplication. For positive semidefinite matrices we have

$$\sum\sum k(x_i,x_j)\alpha_i\alpha_j \geq 0$$

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# Properties

## Distance in Feature Space

Distance between points in feature space via

$$\begin{aligned} d(x, x')^2 :=& \|\Phi(x) - \Phi(x')\|^2 \\ =& \langle \Phi(x), \Phi(x) \rangle - 2\langle \Phi(x), \Phi(x') \rangle + \langle \Phi(x'), \Phi(x') \rangle \\ =& k(x, x) + k(x', x') - 2k(x, x) \end{aligned}$$

## Kernel Matrix

To compare observations we compute dot products, so we study the matrix $K$ given by

$$K_{ij} = \langle \Phi(x_i), \Phi(x_j) \rangle = k(x_i, x_j)$$

where $x_i$ are the training patterns.

## Similarity Measure

The entries $K_{ij}$ tell us the overlap between $\Phi(x_i)$ and $\Phi(x_j)$, so $k(x_i, x_j)$ is a similarity measure.

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# Properties

## $K$ is Positive Semidefinite

Claim: $\alpha^\top K \alpha \geq 0$ for all $\alpha \in \mathbb{R}^m$ and all kernel matrices $K \in \mathbb{R}^{m \times m}$. Proof:

$$\sum_{i,j}^{m} \alpha_i \alpha_j K_{ij} = \sum_{i,j}^{m} \alpha_i \alpha_j \langle \Phi(x_i), \Phi(x_j) \rangle$$

$$= \left\langle \sum_{i}^{m} \alpha_i \Phi(x_i), \sum_{j}^{m} \alpha_j \Phi(x_j) \right\rangle = \left\| \sum_{i=1}^{m} \alpha_i \Phi(x_i) \right\|^2$$

## Kernel Expansion

If $w$ is given by a linear combination of $\Phi(x_i)$ we get

$$\langle w, \Phi(x) \rangle = \left\langle \sum_{i=1}^{m} \alpha_i \Phi(x_i), \Phi(x) \right\rangle = \sum_{i=1}^{m} \alpha_i k(x_i, x).$$

# Examples

**Examples of kernels** $k(x, x')$

| | |
|---|---|
| Linear | $\langle x, x' \rangle$ |
| Laplacian RBF | $\exp\left(-\lambda \lVert x - x' \rVert\right)$ |
| Gaussian RBF | $\exp\left(-\lambda \lVert x - x' \rVert^2\right)$ |
| Polynomial | $\left(\langle x, x' \rangle + c\rangle\right)^d, c \geq 0,\ d \in \mathbb{N}$ |
| B-Spline | $B_{2n+1}(x - x')$ |
| Cond. Expectation | $\mathbf{E}_c[p(x\|c)p(x'\|c)]$ |

**Simple trick for checking Mercer's condition**

Compute the Fourier transform of the kernel and check that it is nonnegative.

