Photo by Arthur Gretton, CMU Machine Learning Protestors at G20

BBM406

Fundamentals of Machine Learning

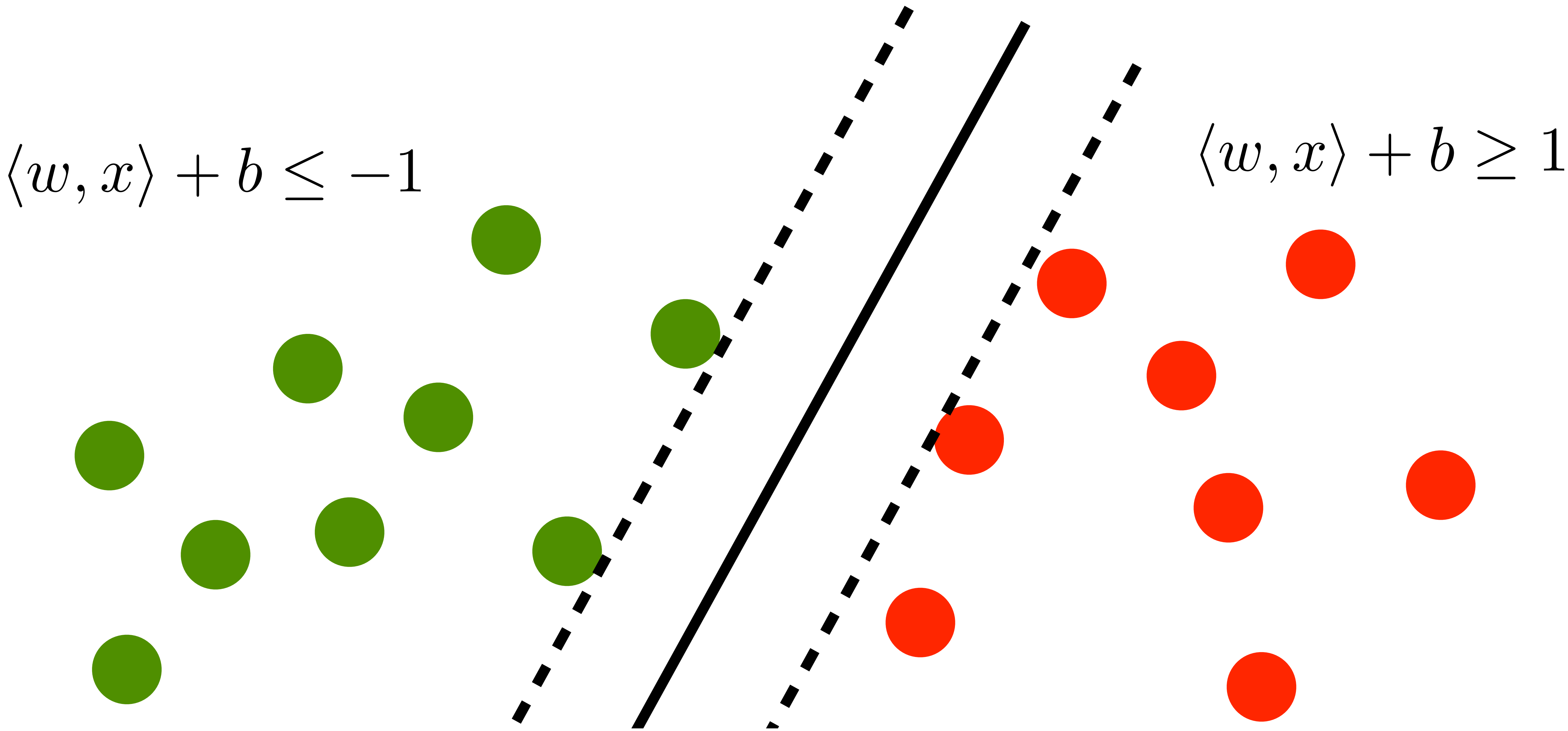
Lecture 16:

Soft Margin Classification
Multi-class SVMs
Kernels

HACETTEPE UNIVERSITY COMPUTER VISION LAB

Erkut Erdem // Hacettepe University // Spring 2021

Last time… **Support Vector Machines**



linear function

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

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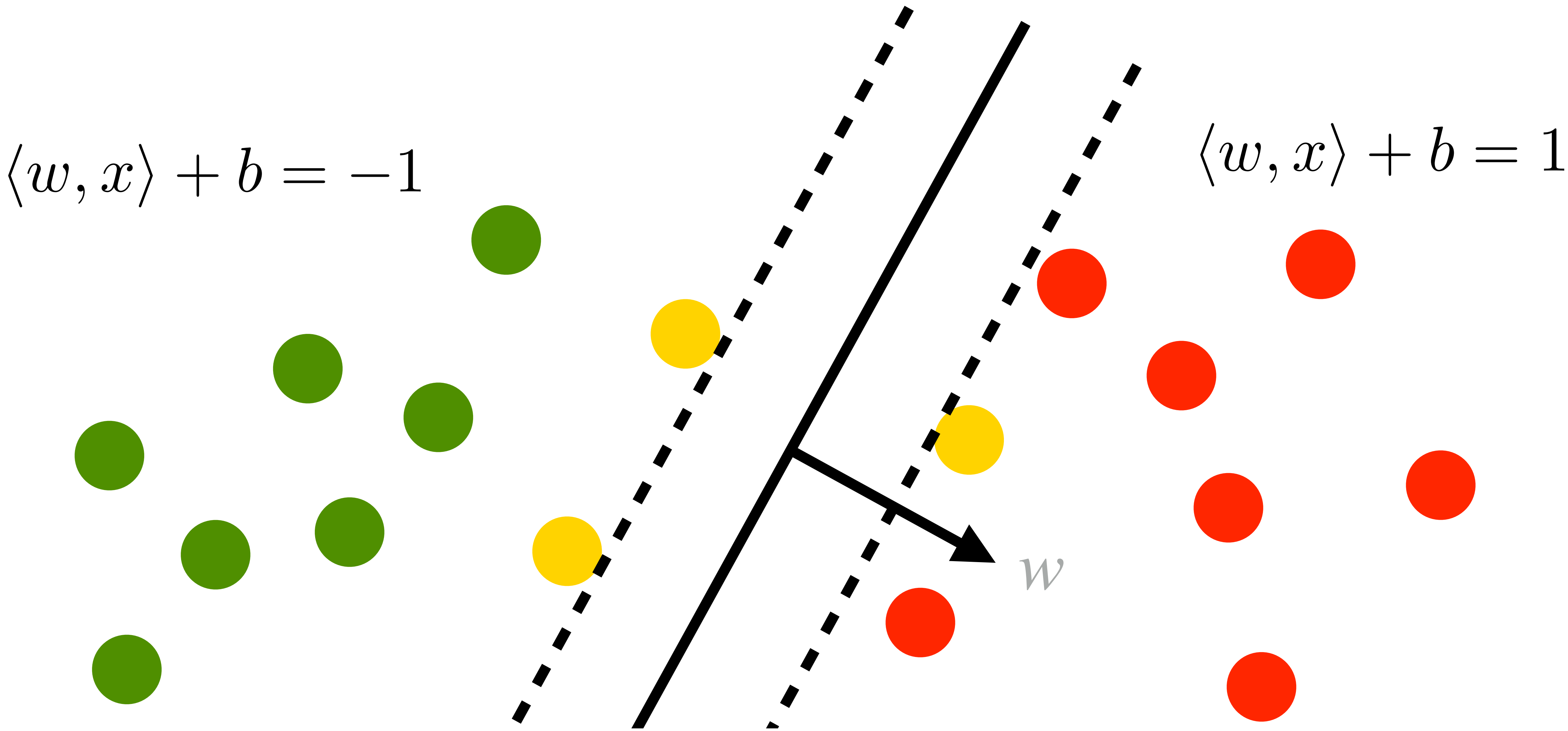
Last time... **Support Vector Machines**



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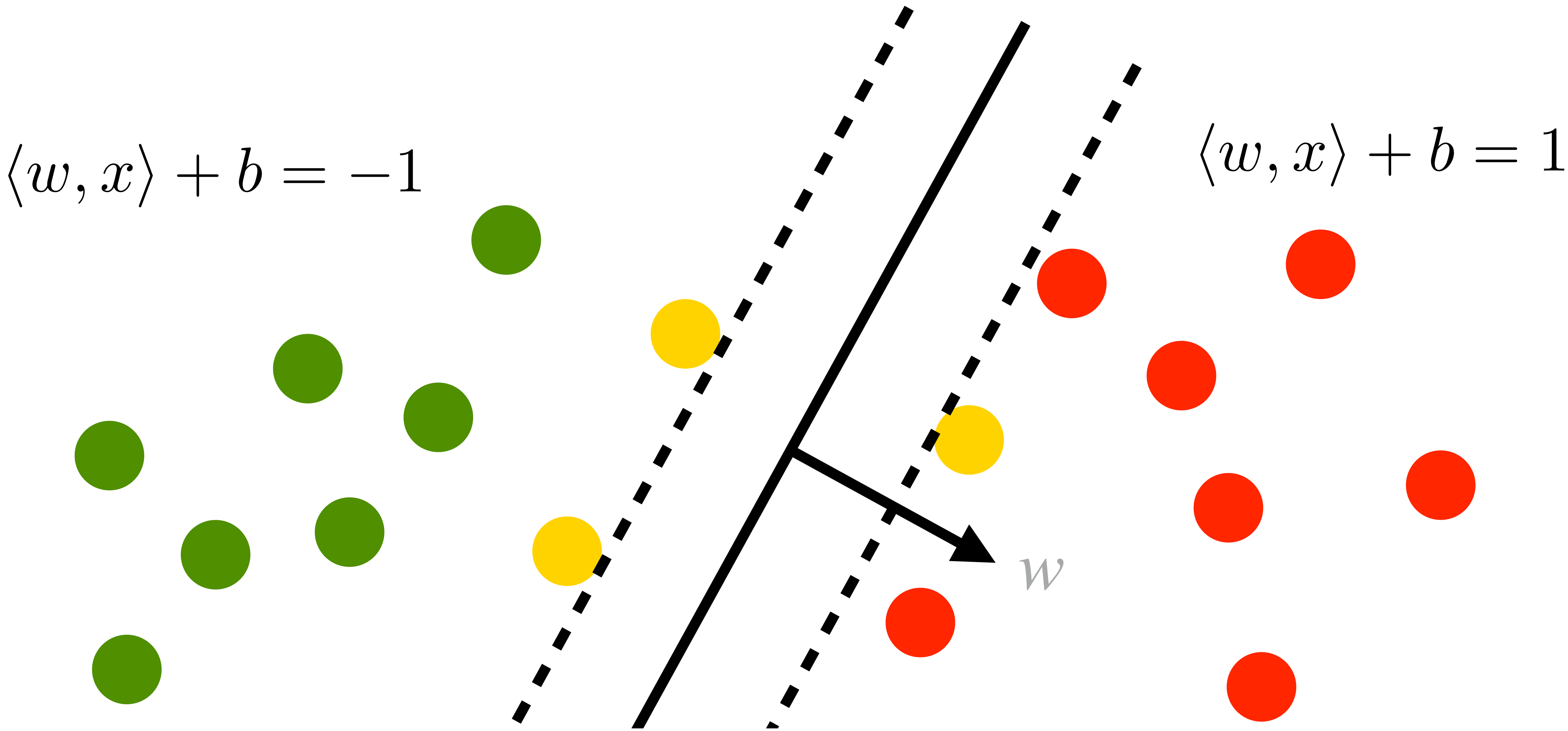
Last time... **Support Vector Machines**



optimization problem

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

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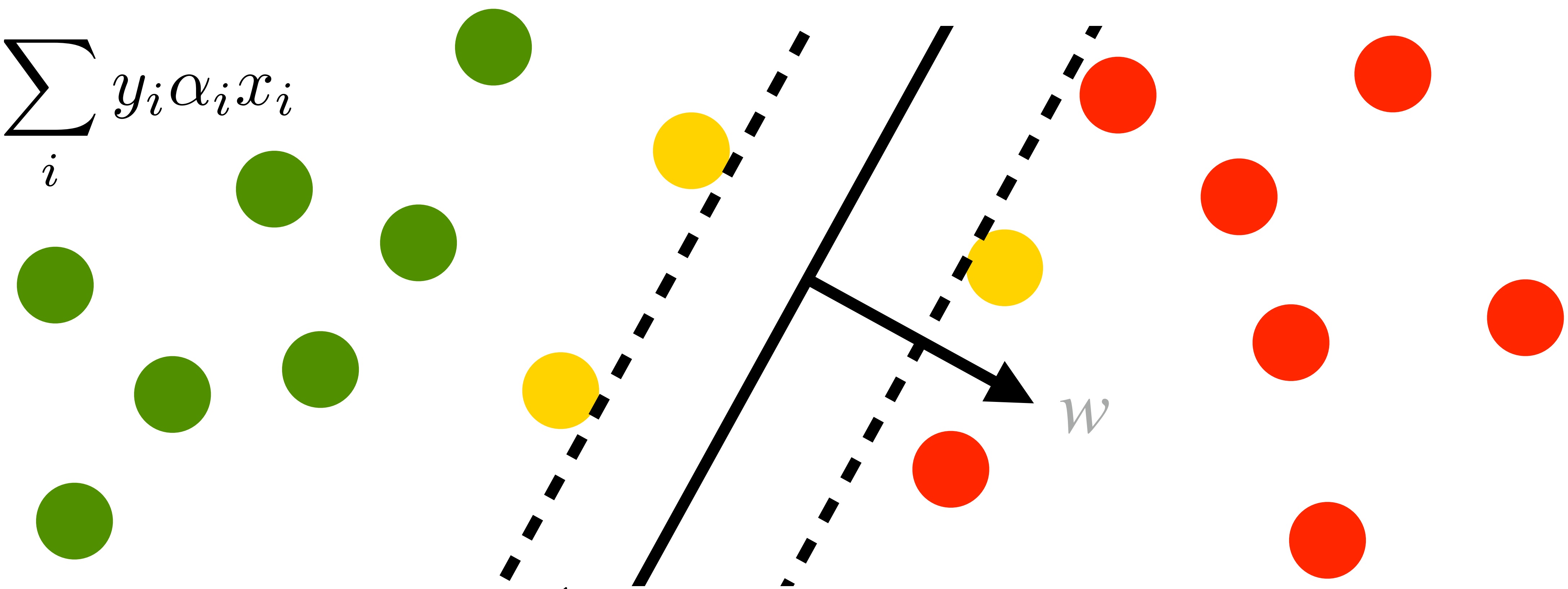
Last time... **Support Vector Machines**

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

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



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

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

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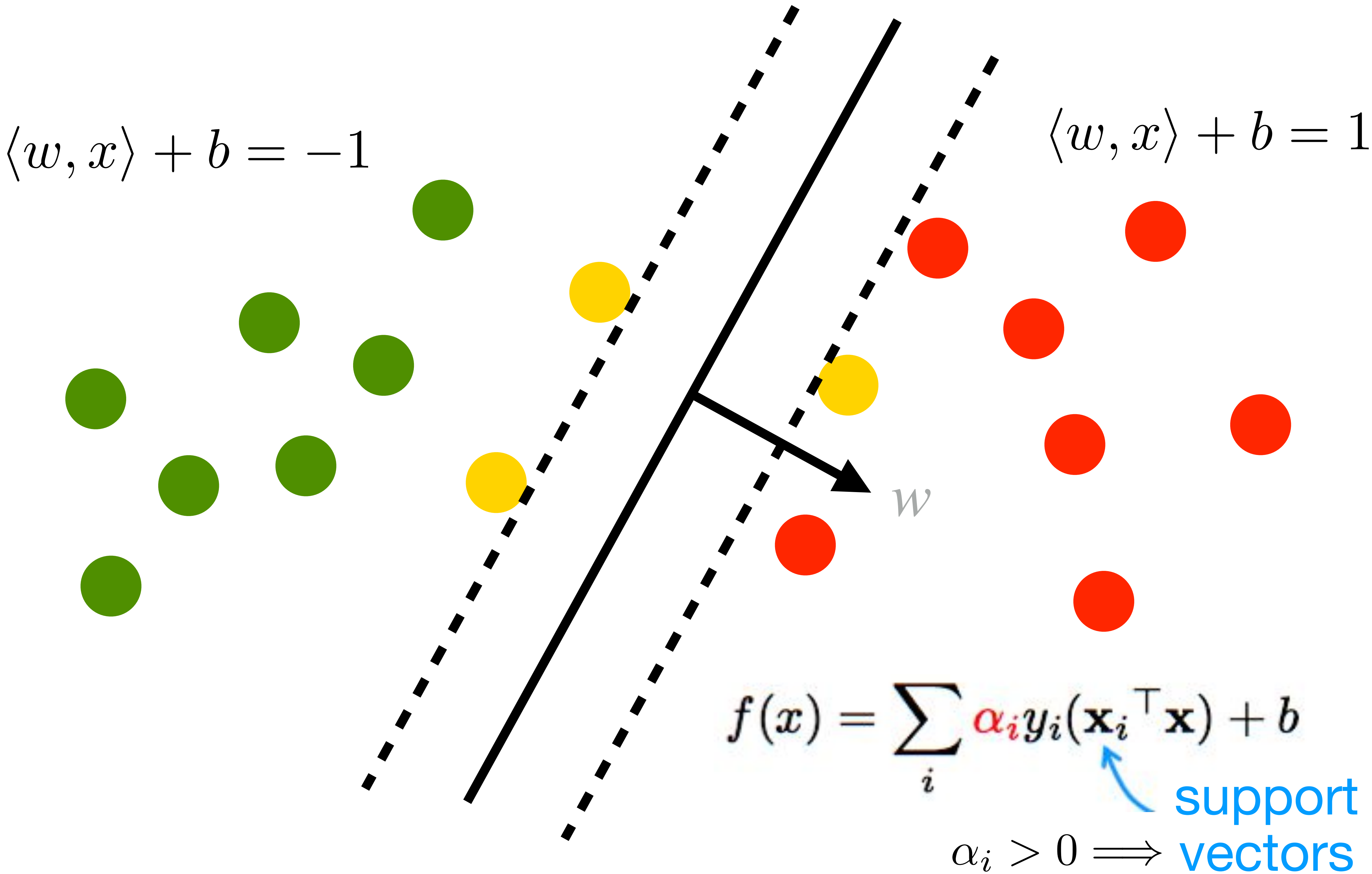
Last time… **Large Margin Classifier**

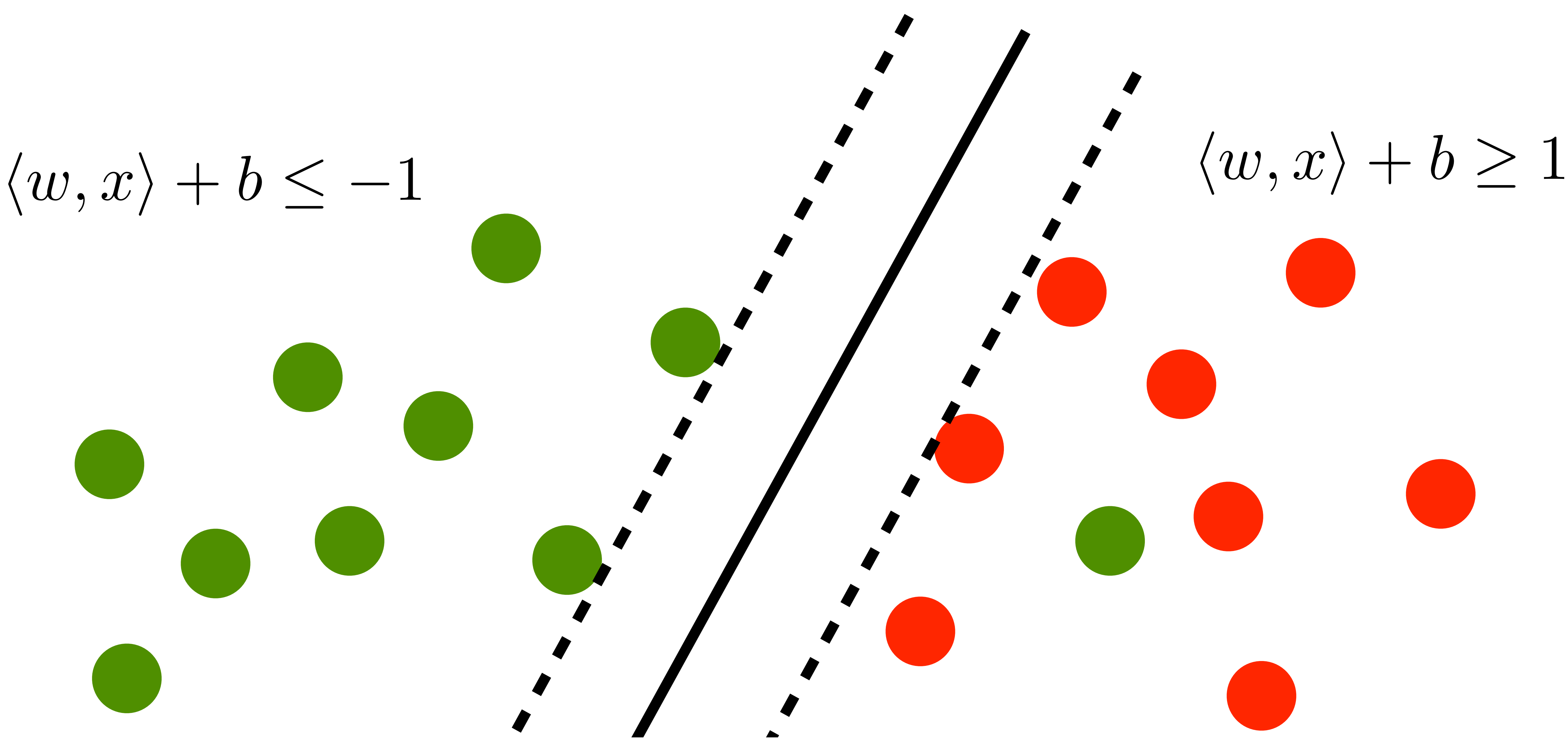


Today

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

Soft Margin Classification

Large Margin Classifier



linear function

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

linear separator
is impossible

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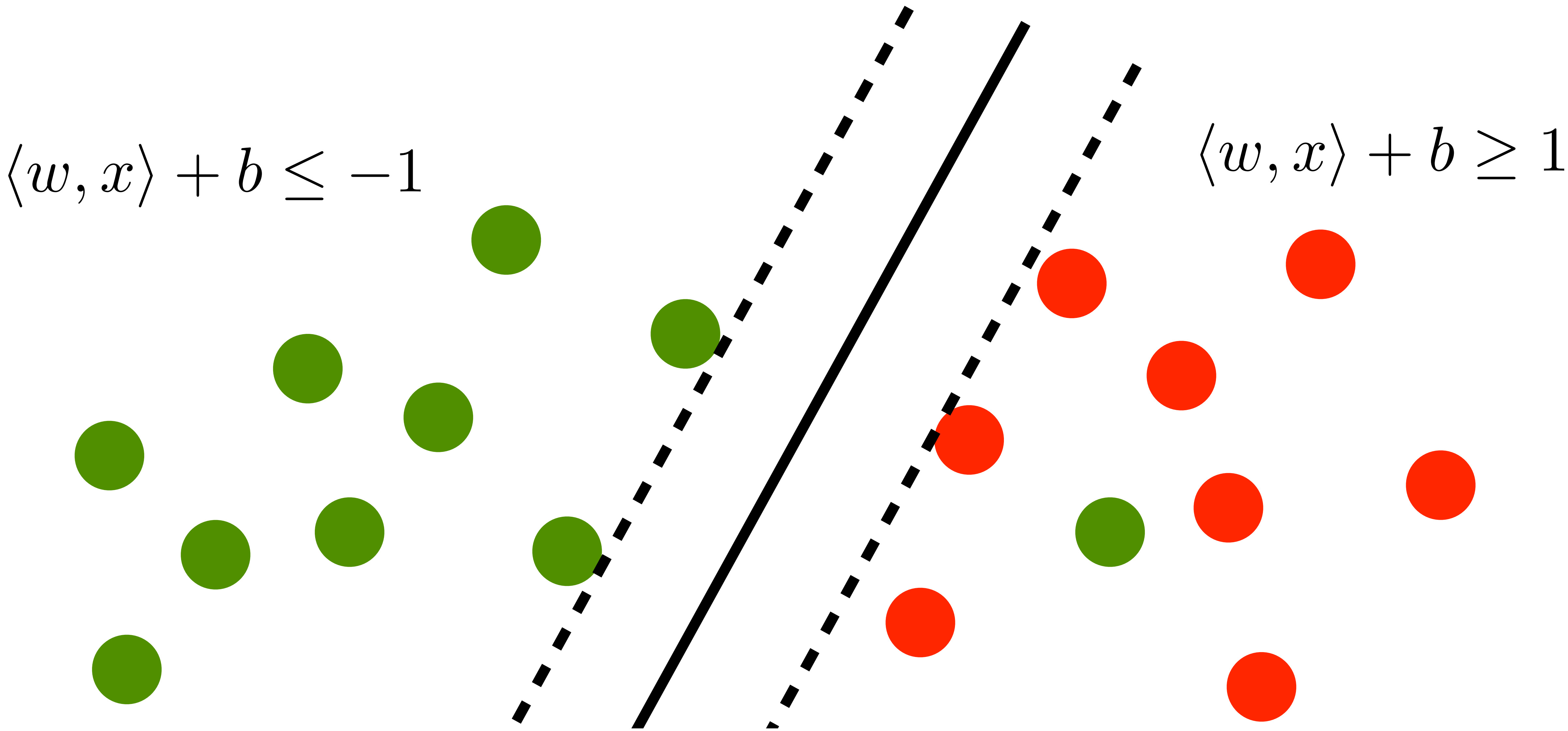
Large Margin Classifier



minimum error separator is impossible

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

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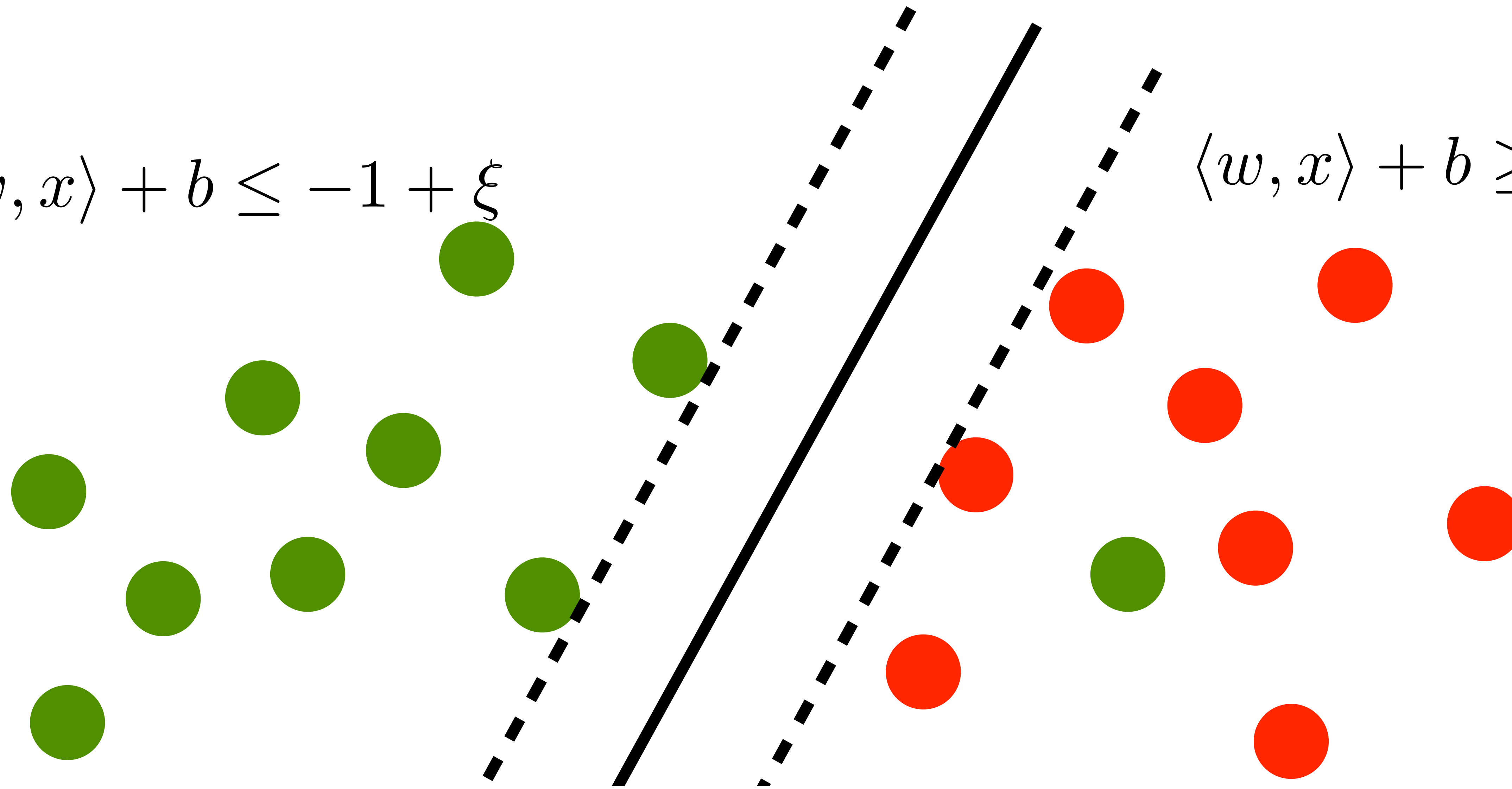
Adding Slack Variables

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

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



minimize amount of slack

Convex optimization problem

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Convex Programs for Dummies

- Primal optimization problem

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

- 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

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

(keep explicit constraints)

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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:

$w = 0$ and $b = 0$ 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,ξ is at saddle point with α,η

- Derivatives in w,b,ξ 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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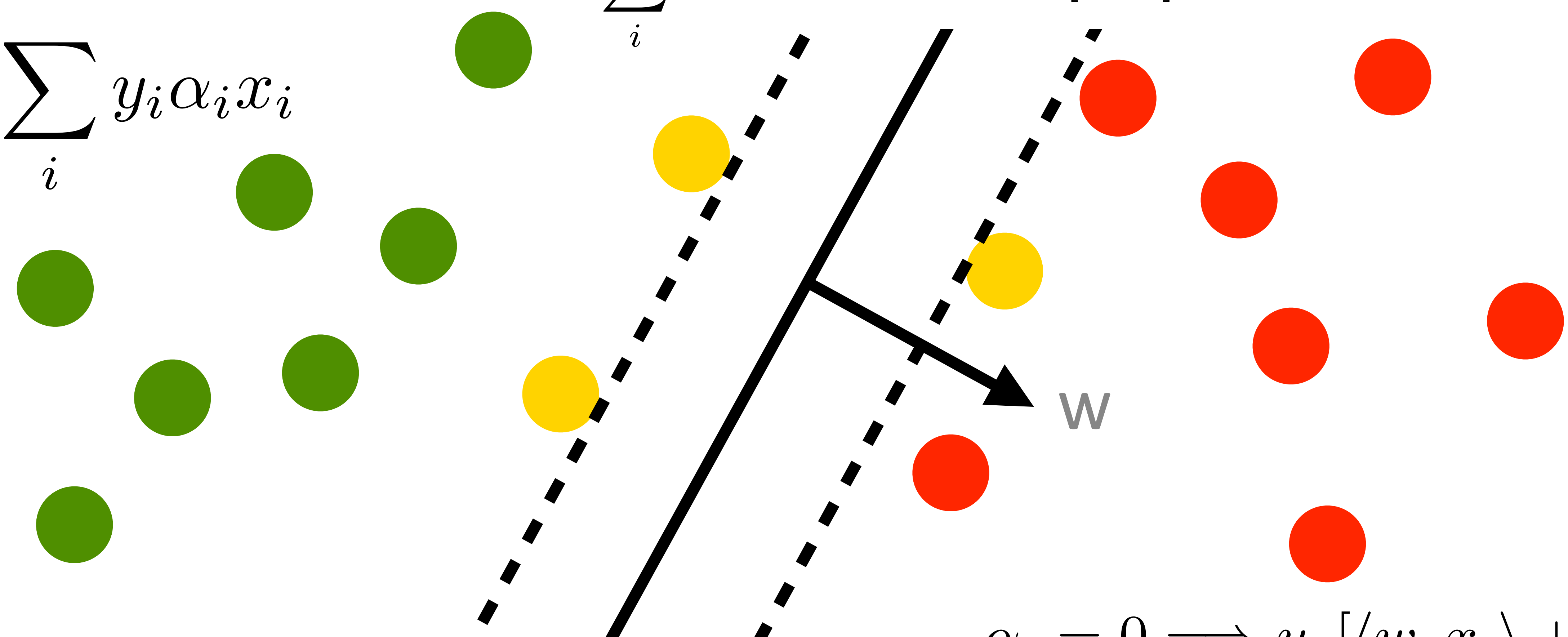
Karush Kuhn Tucker Conditions

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

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

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



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

$$\eta_i \xi_i = 0$$

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

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

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

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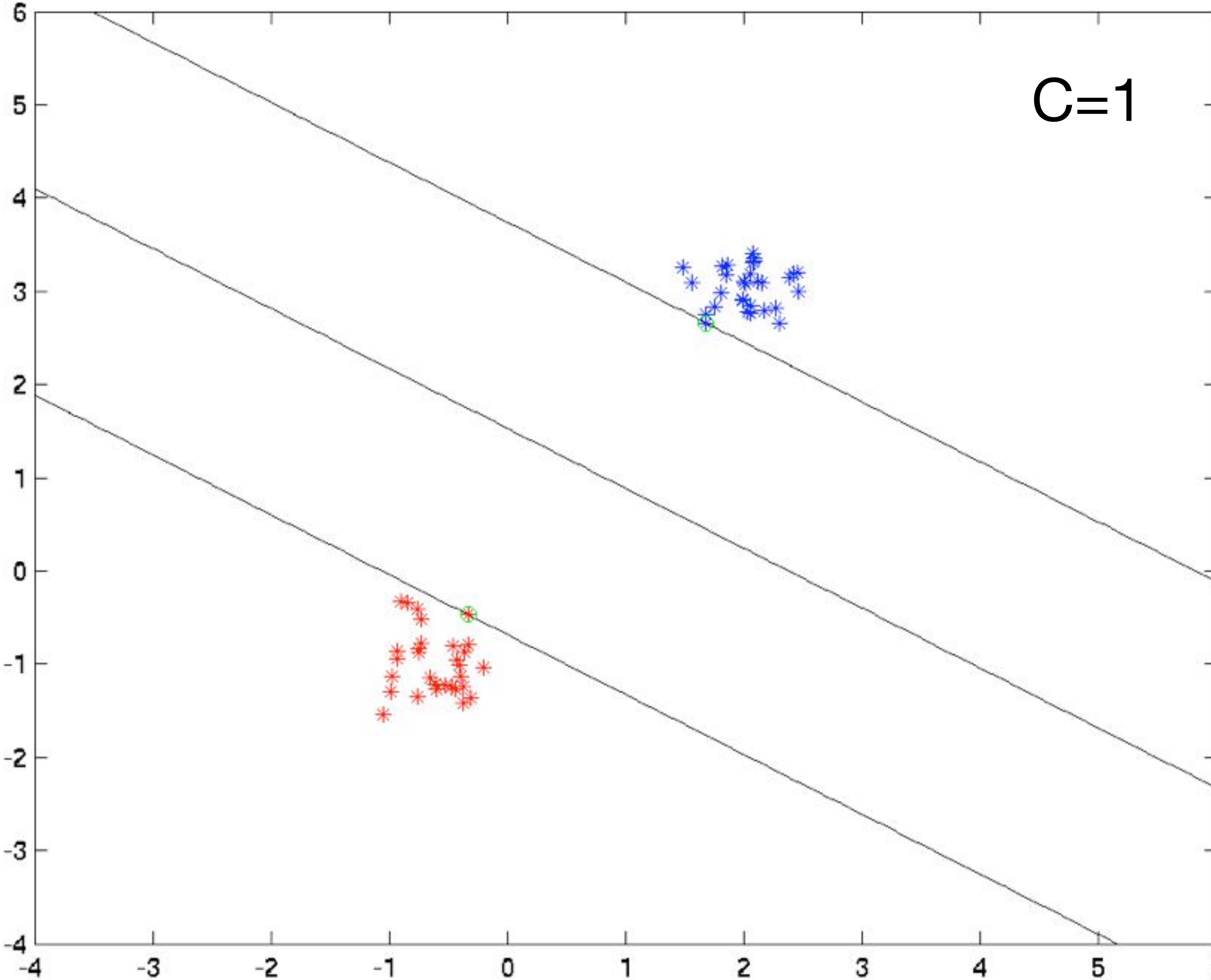

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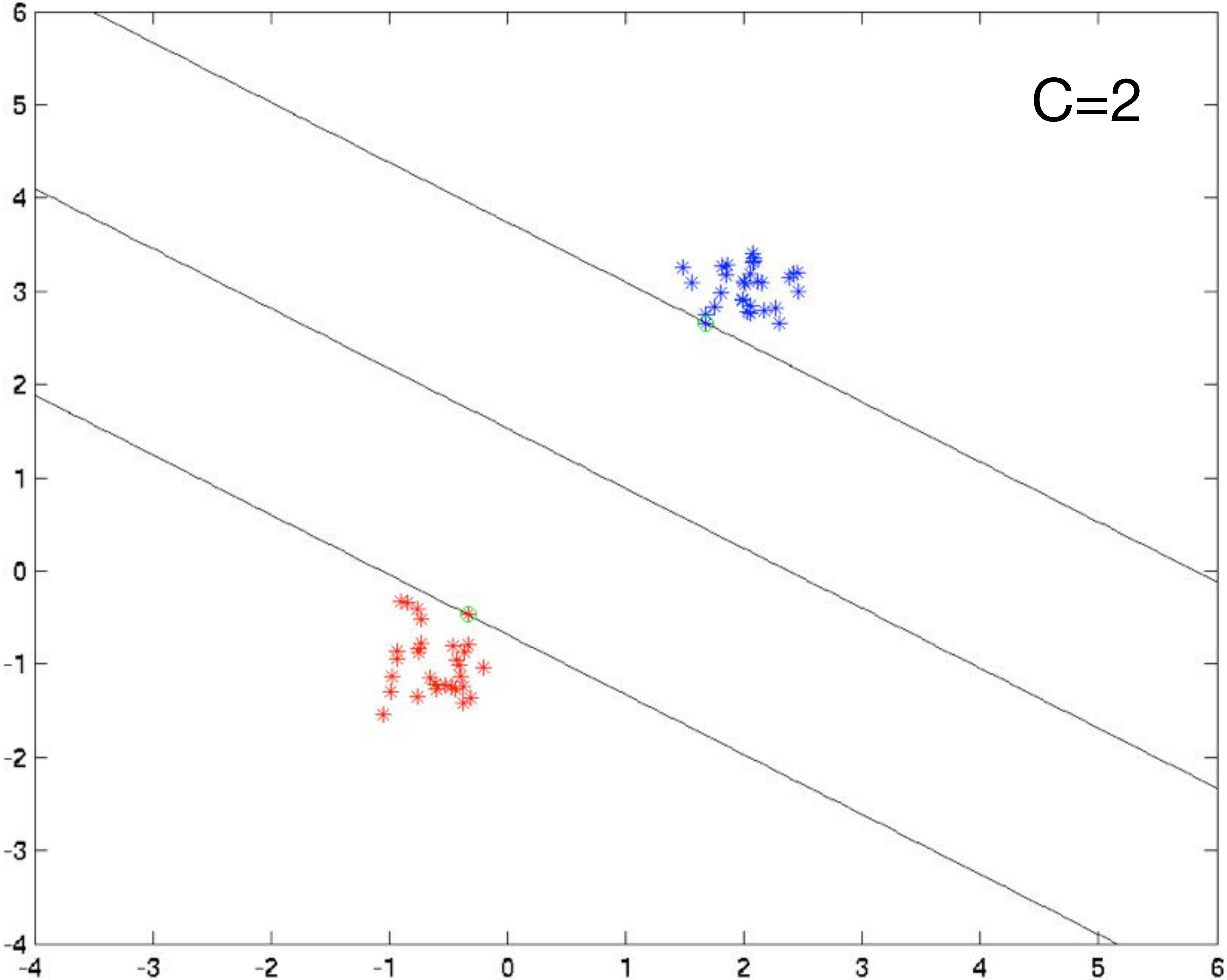

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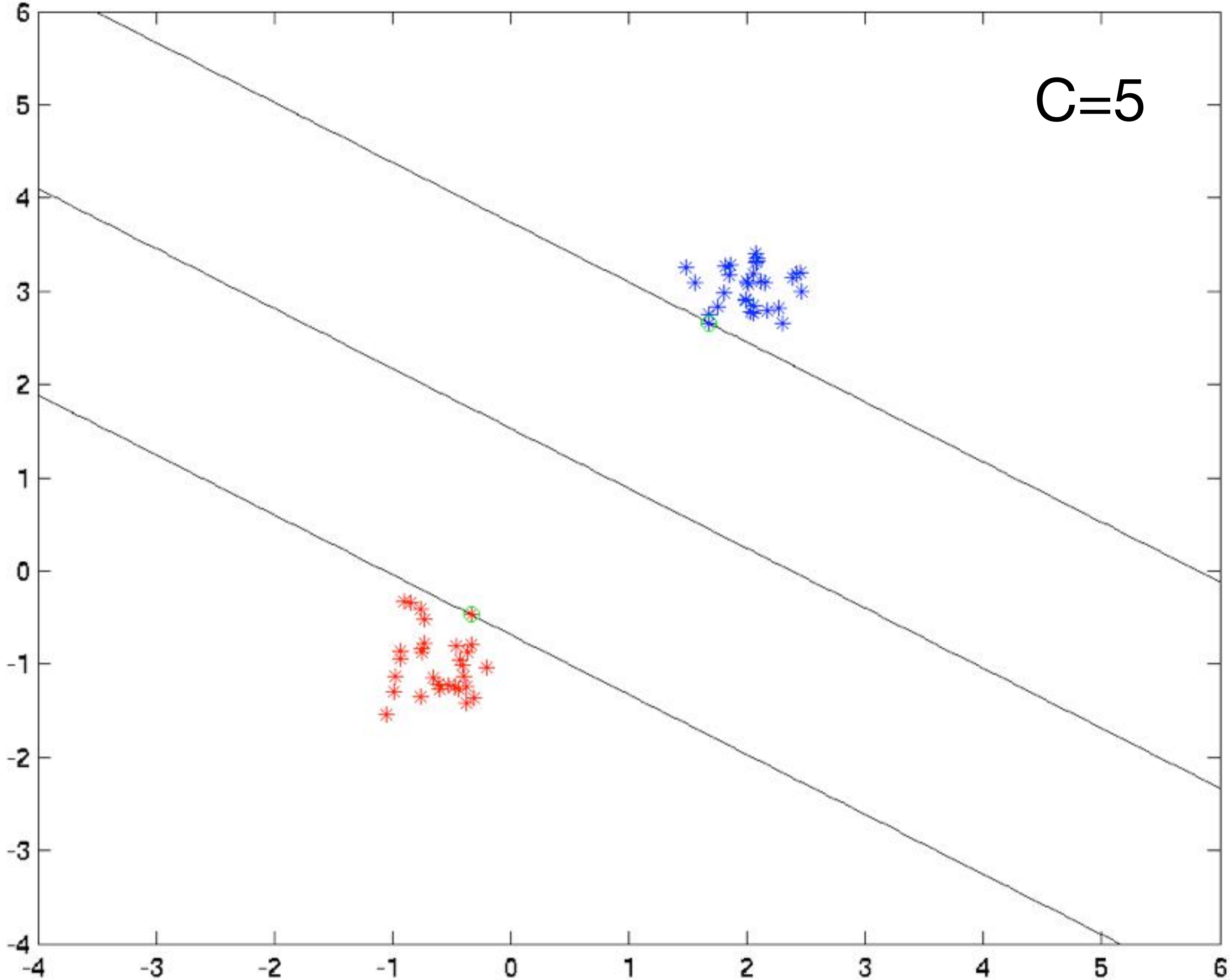

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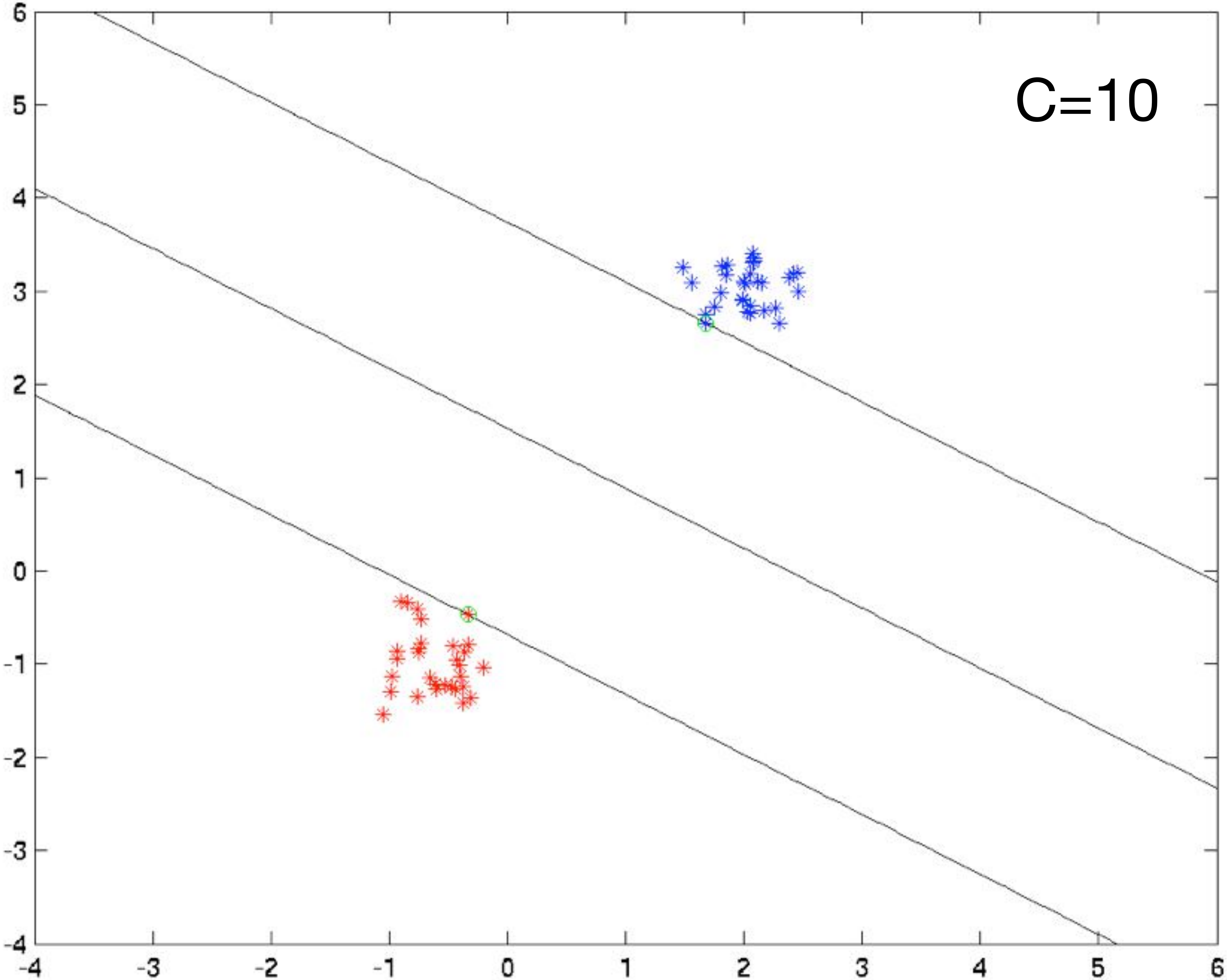