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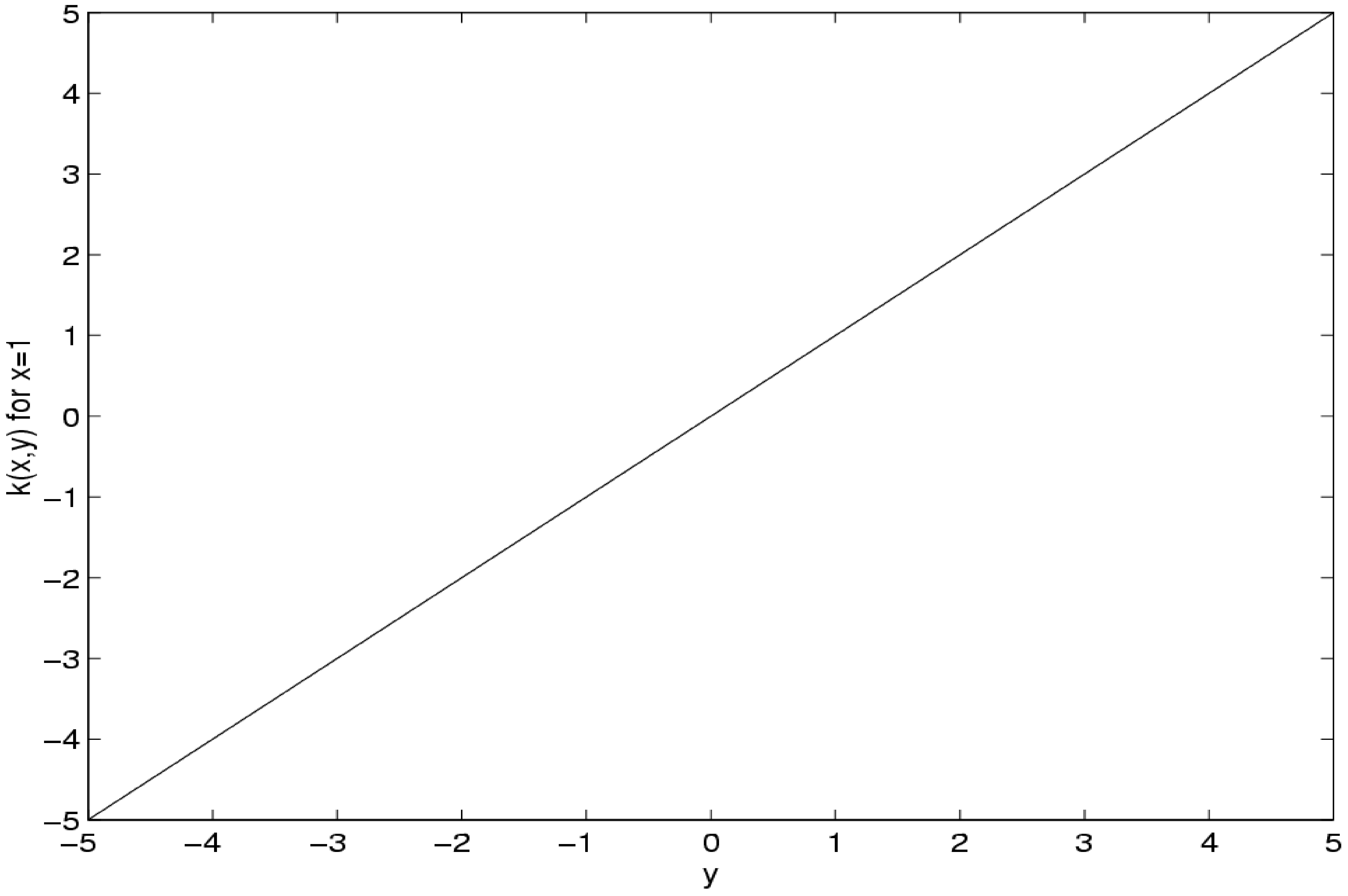
# Linear Kernel