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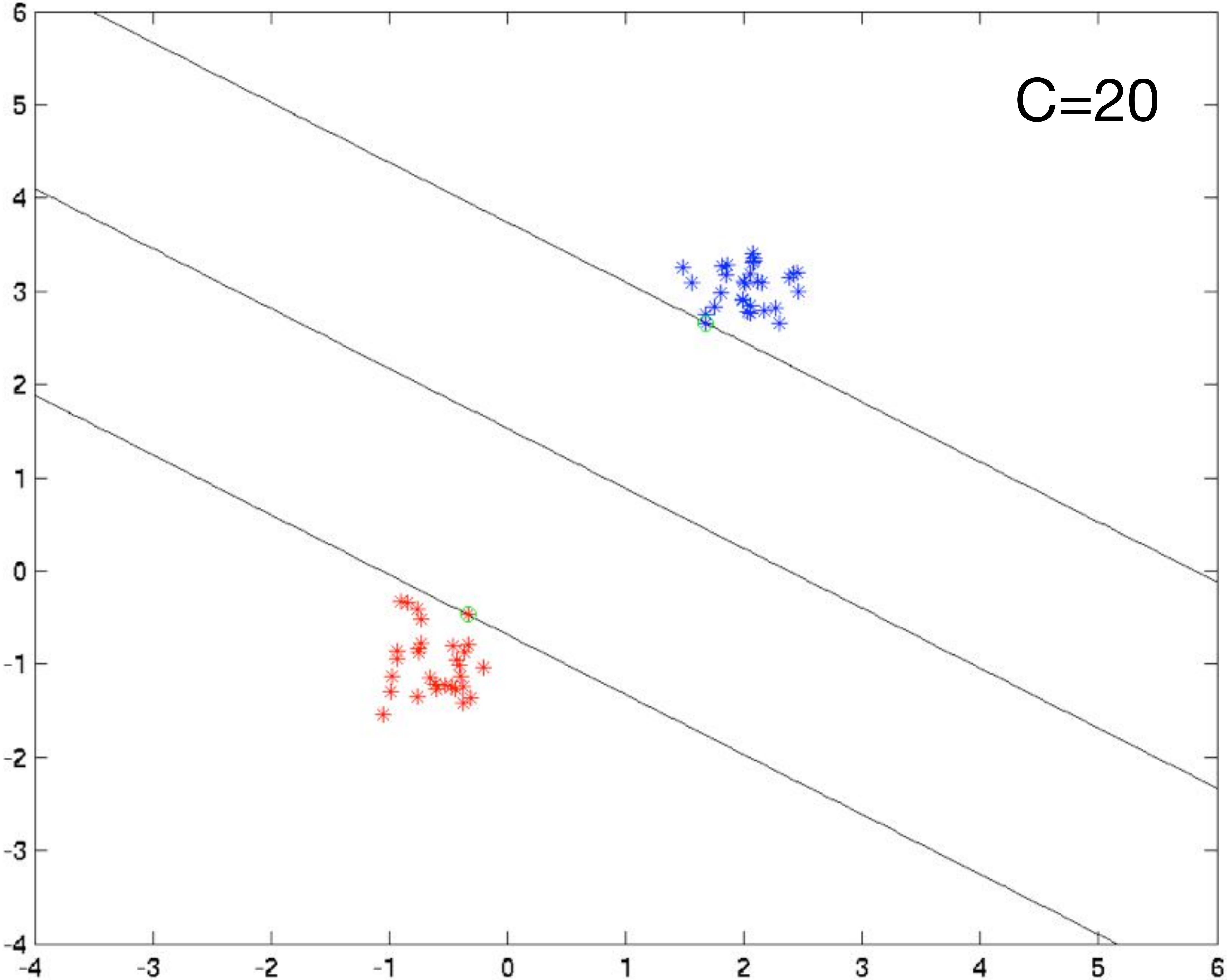

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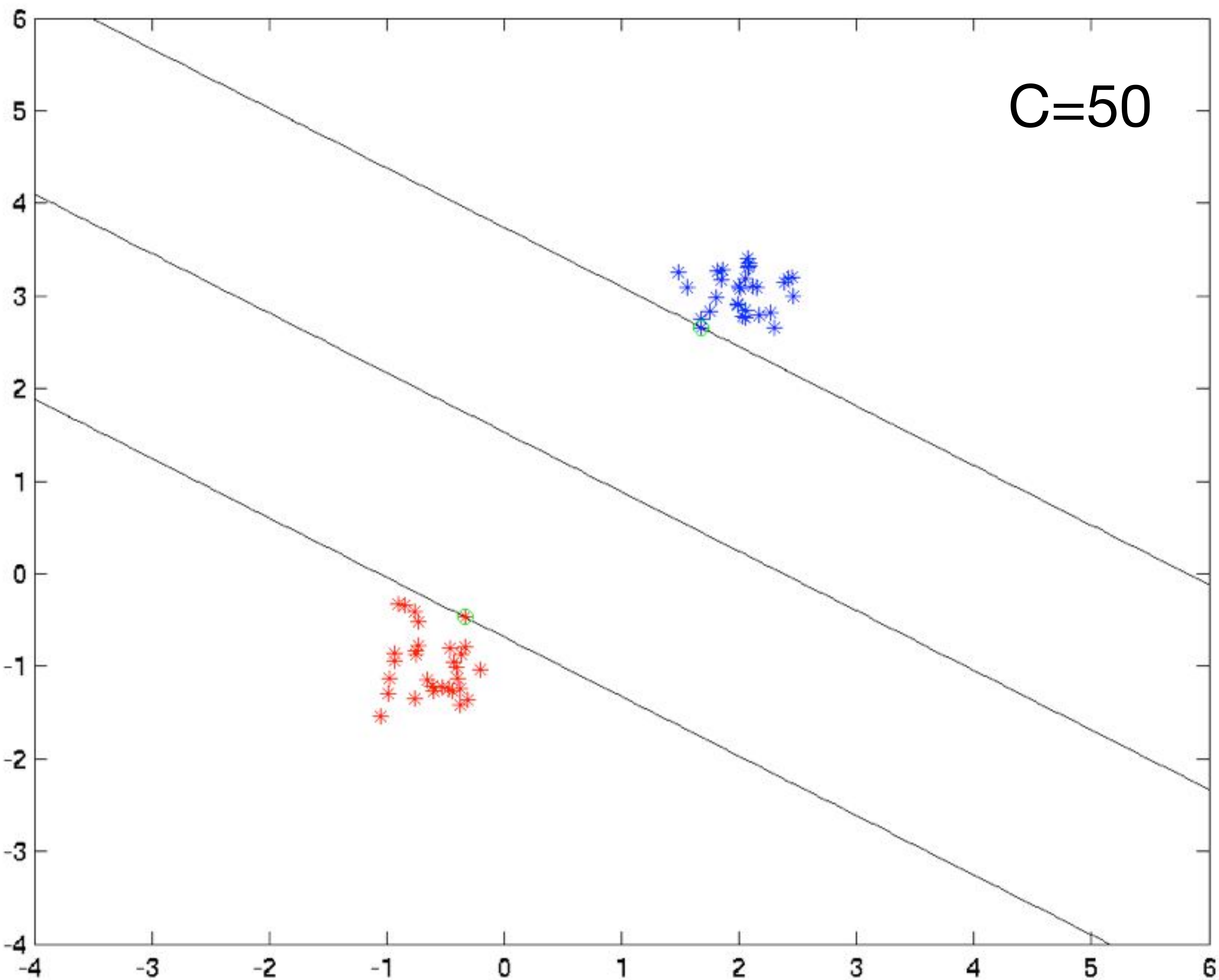

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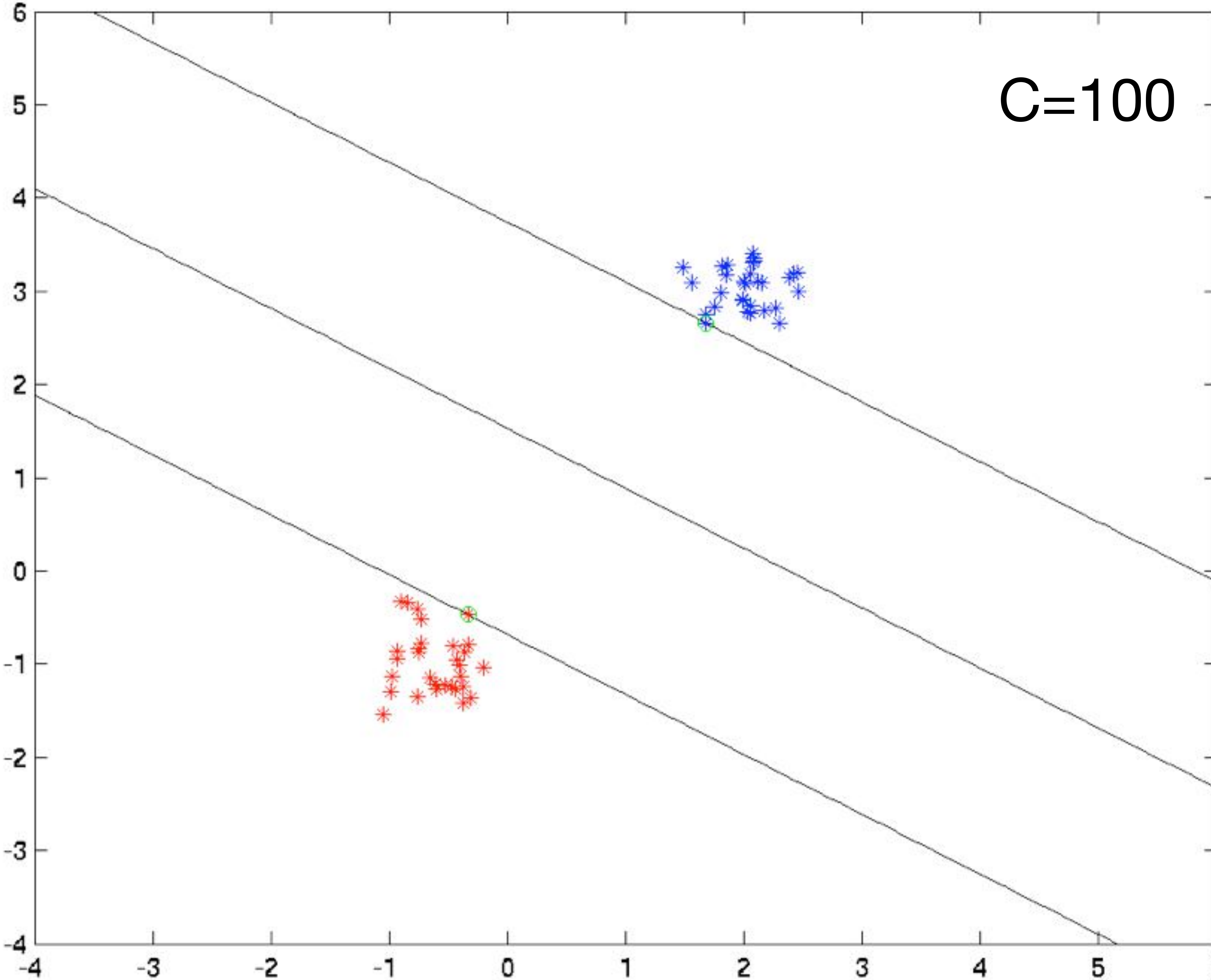

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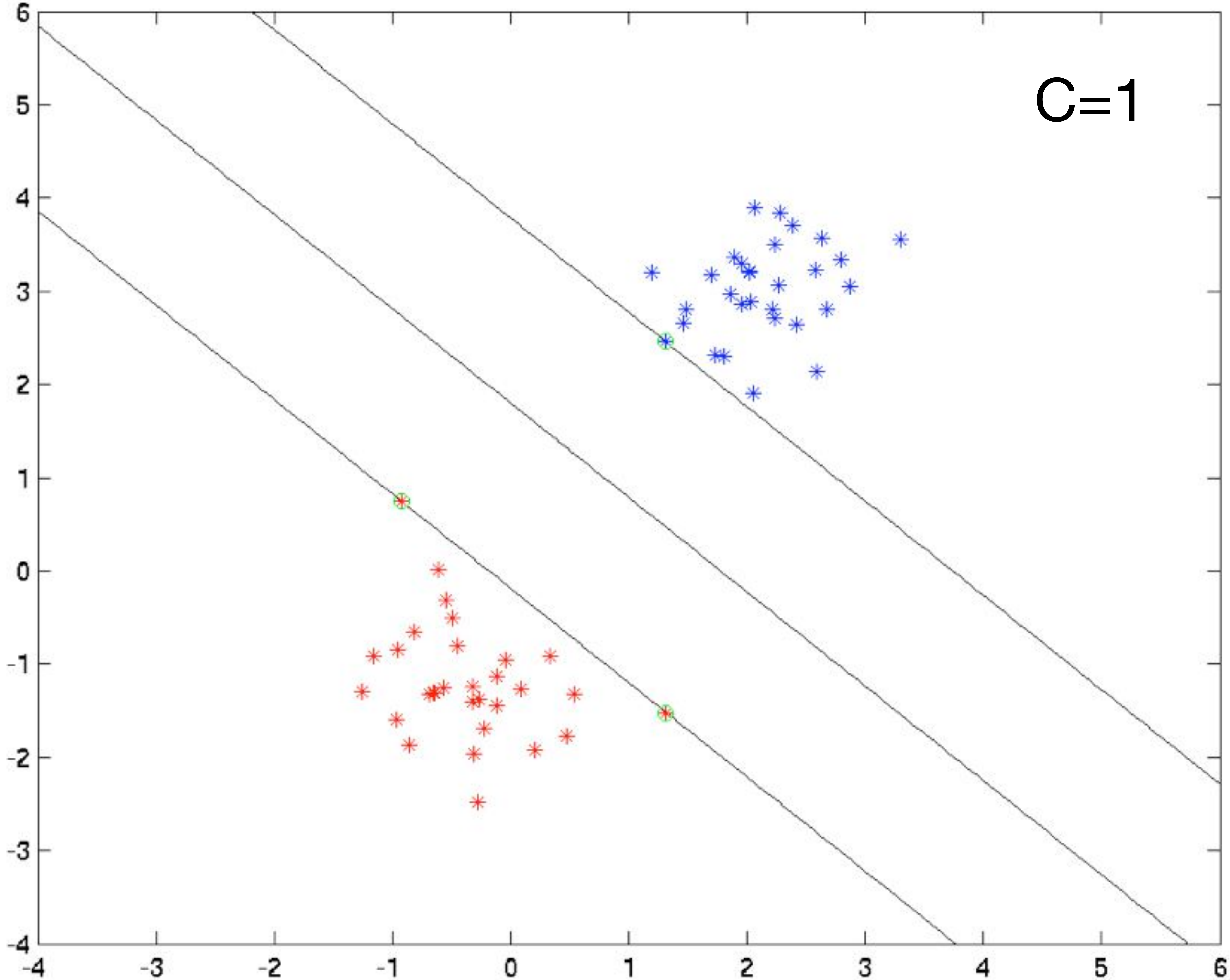

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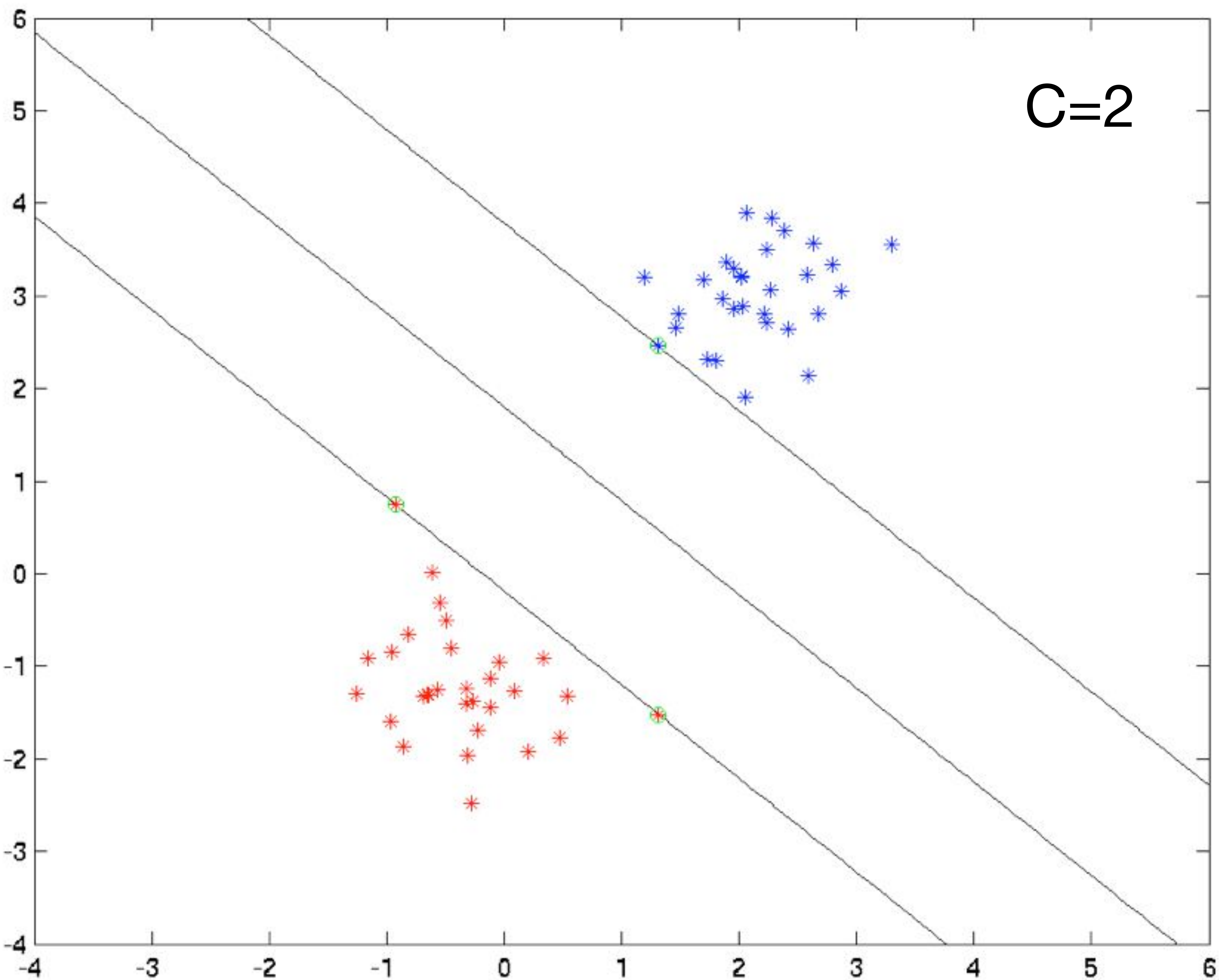

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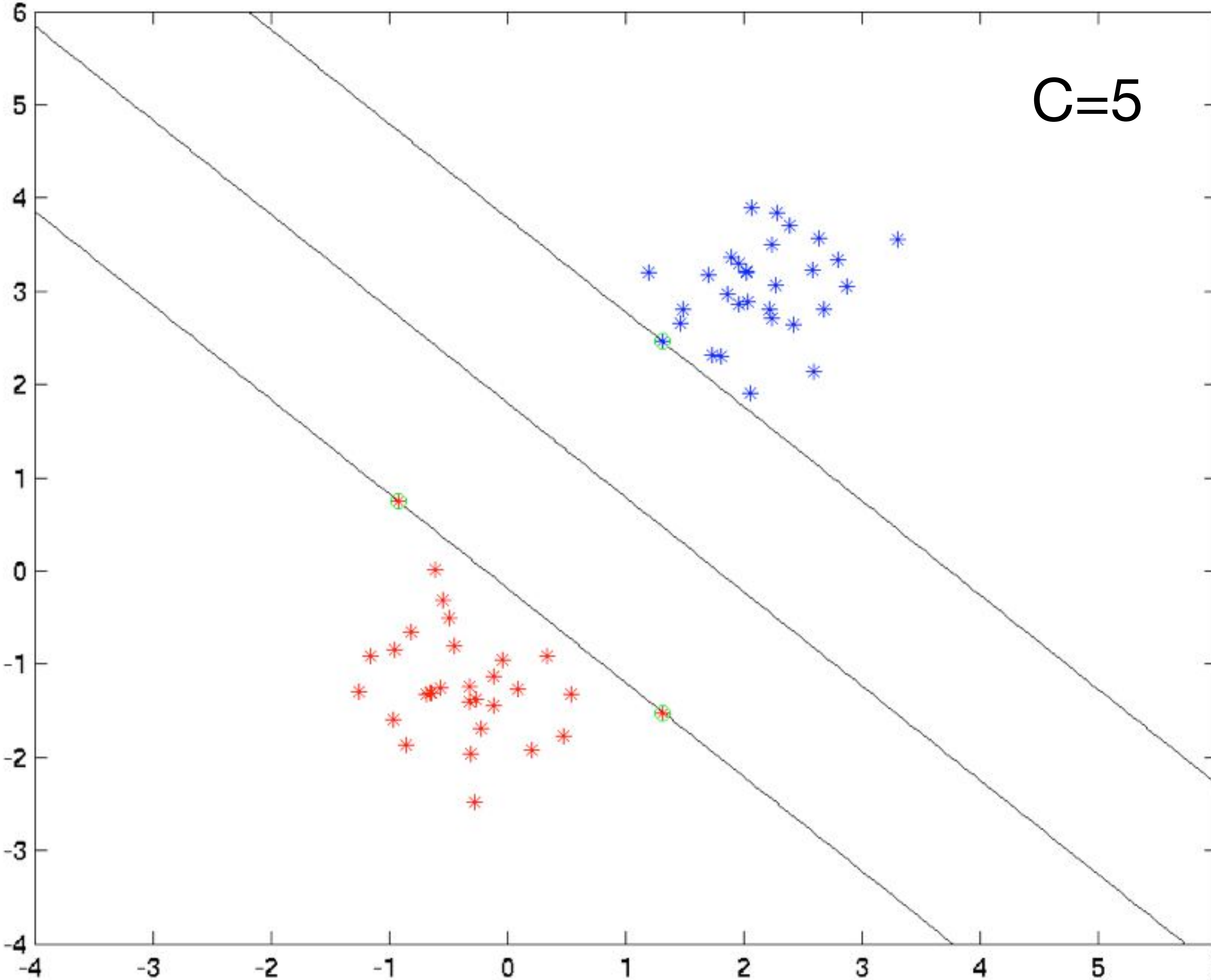