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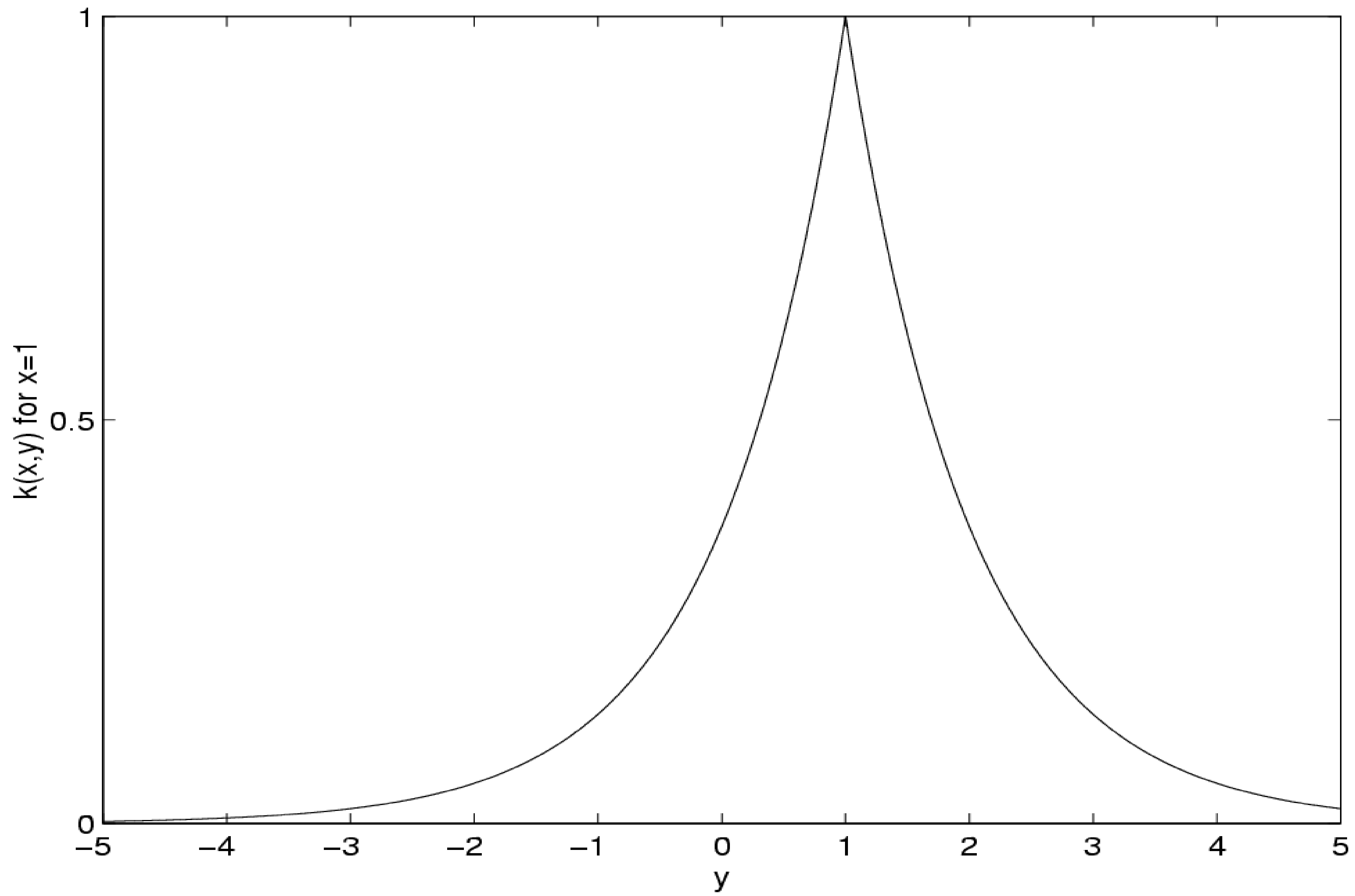
# Laplacian Kernel



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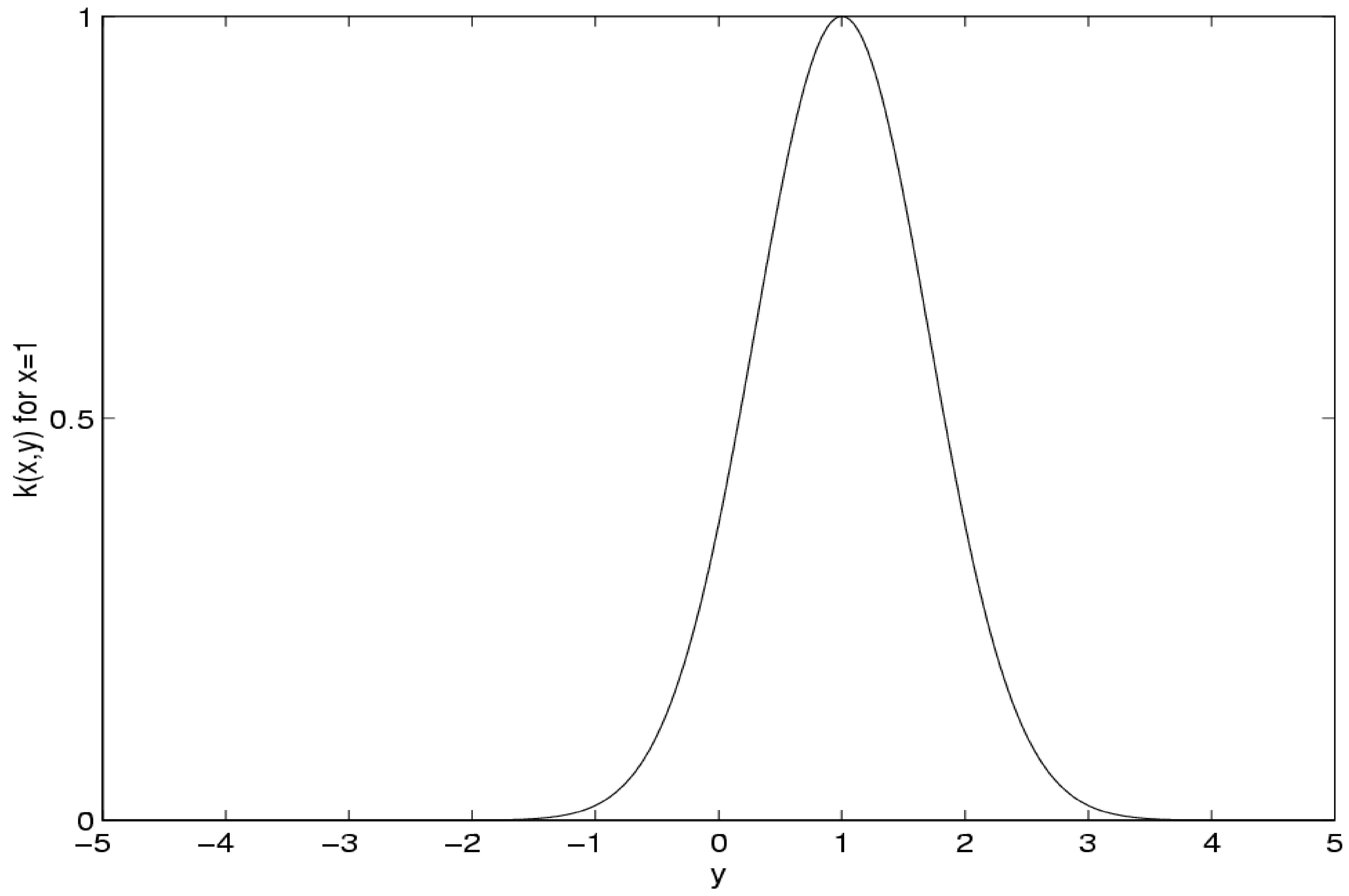
# Gaussian Kernel