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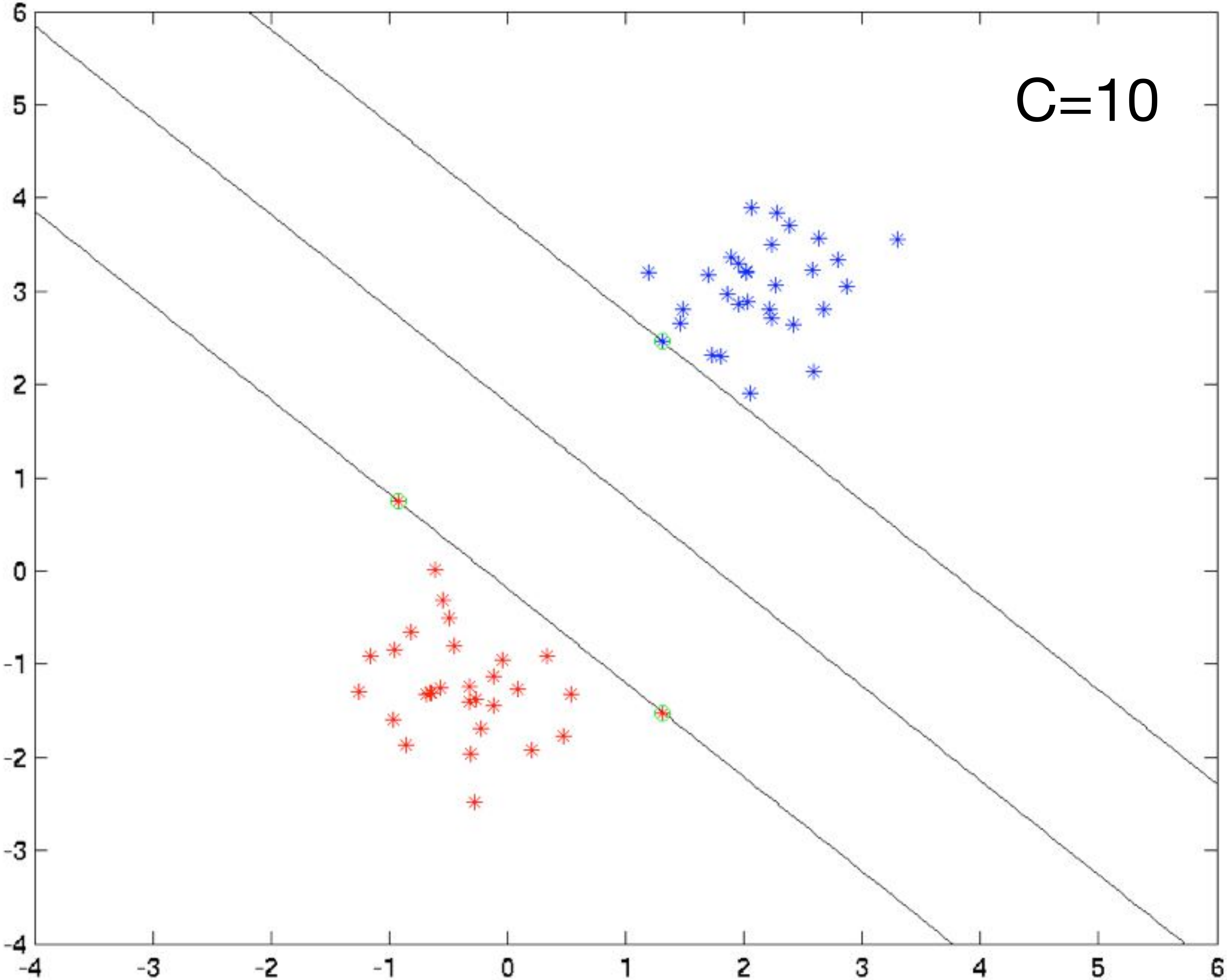

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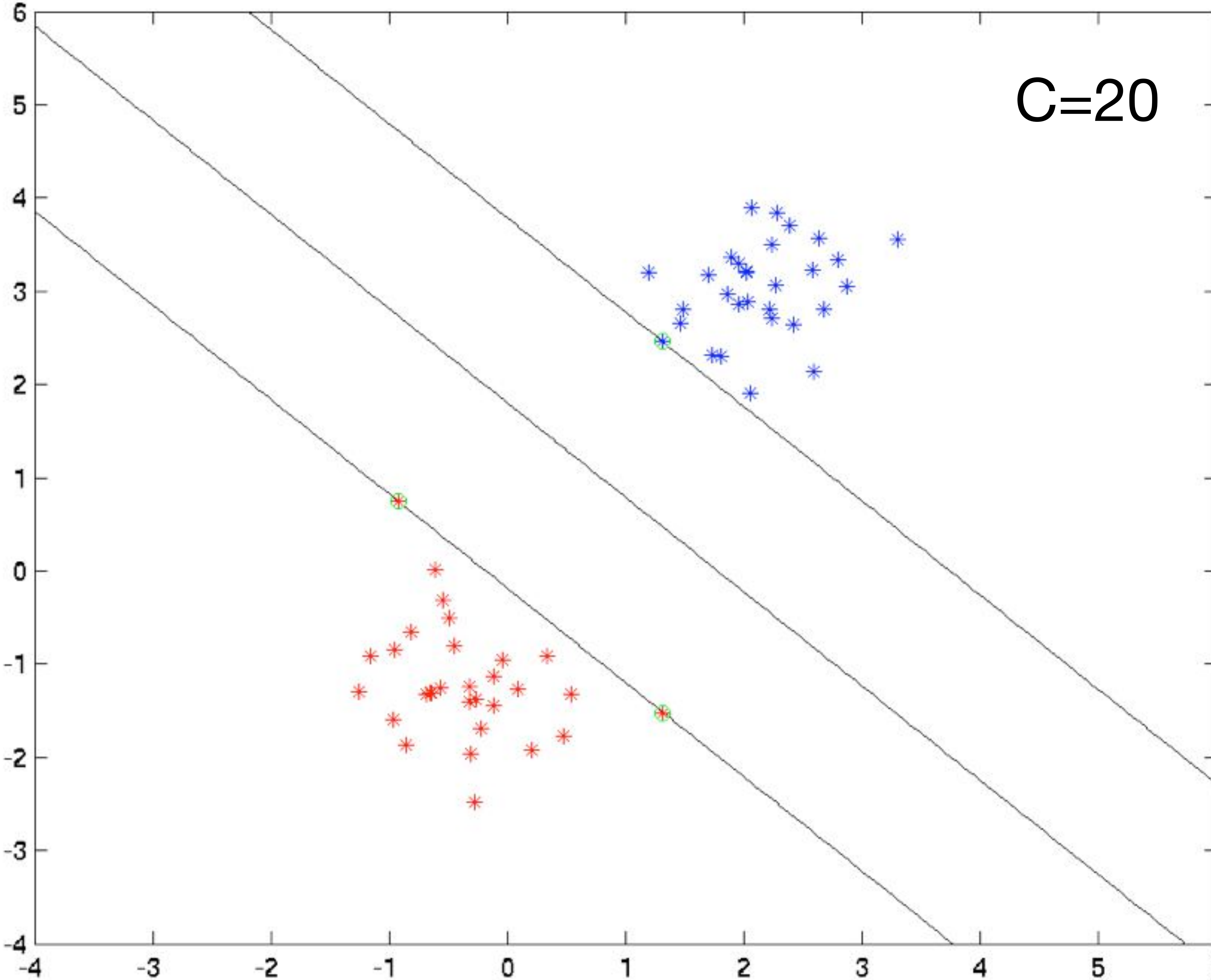

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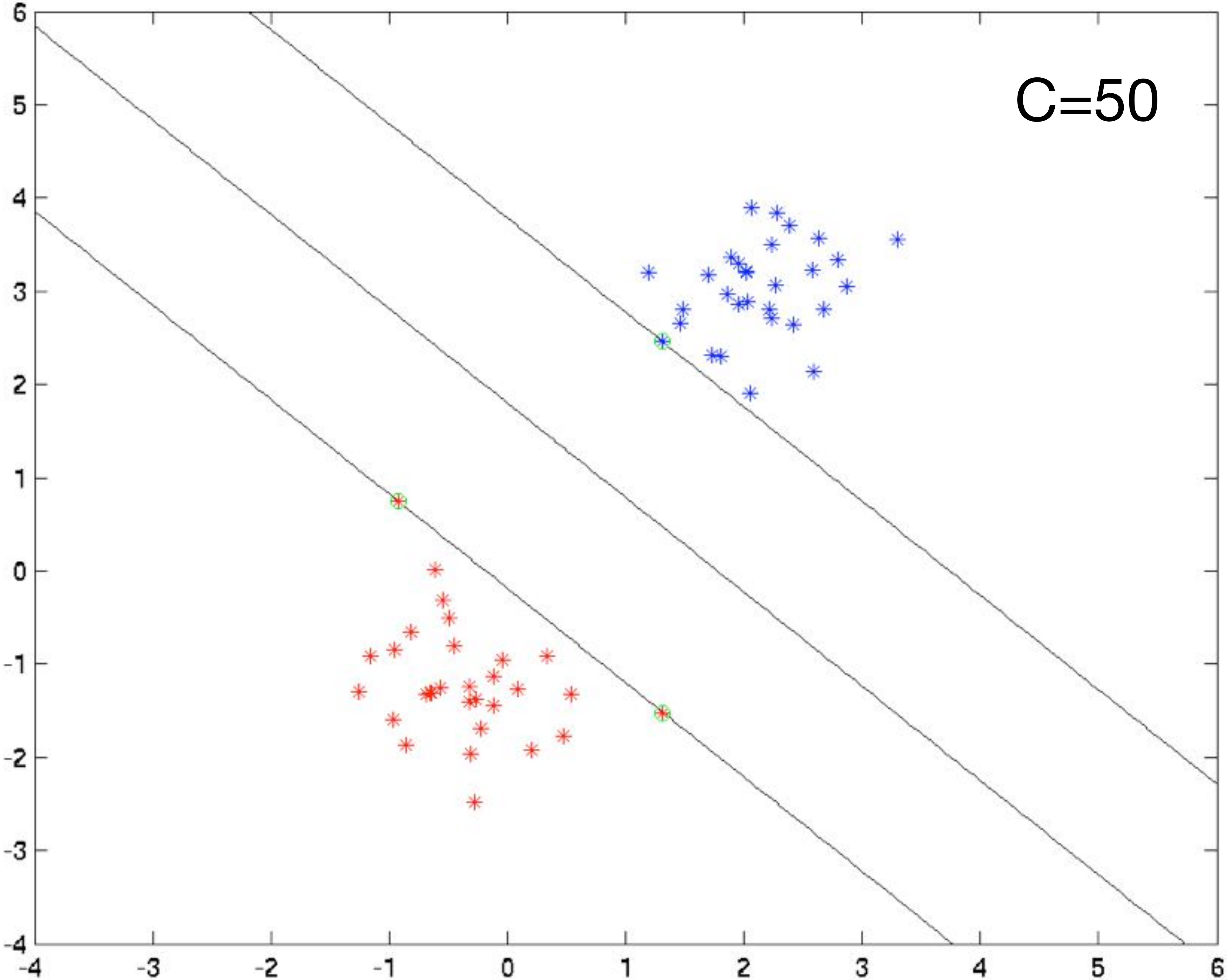

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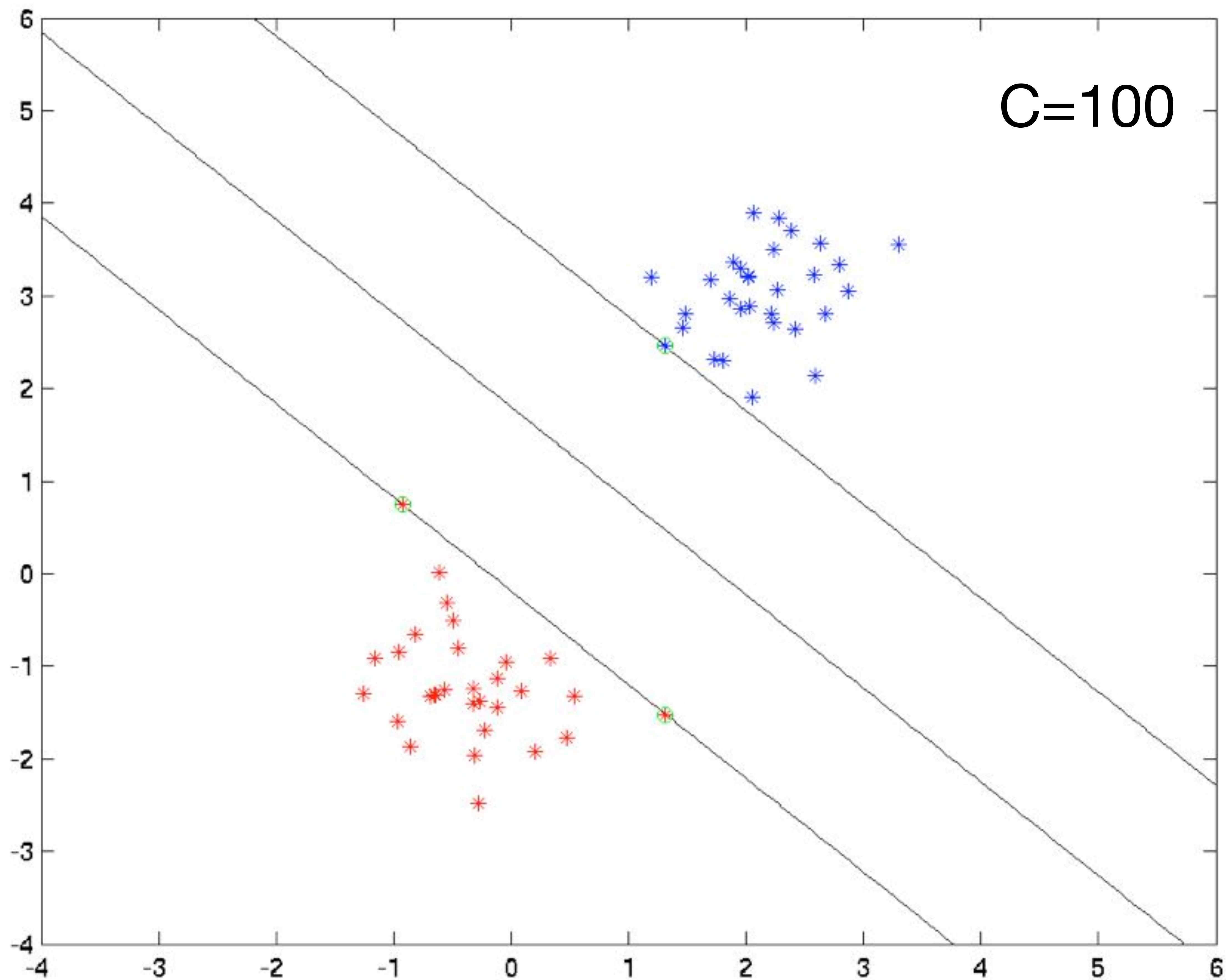

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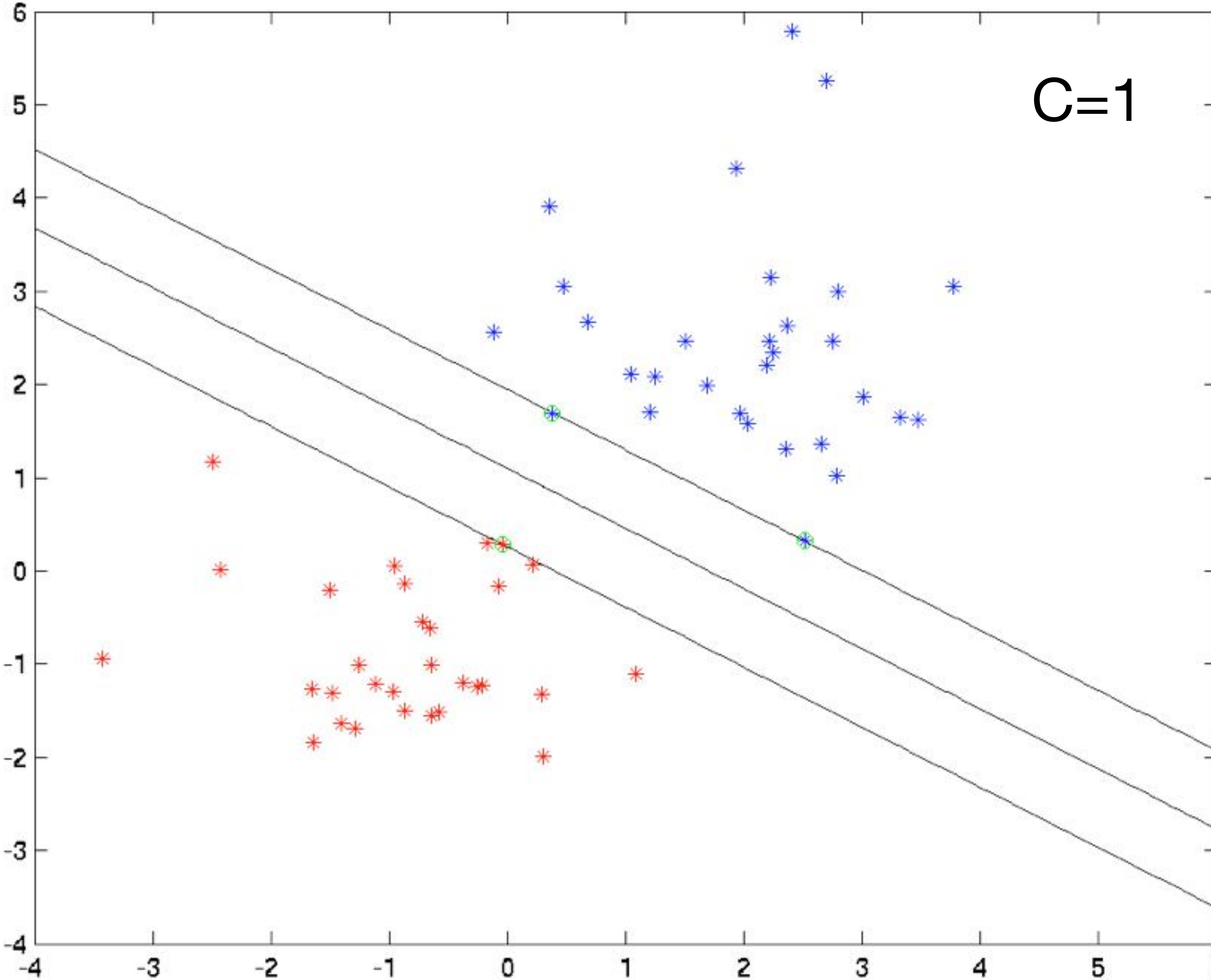

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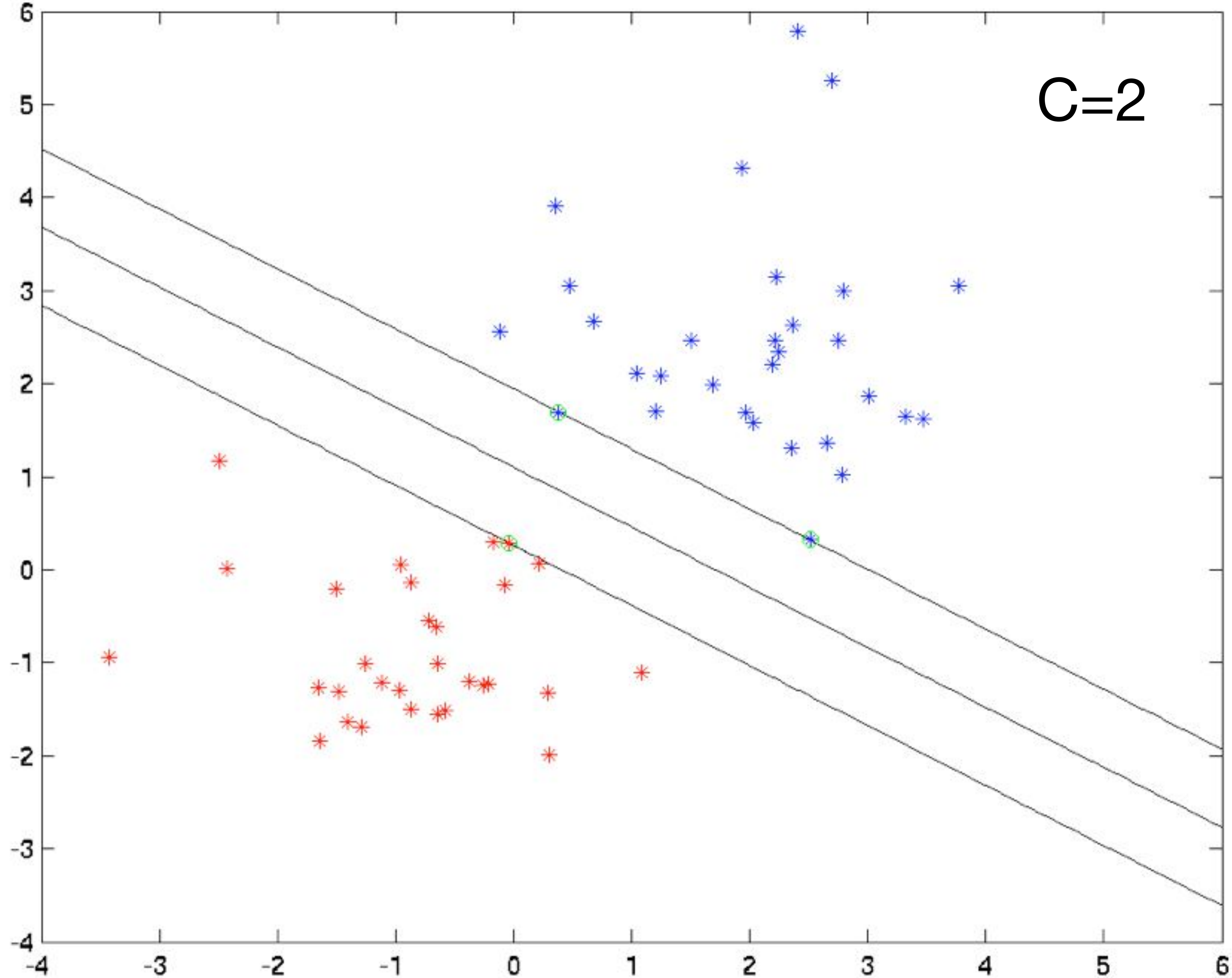