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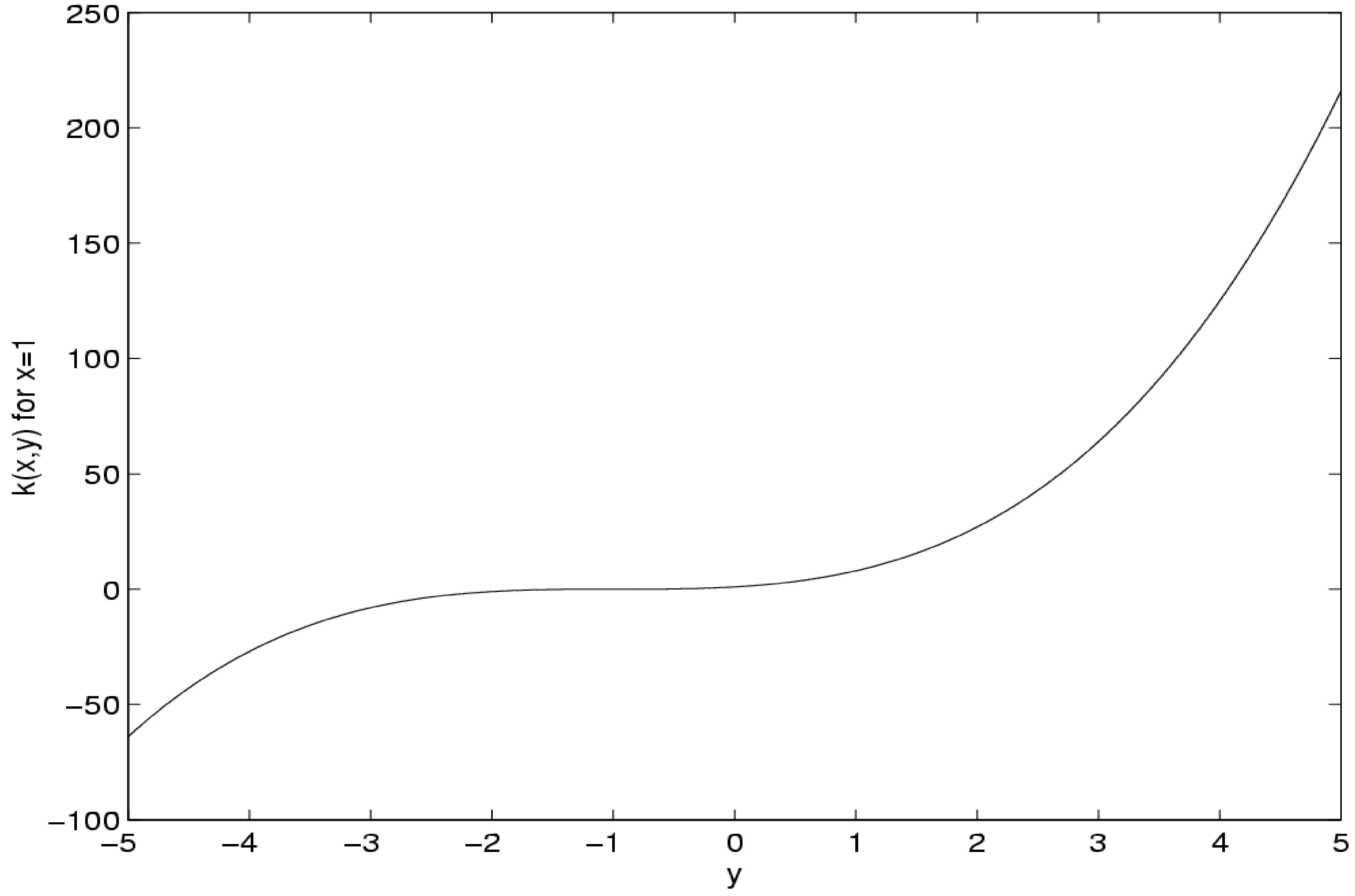
# Polynomial of order 3