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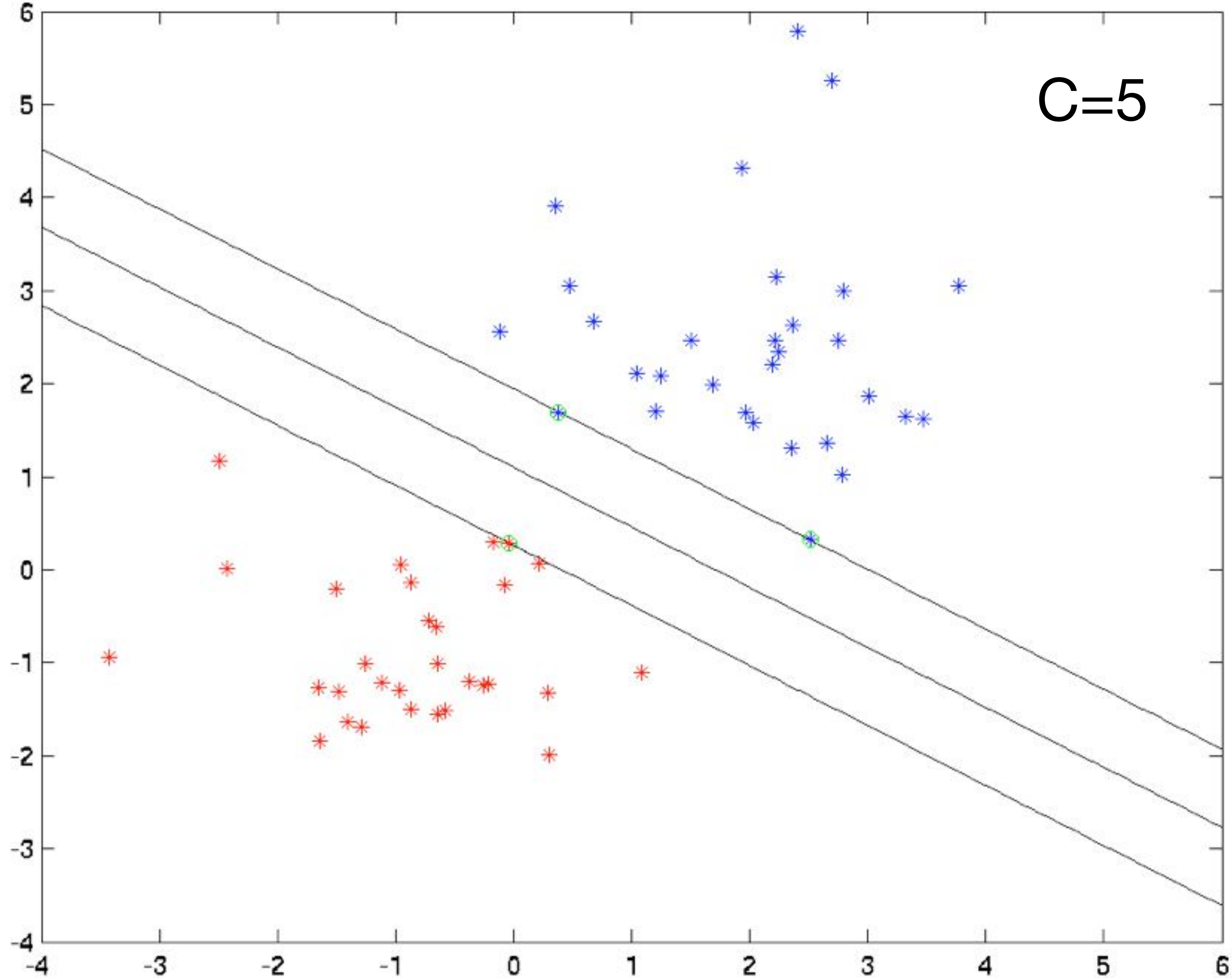

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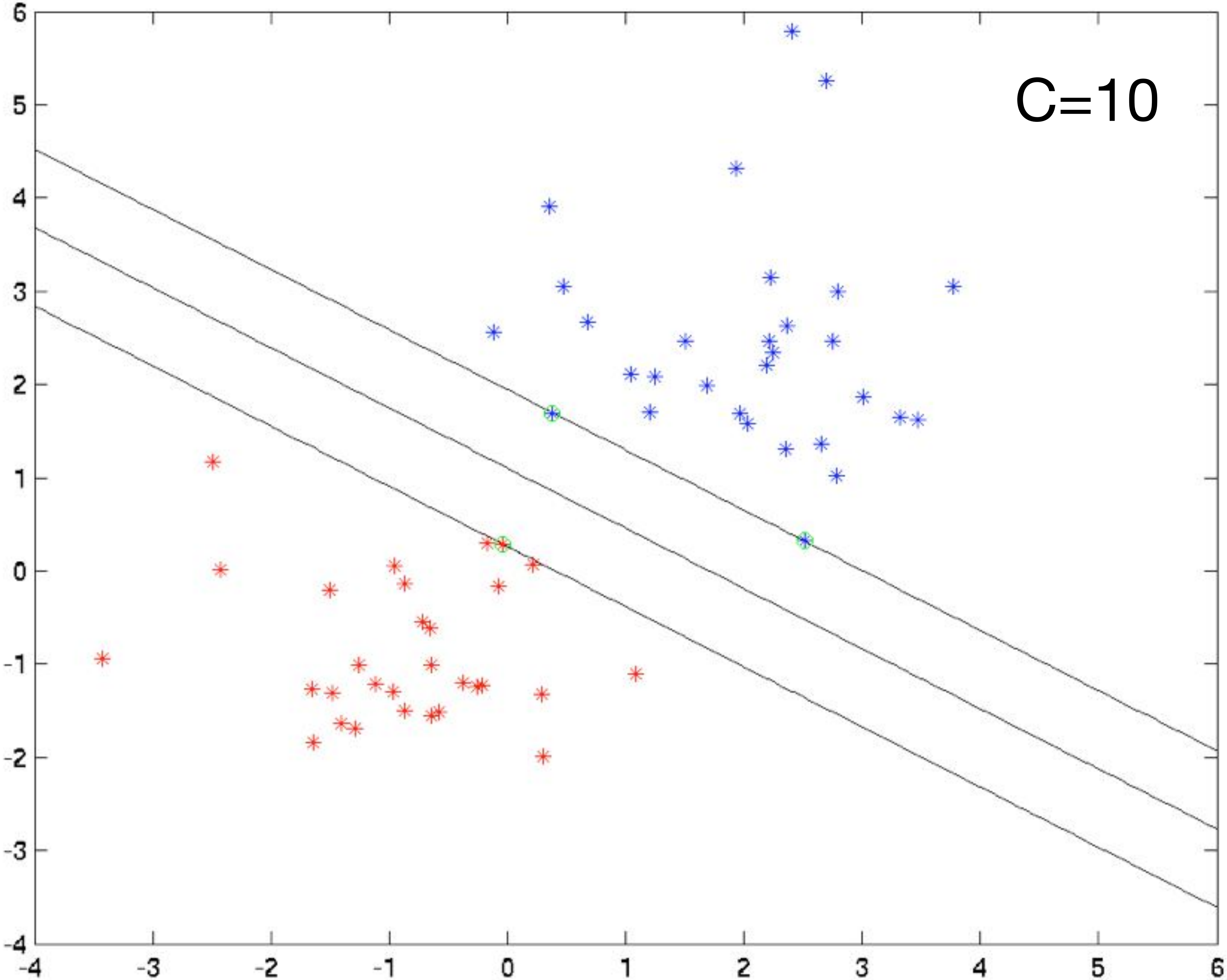

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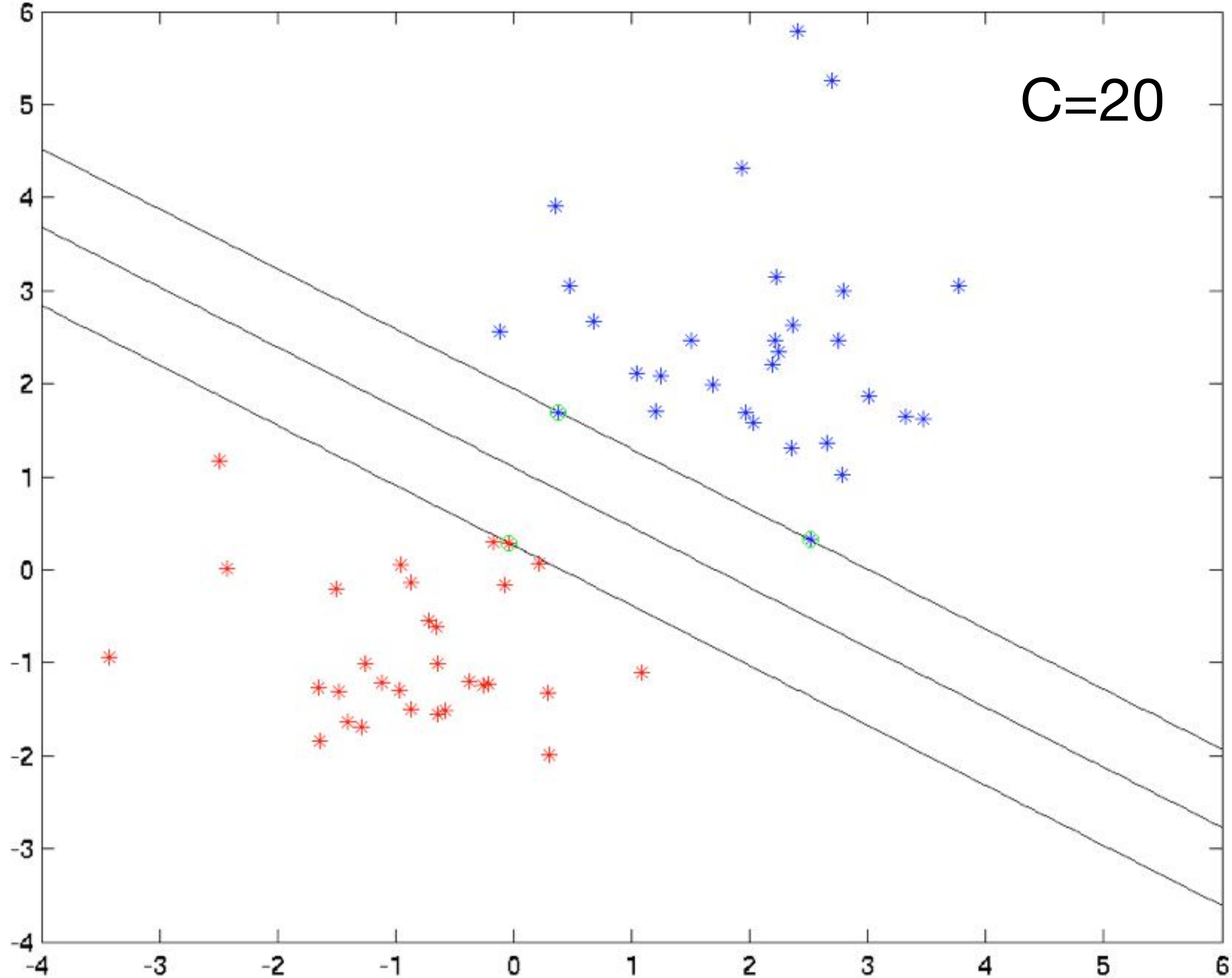

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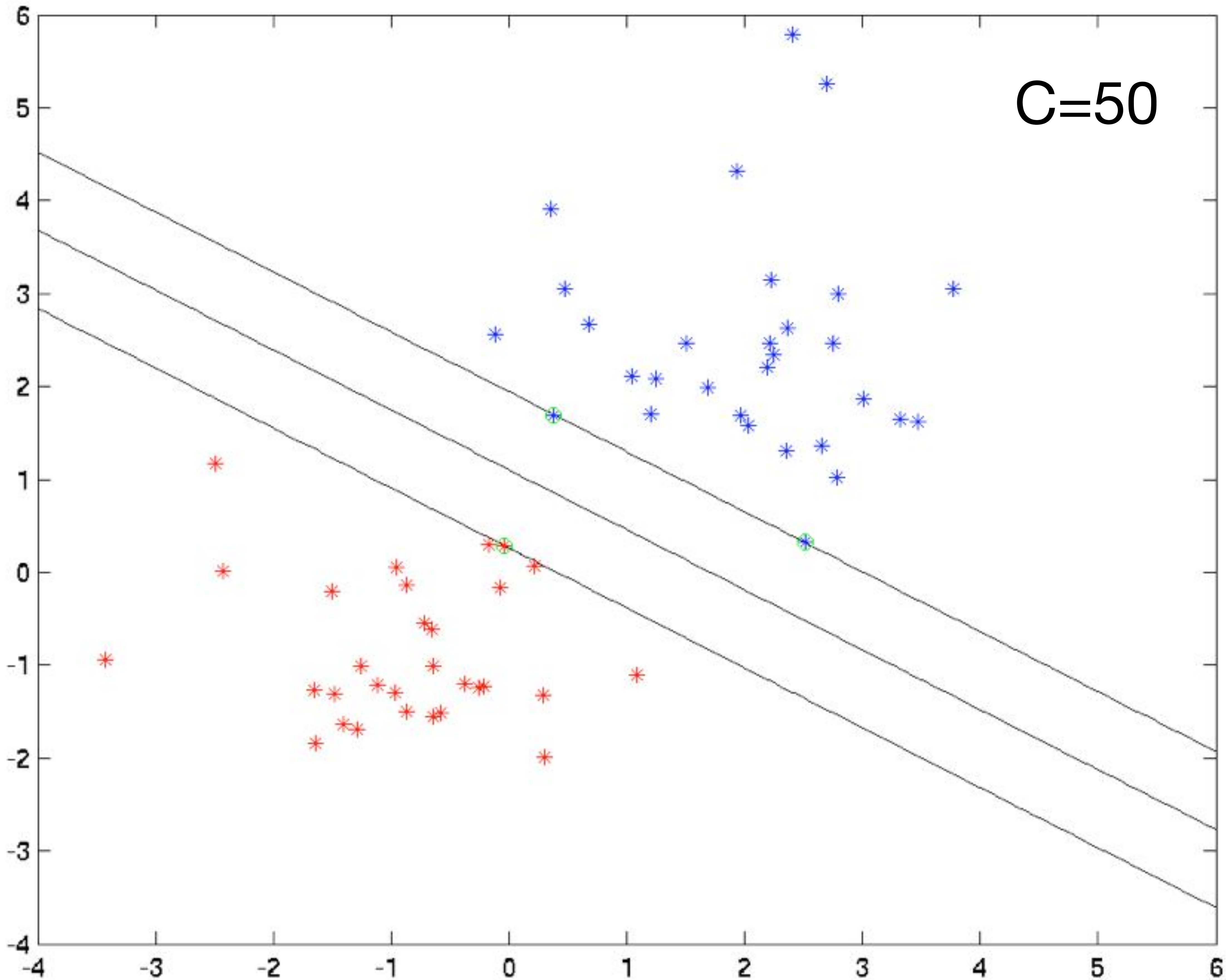

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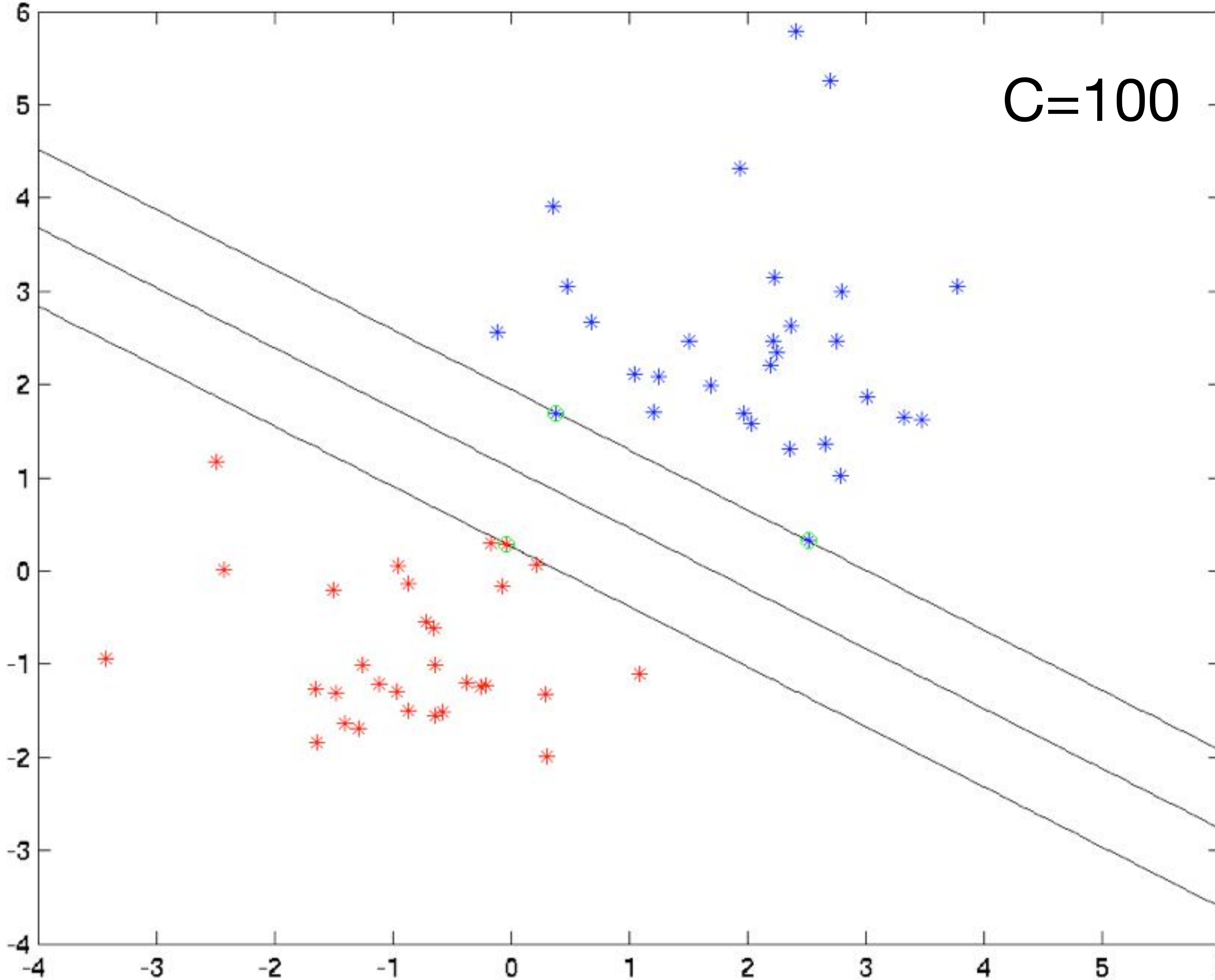

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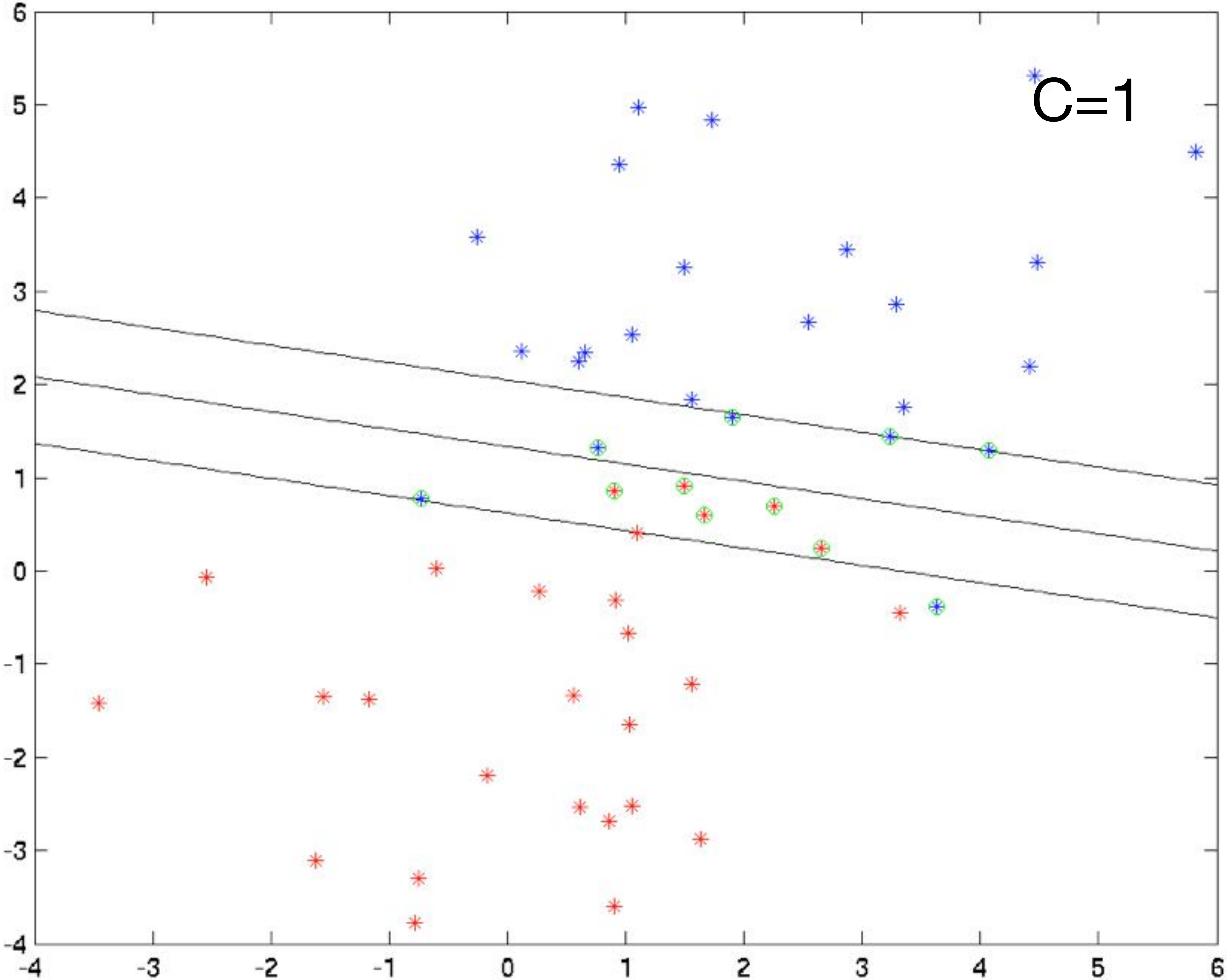

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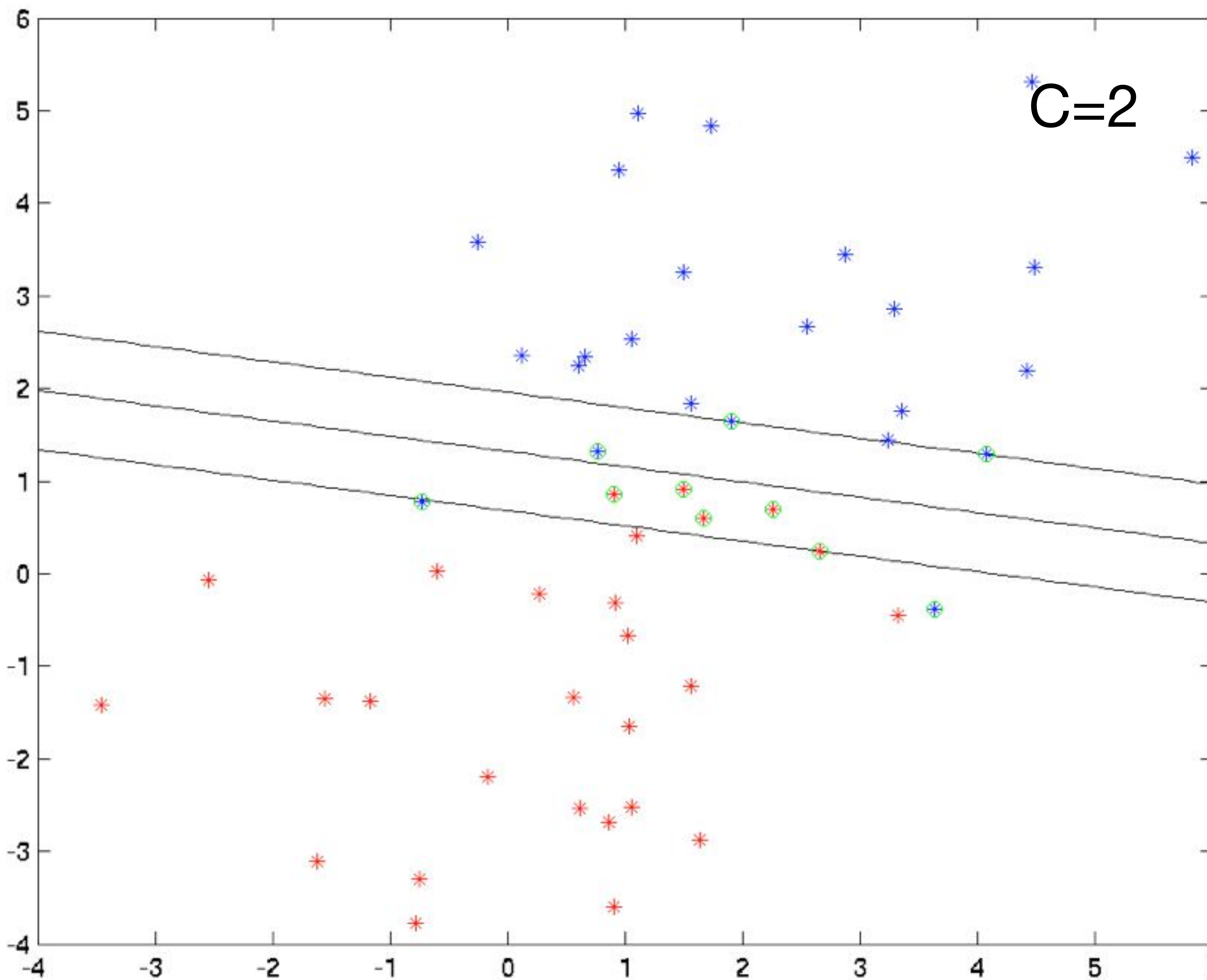

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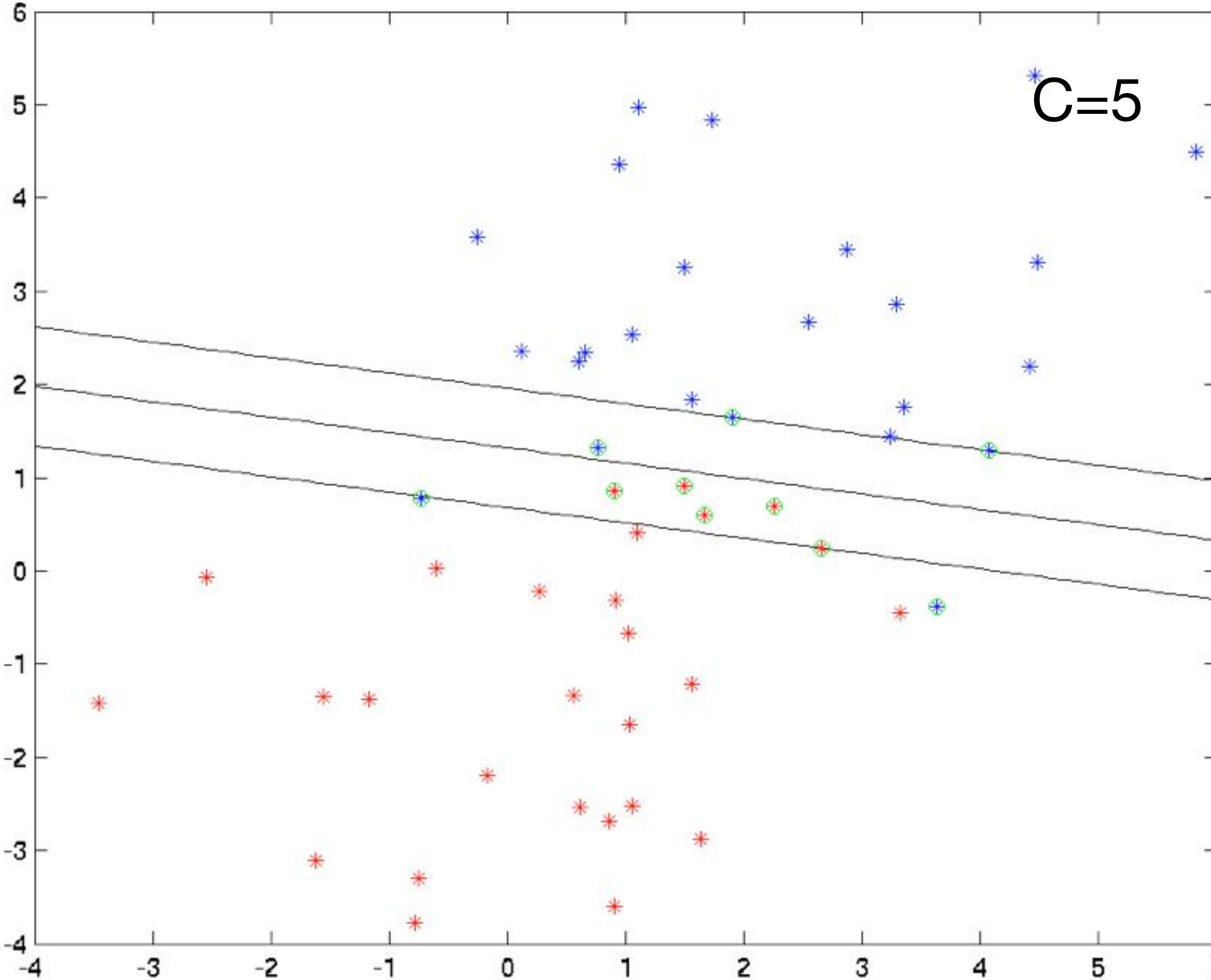

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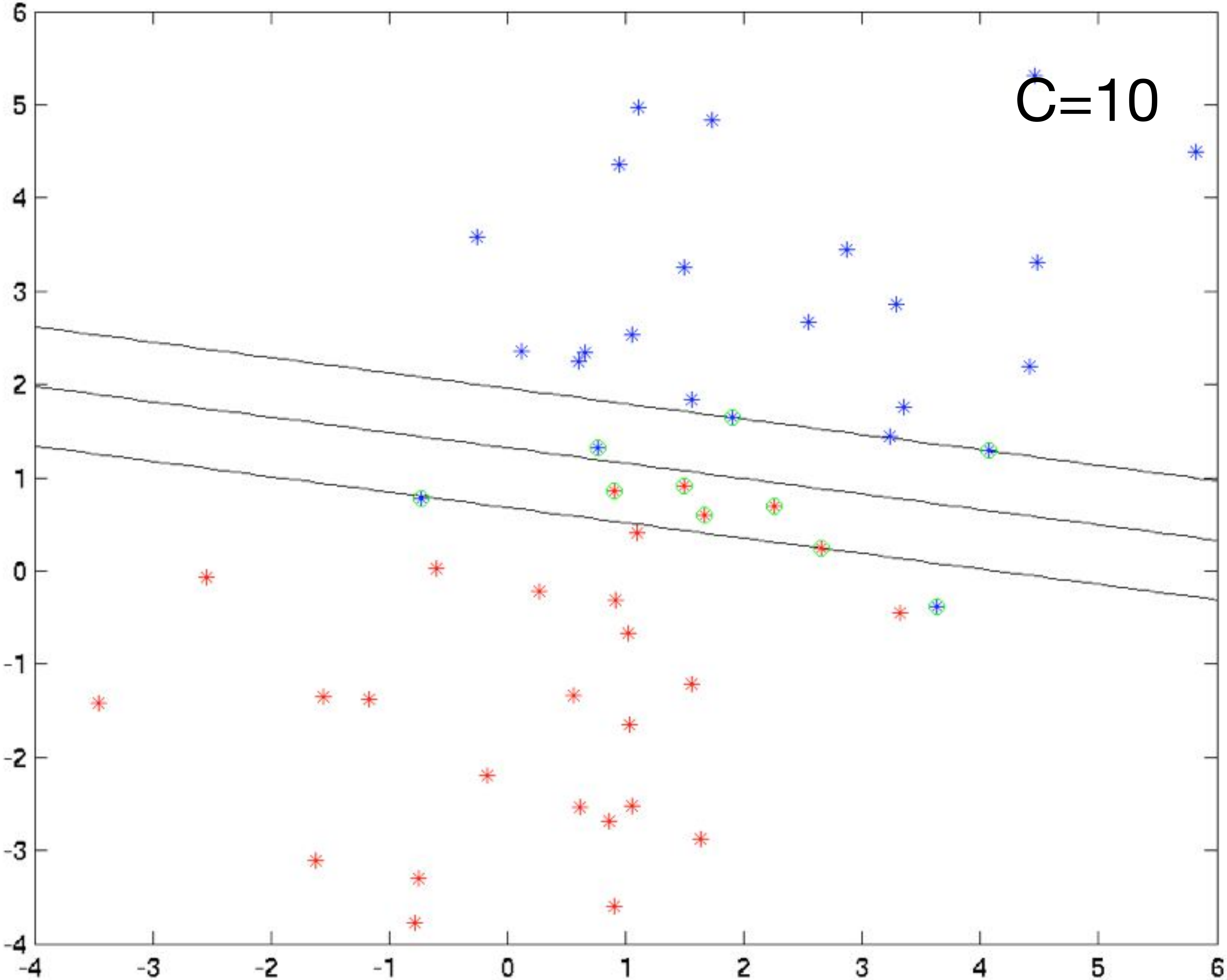

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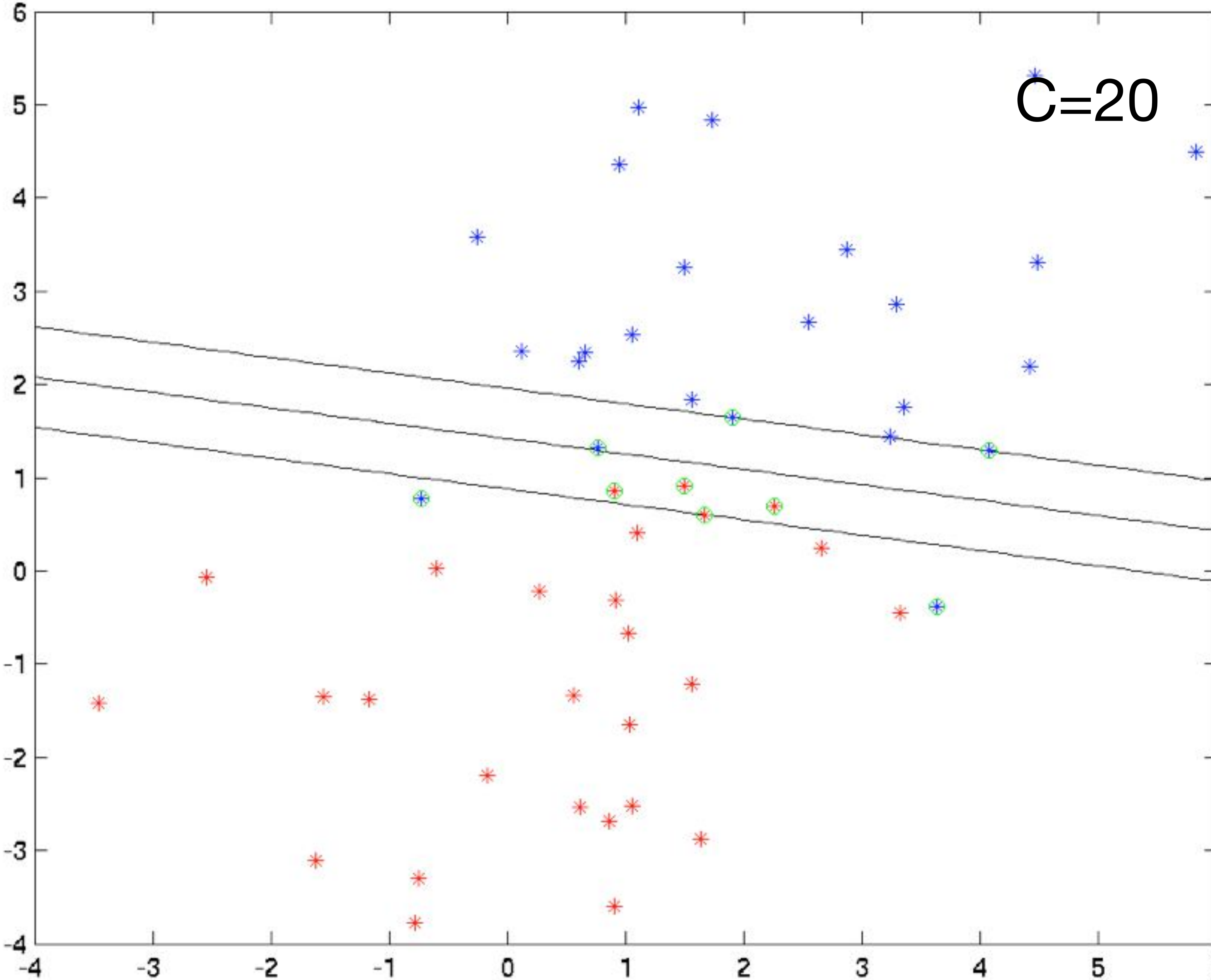

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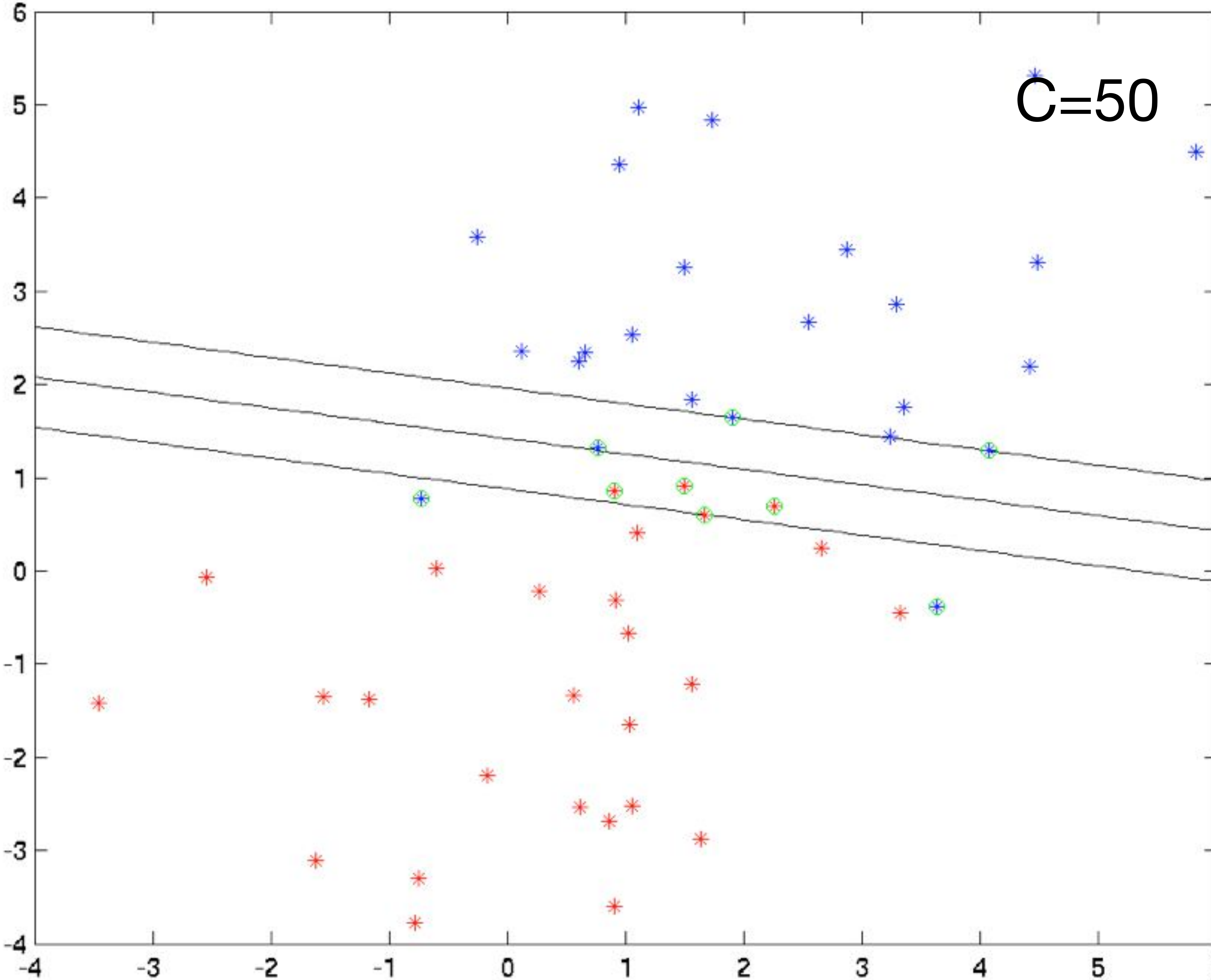

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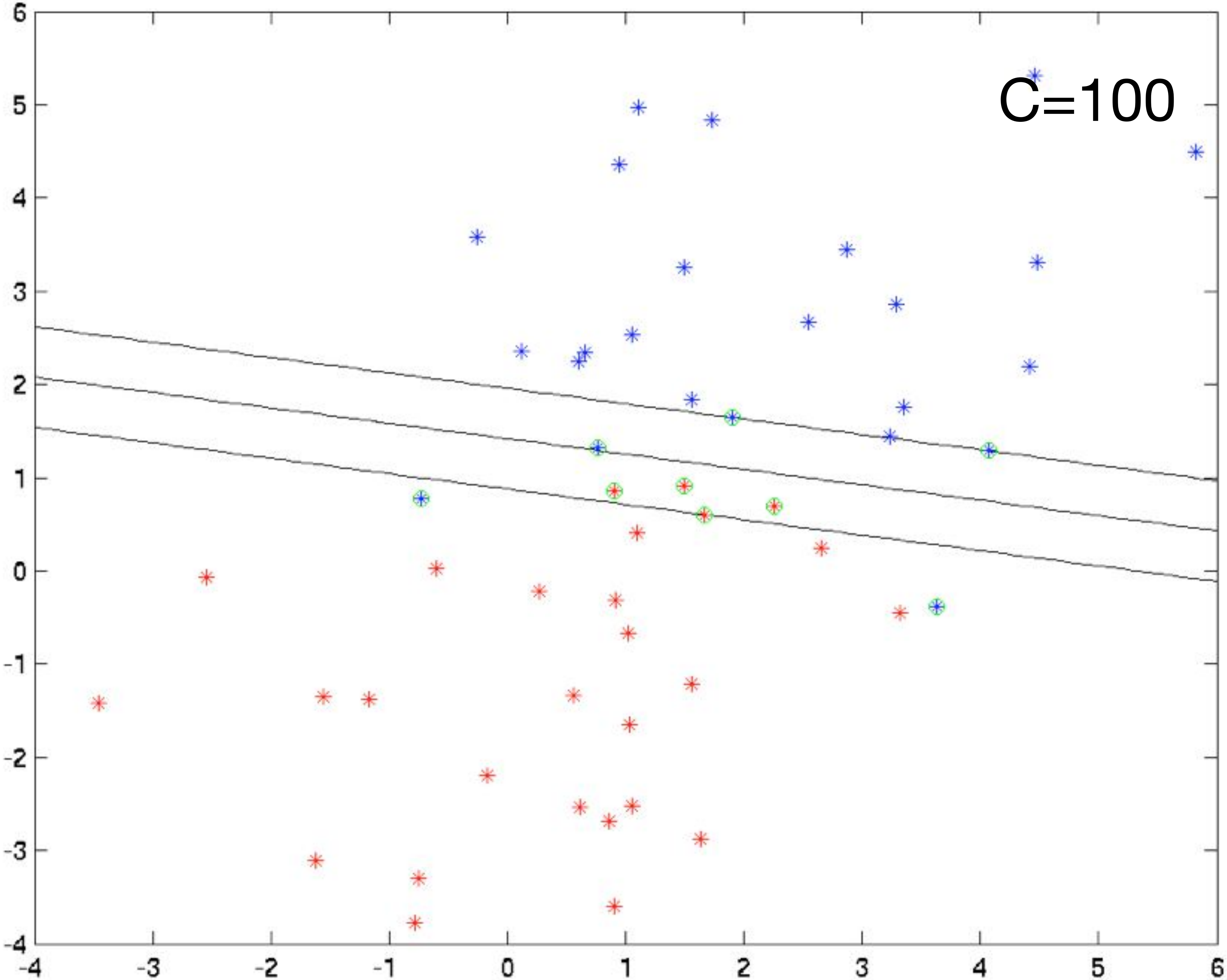

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Solving the optimization problem