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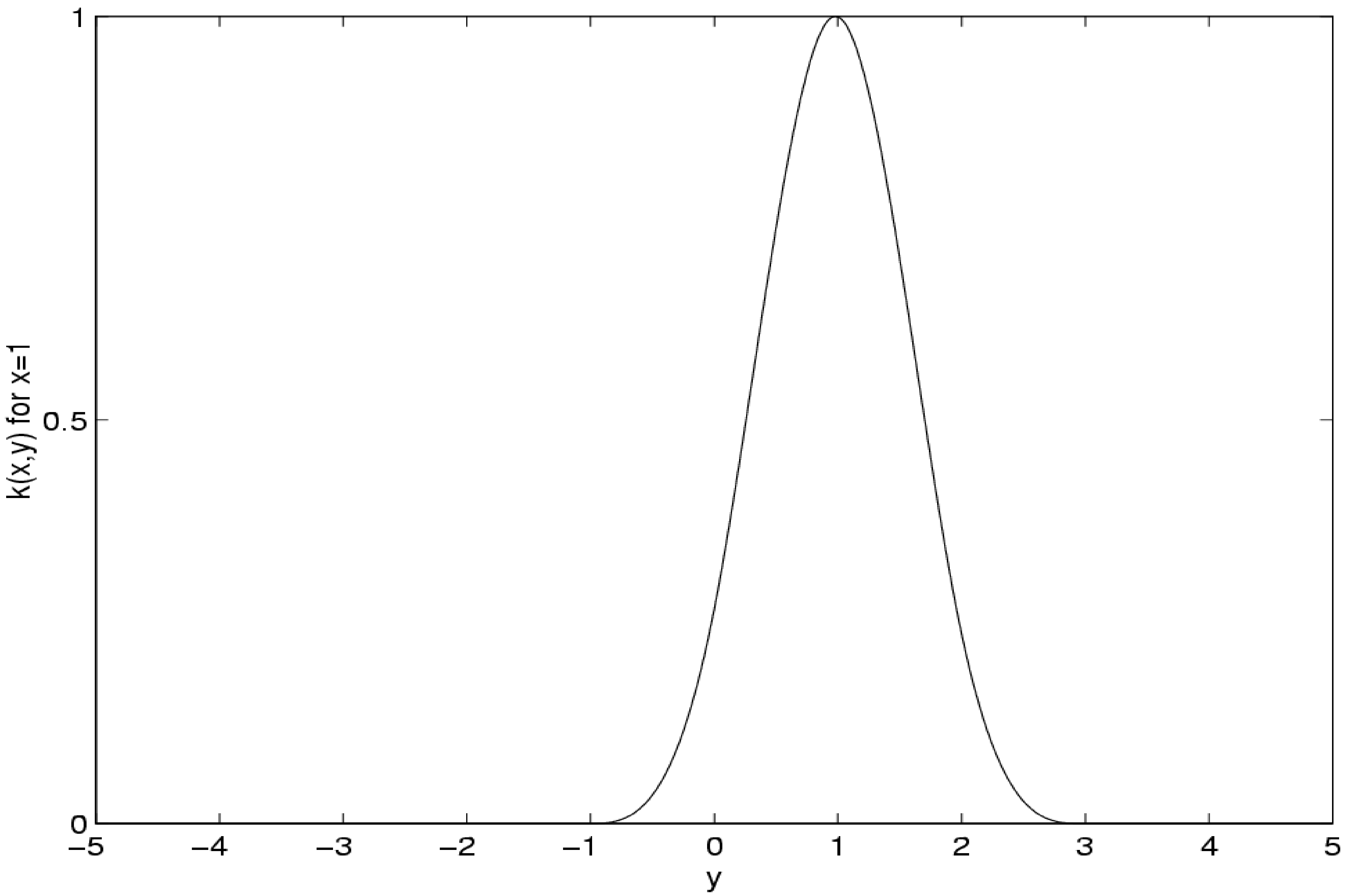
# $B_3$ Spline Kernel



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# Kernels in Computer Vision

- Features x = histogram (of color, texture, etc)

- Common Kernels
  - Intersection Kernel
  - Chi-square Kernel

$$K_{\text{intersect}}(\boldsymbol{u}, \boldsymbol{v}) = \sum_i \min(u_i, v_i)$$

$$K_{\chi^2}(\boldsymbol{u}, \boldsymbol{v}) = \sum_i \frac{2u_i v_i}{u_i + v_i}$$