- 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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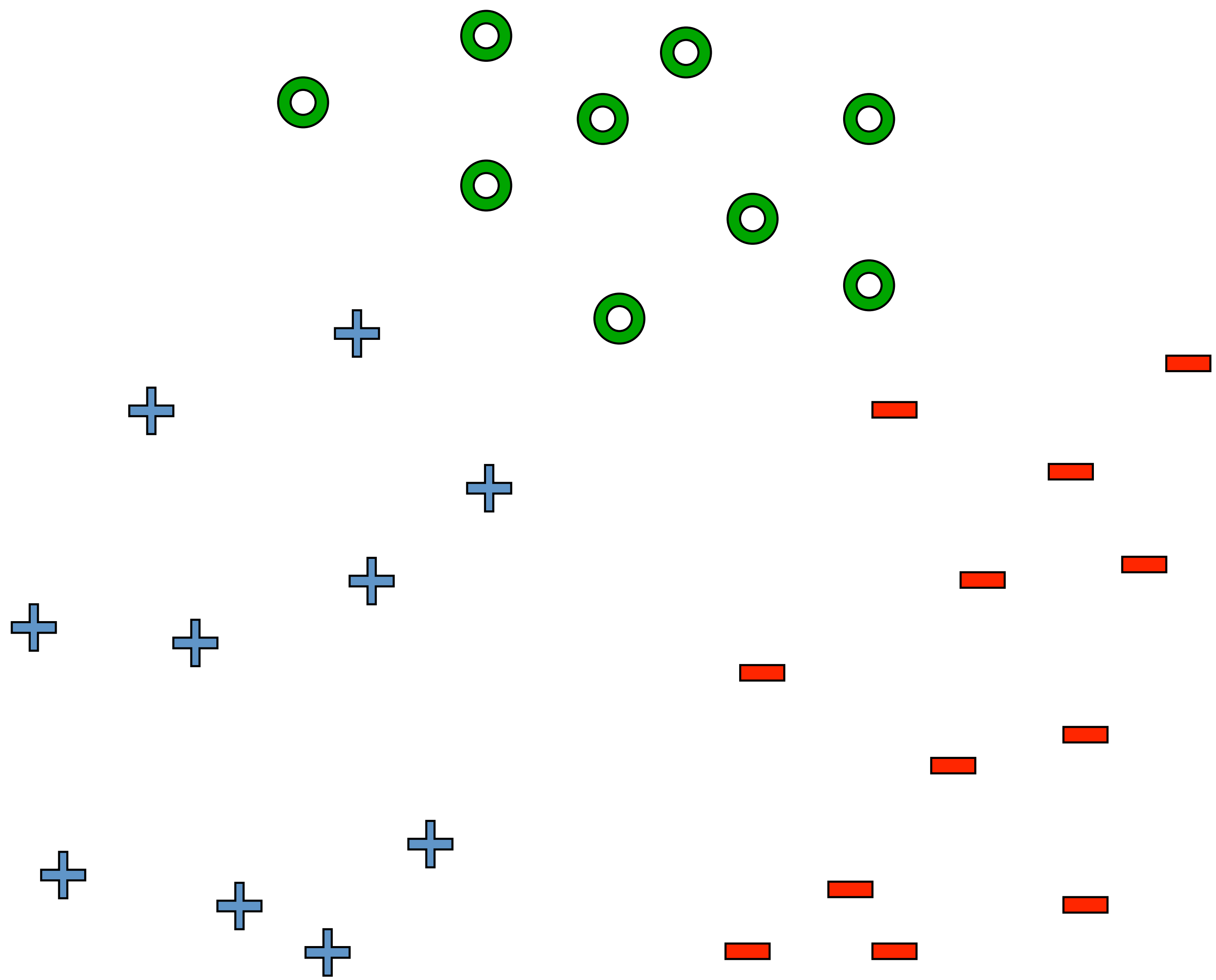
Multi-class classification



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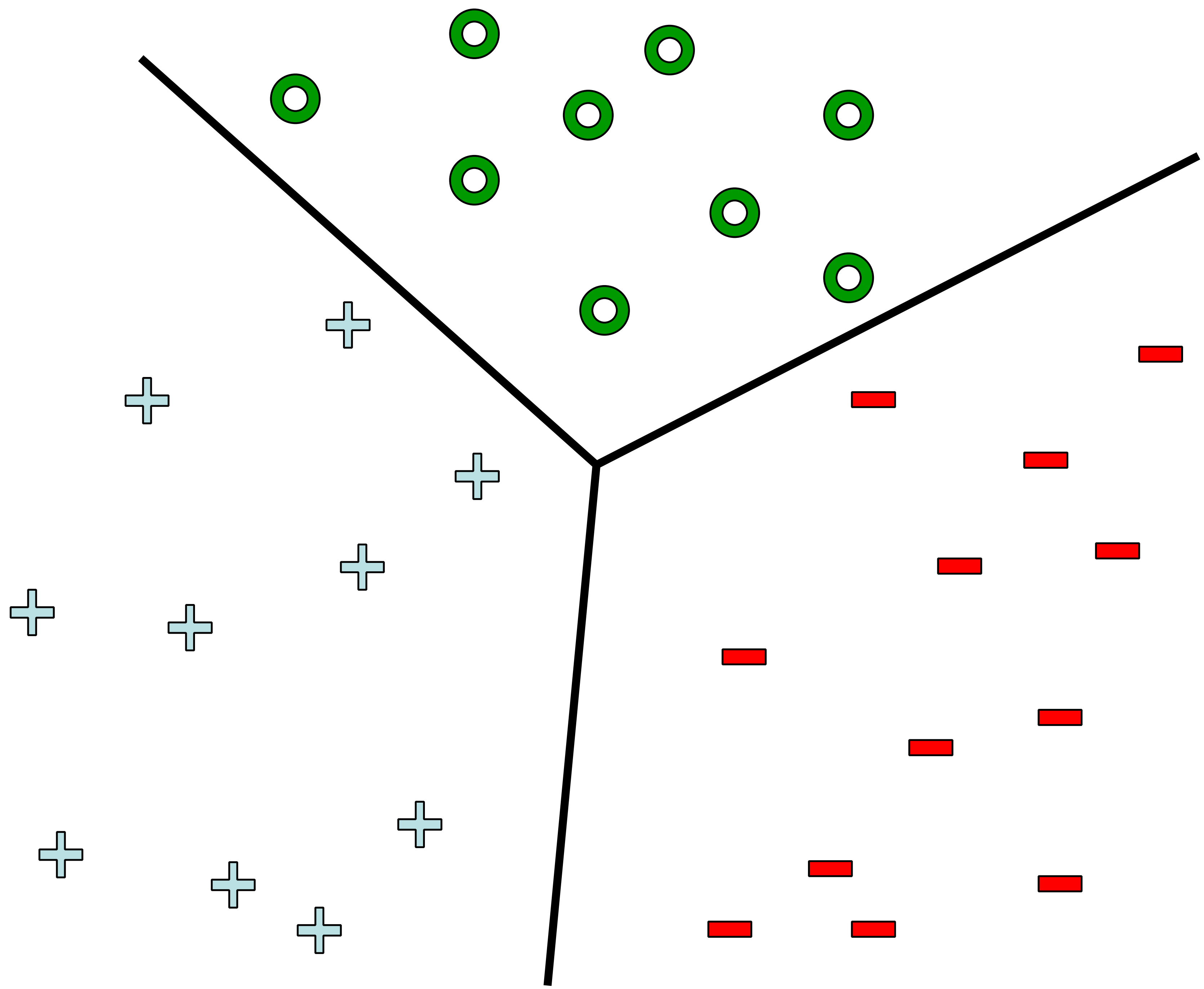
Multi-class classification



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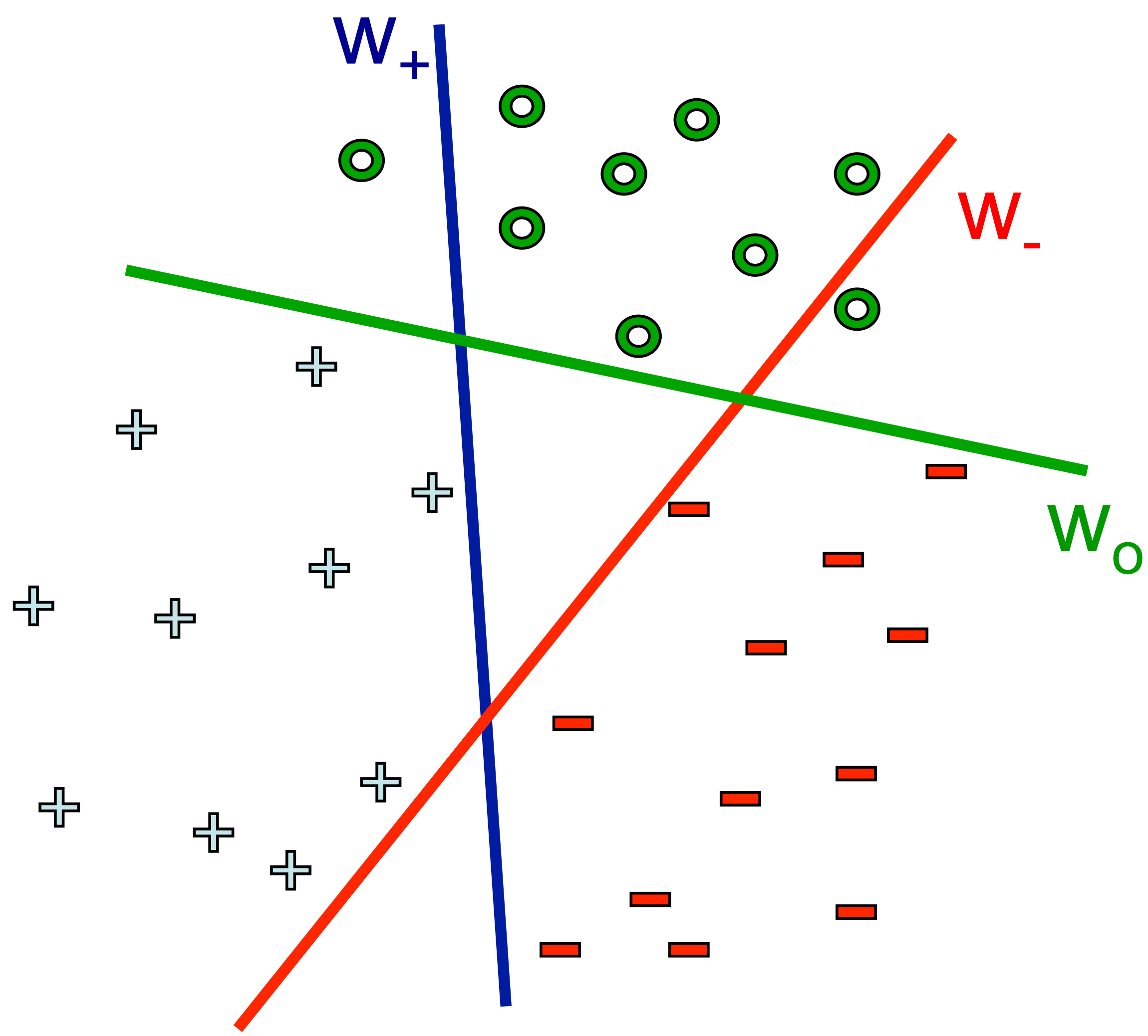
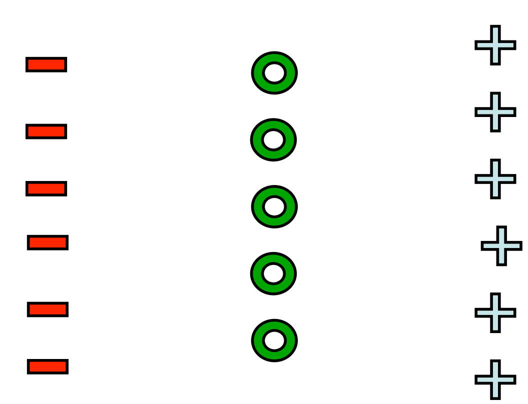
One versus all classification



- 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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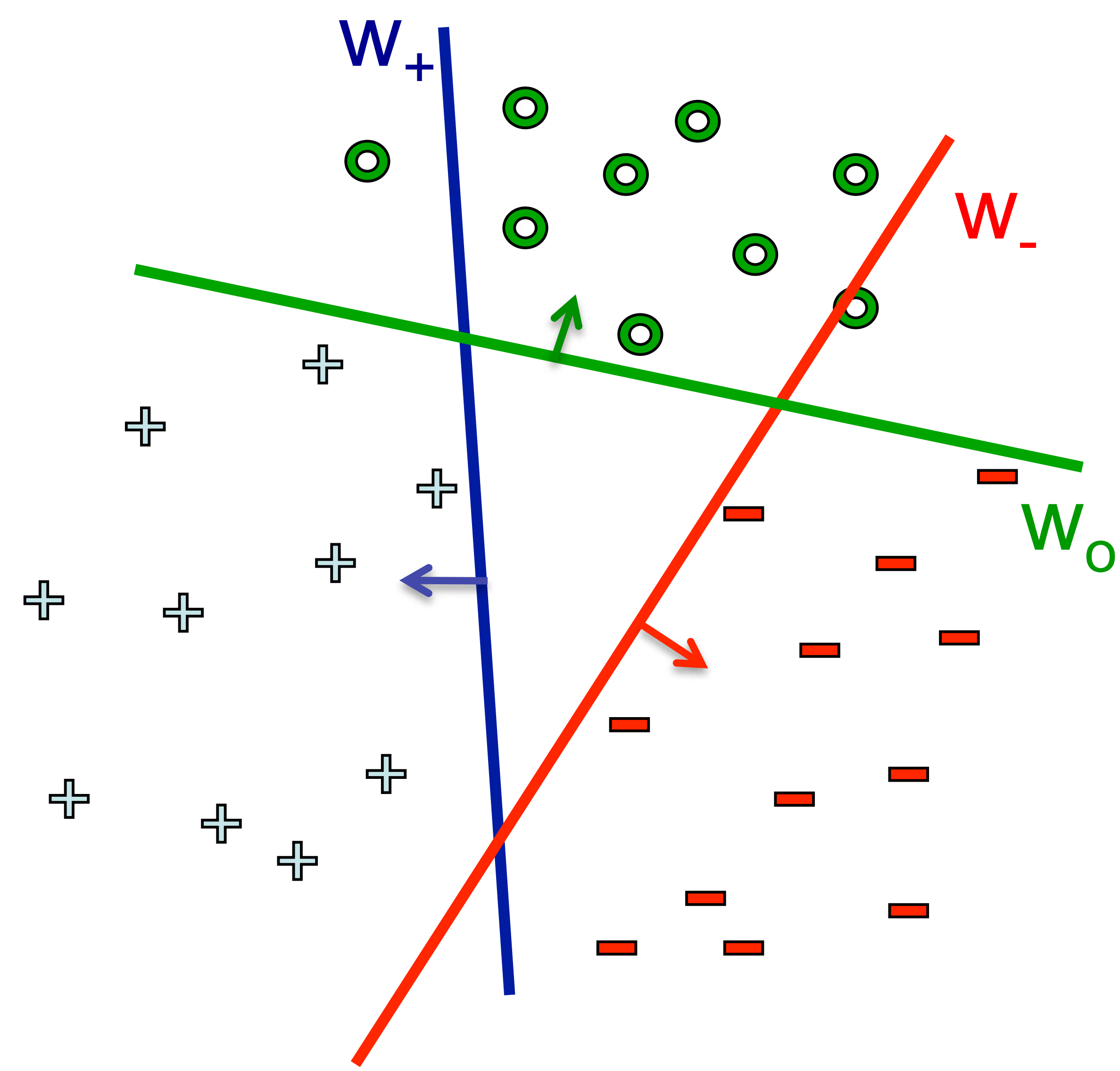
Multi-class SVM

- 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

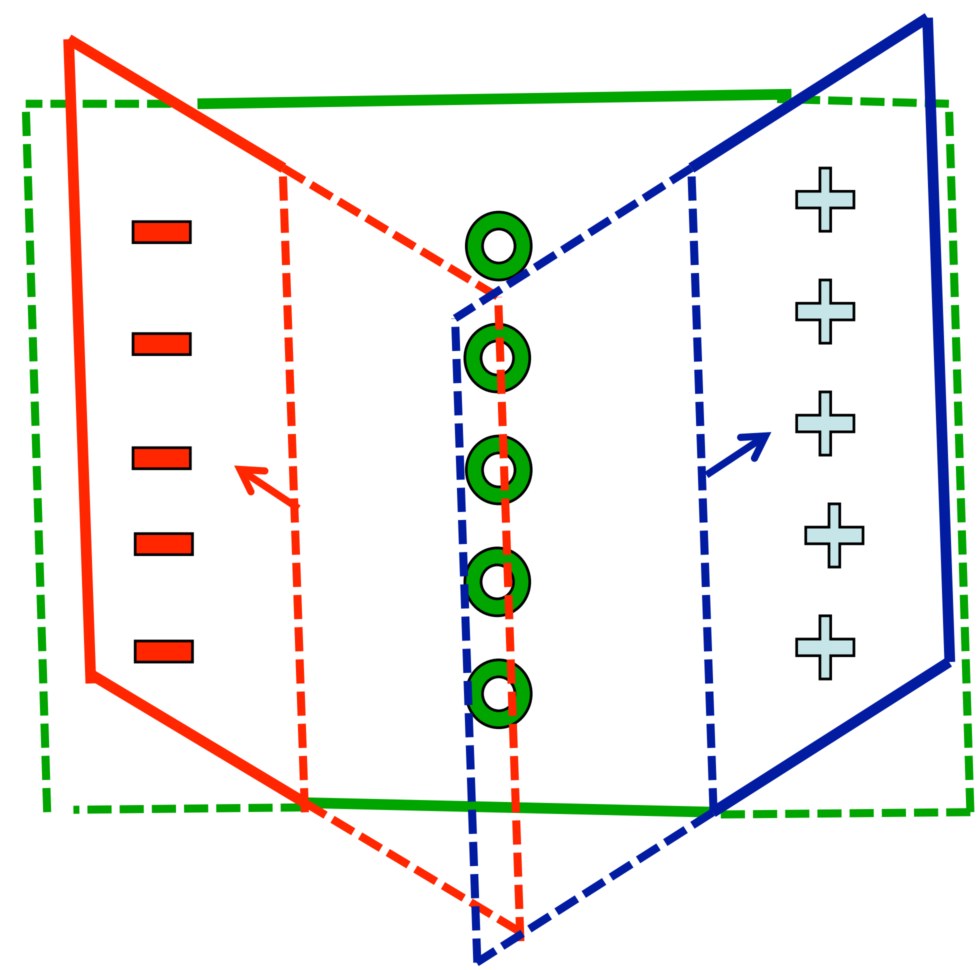
- As for the SVM, we introduce slack variables and maximize margin:

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

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

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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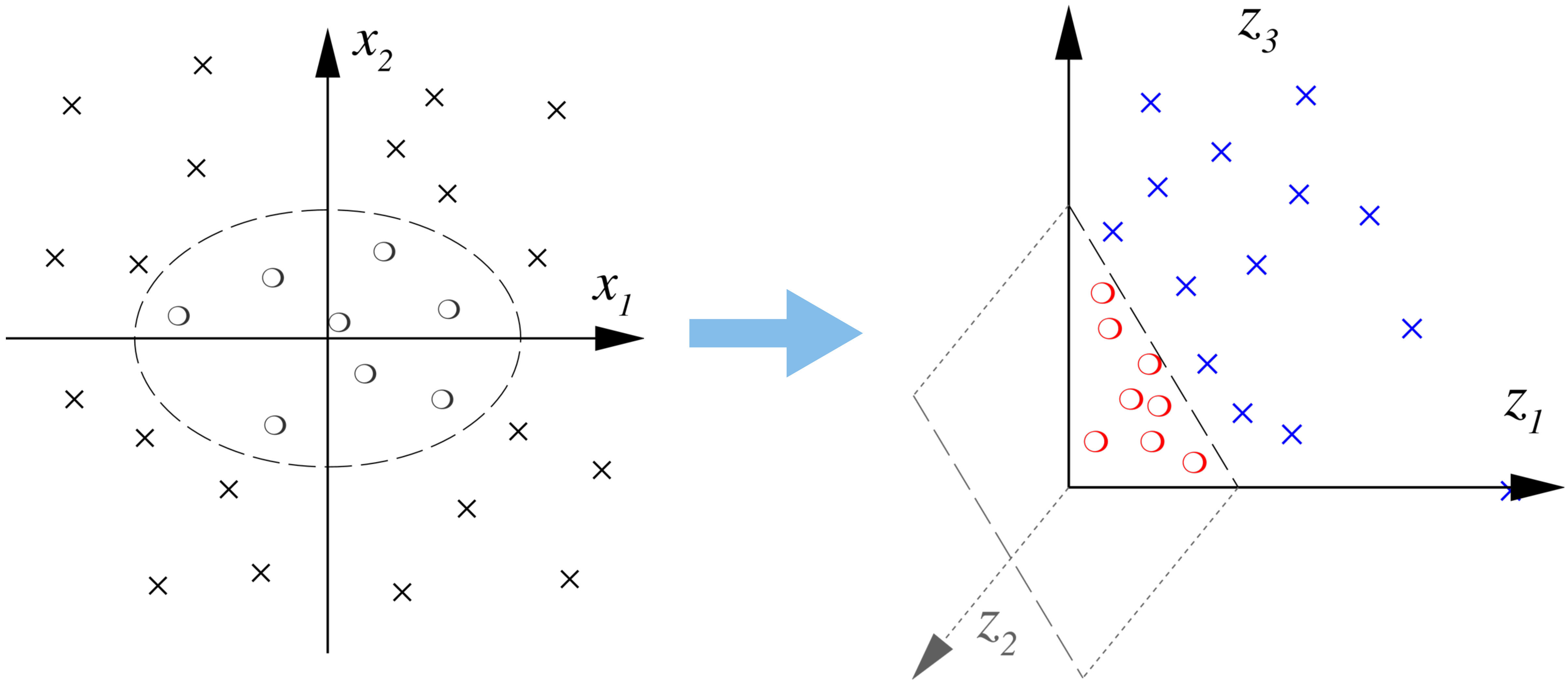
Non-linear features