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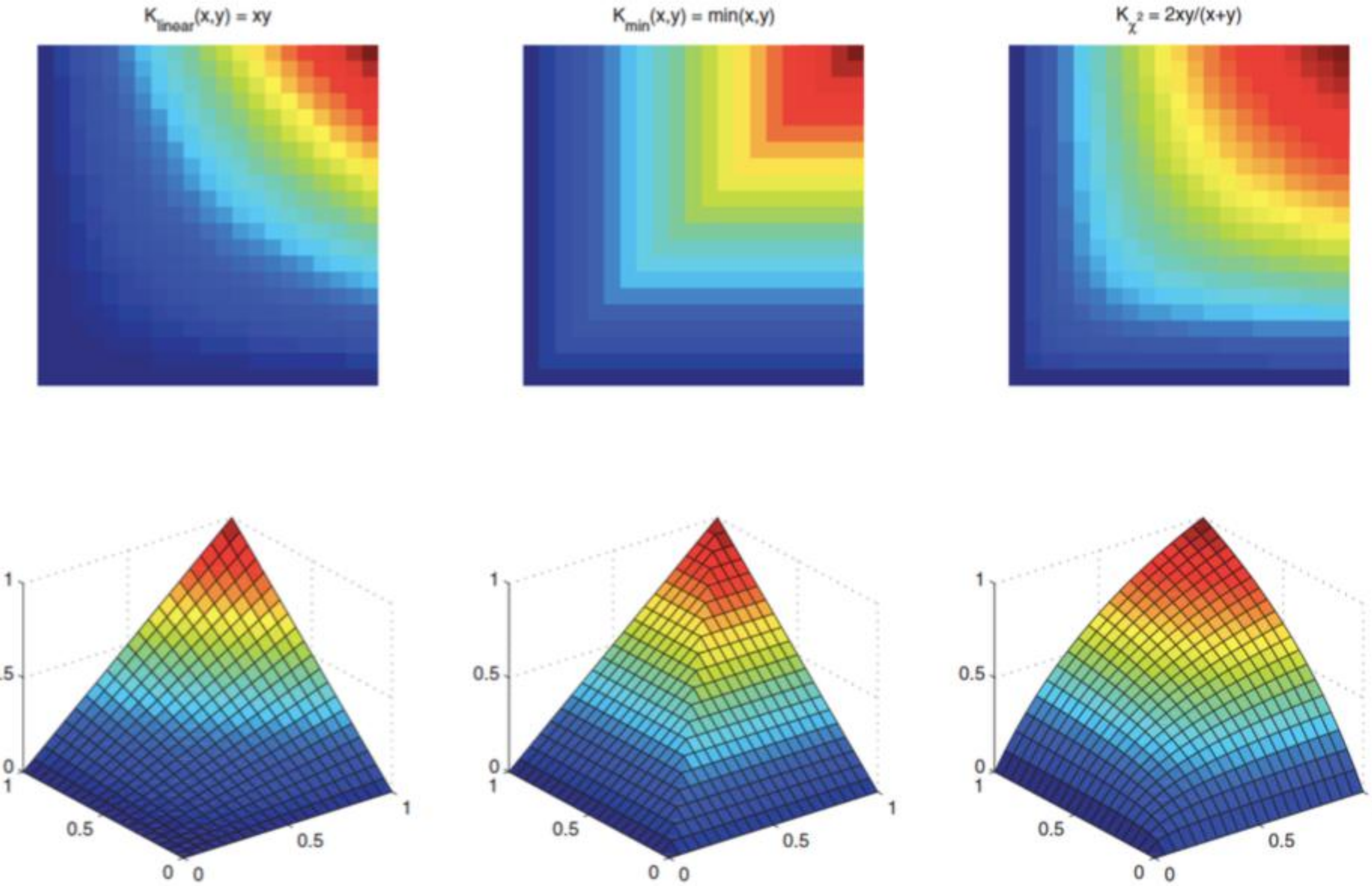

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Image credit: Subhransu Maji

## **Next Lecture:**

Kernel Trick for SVMs,
Support Vector Regression