- Separating surfaces are
  Circles, hyperbolae, parabolae

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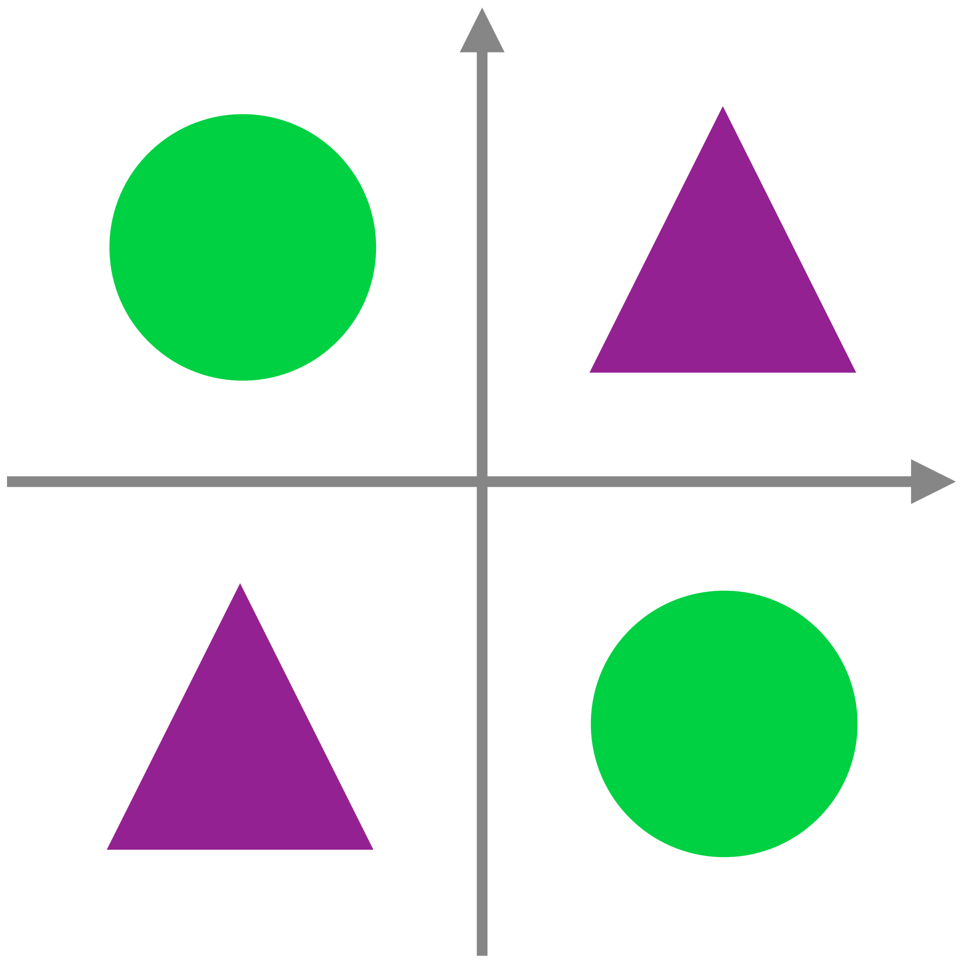
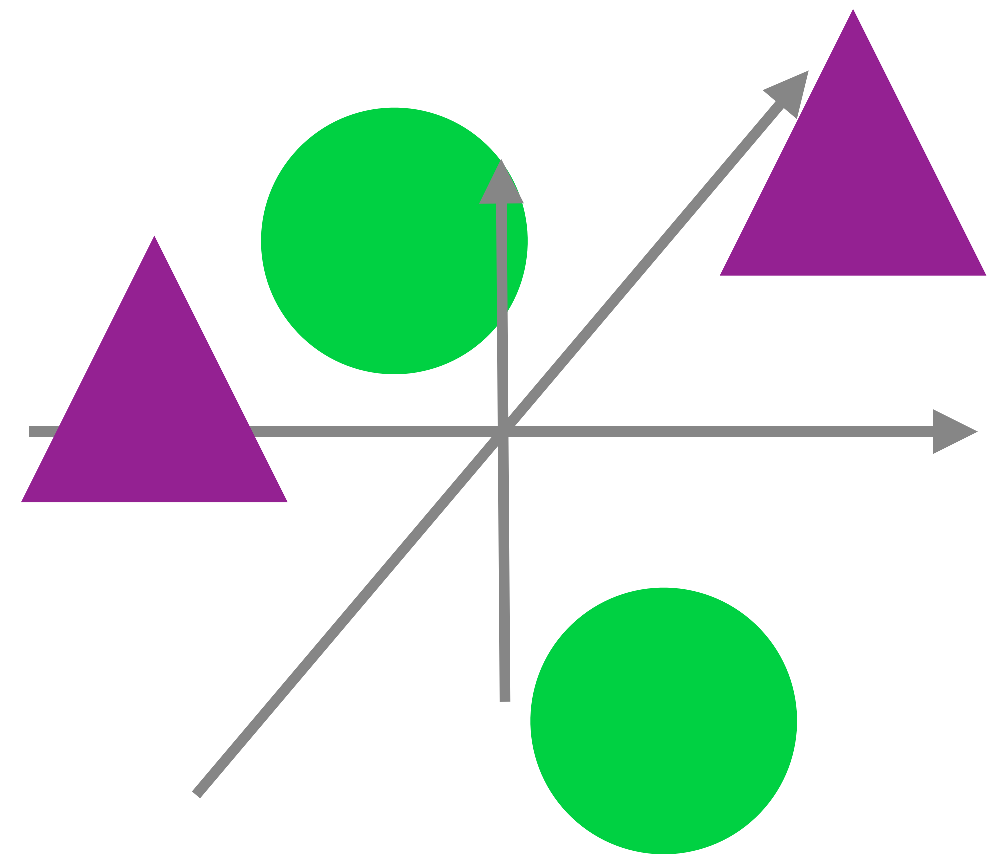
Solving XOR



(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 $\mathbb{R}^2$

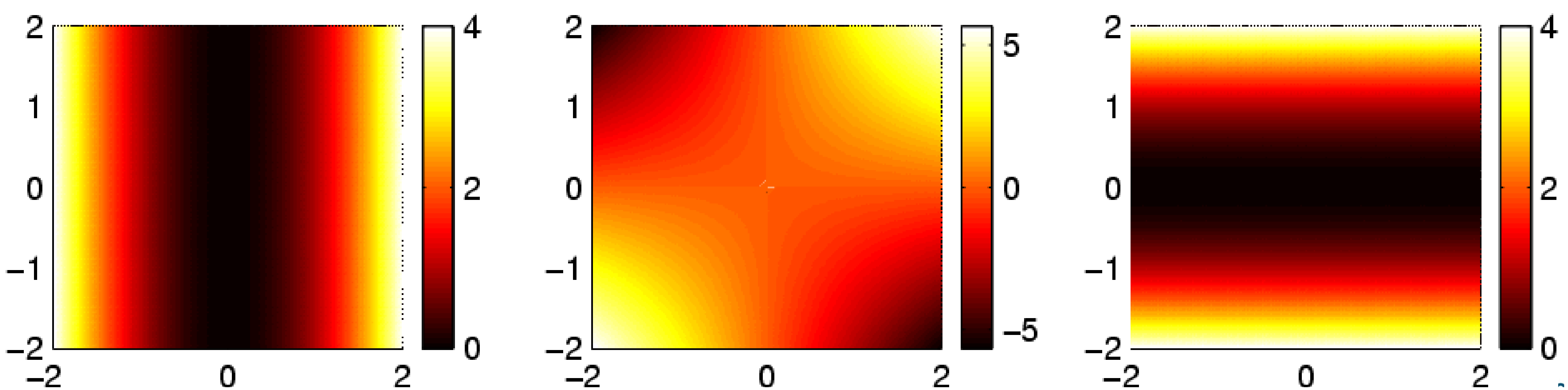
$$\Phi(x) := \left(x_1^2, \sqrt{2}x_1x_2, x_2^2\right)$$

Dot Product

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

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

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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

$$\begin{aligned} w' &= w + y_i \Phi(x_i) \\ b' &= b + y_i \end{aligned}$$

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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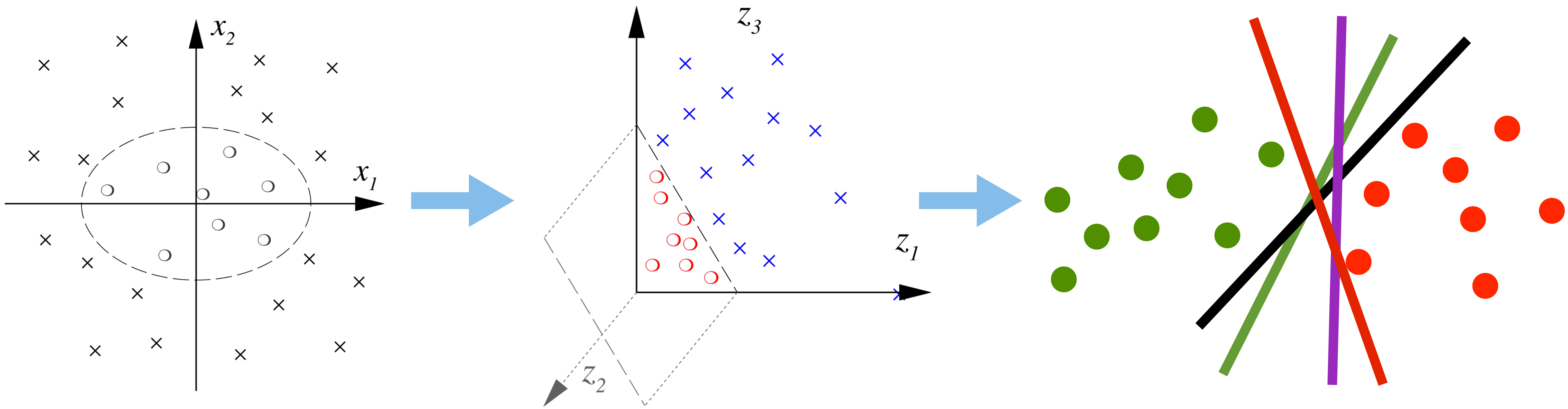
Processing Pipeline



- 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 Φ 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:

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

Kernel Expansion

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

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

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Examples

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

Linear	$\langle x, x' \rangle$
Laplacian RBF	$\exp\left(-\lambda \|x - x'\|\right)$
Gaussian RBF	$\exp\left(-\lambda \|x - x'\|^2\right)$
Polynomial	$(\langle x, x' \rangle + c \rangle)^d,\ c \geq 0,\ d \in \mathbb{N}$
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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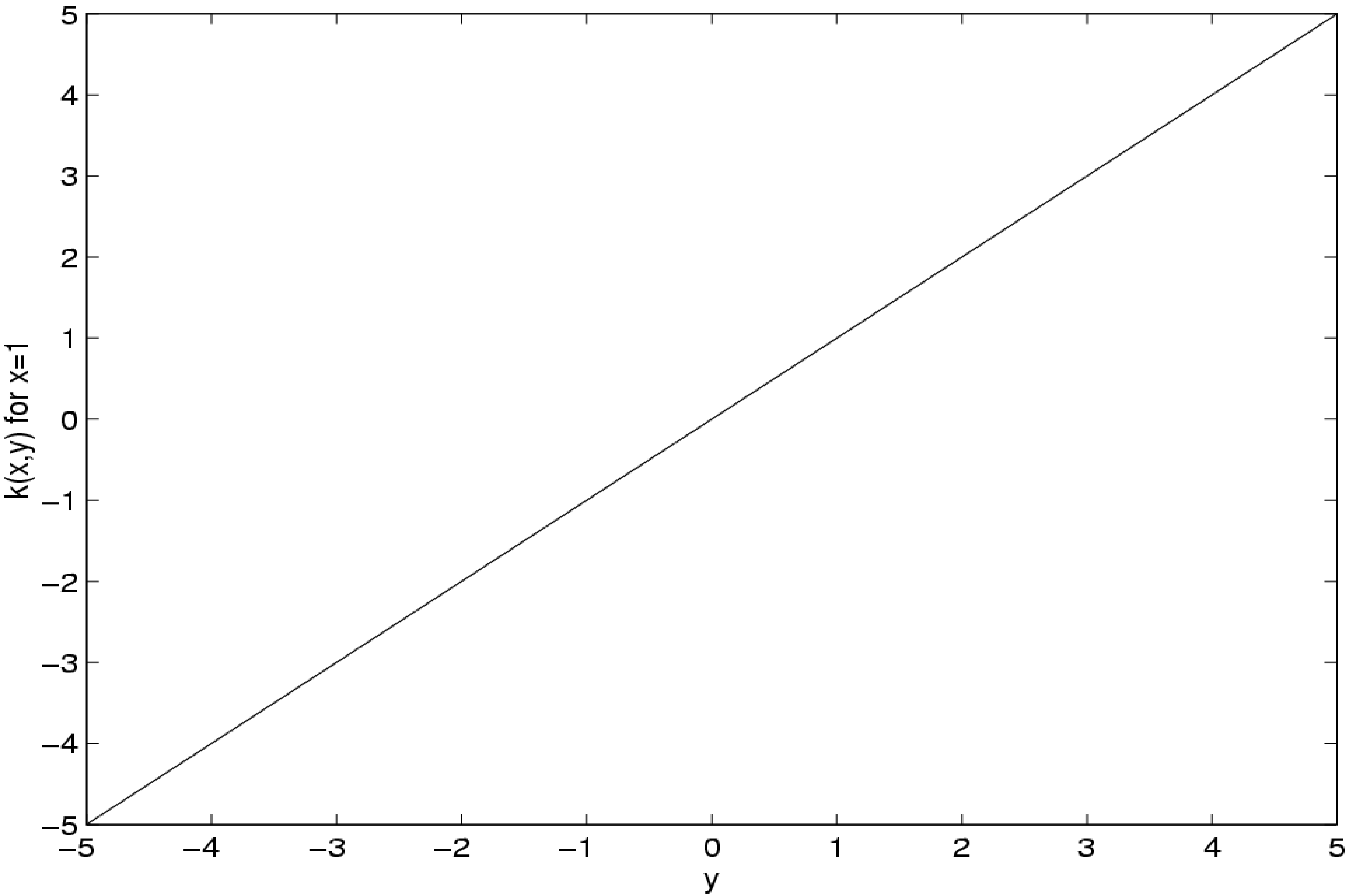
Linear Kernel



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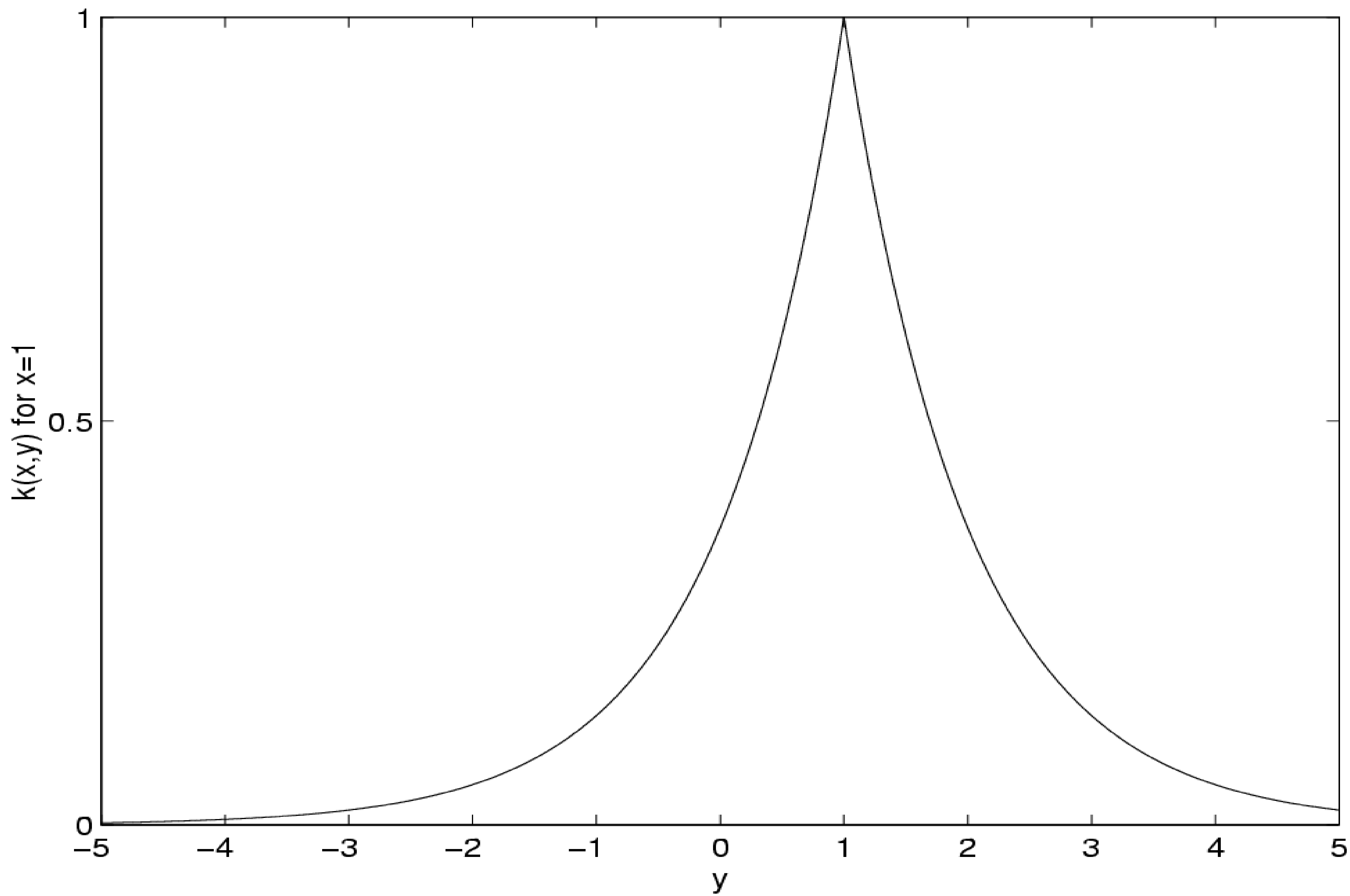
Laplacian Kernel



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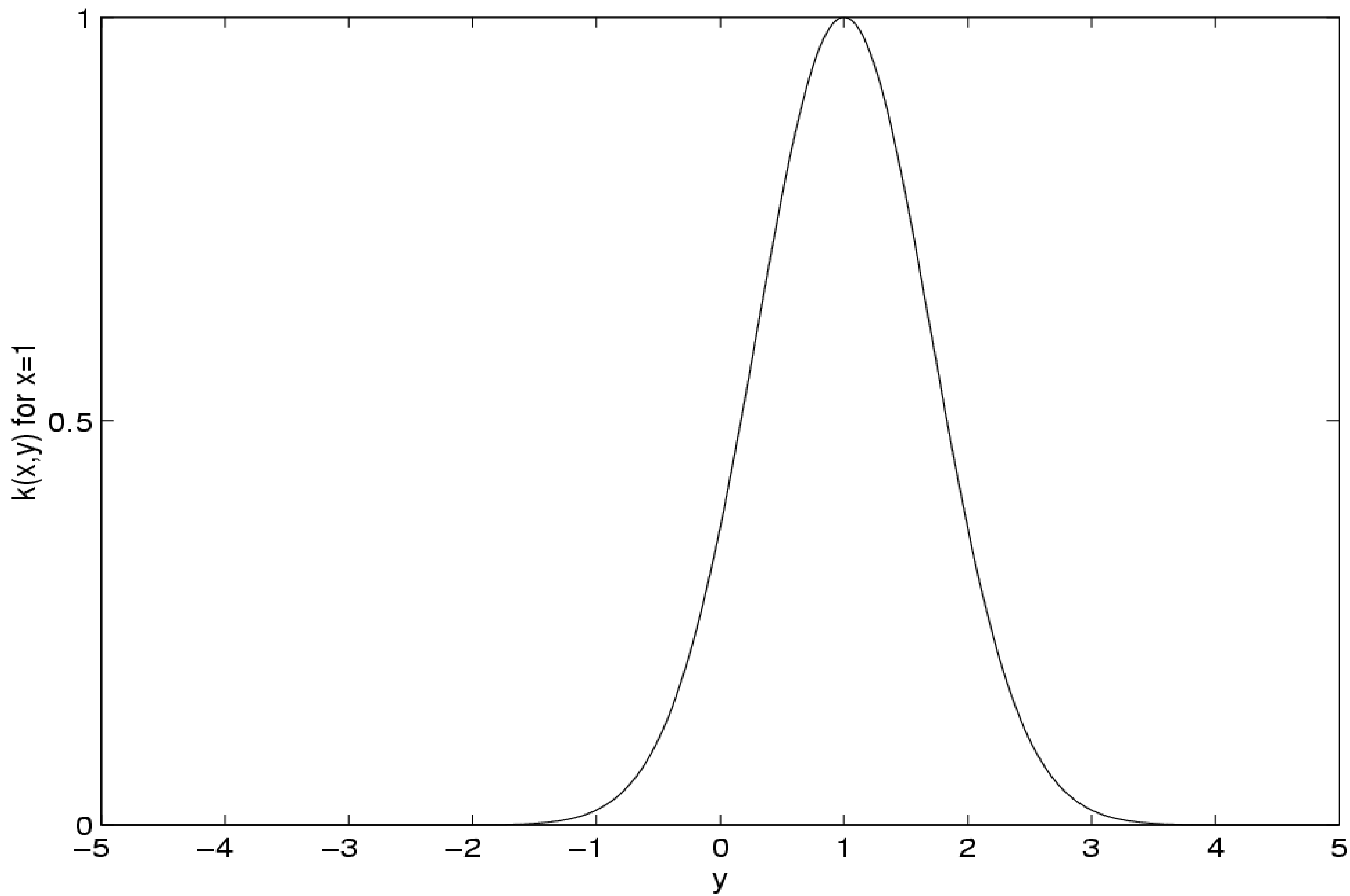
Gaussian Kernel



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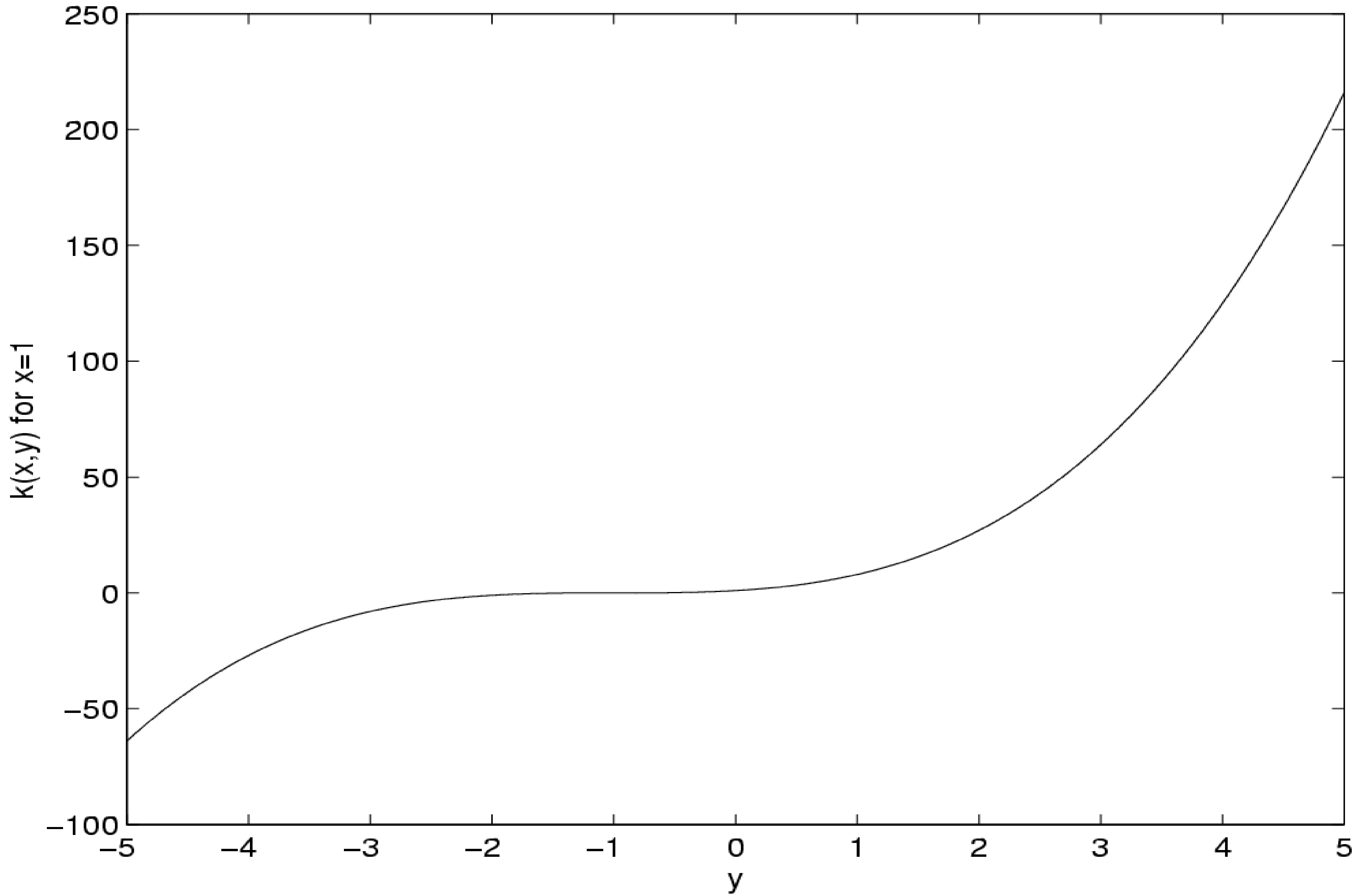
Polynomial of order 3



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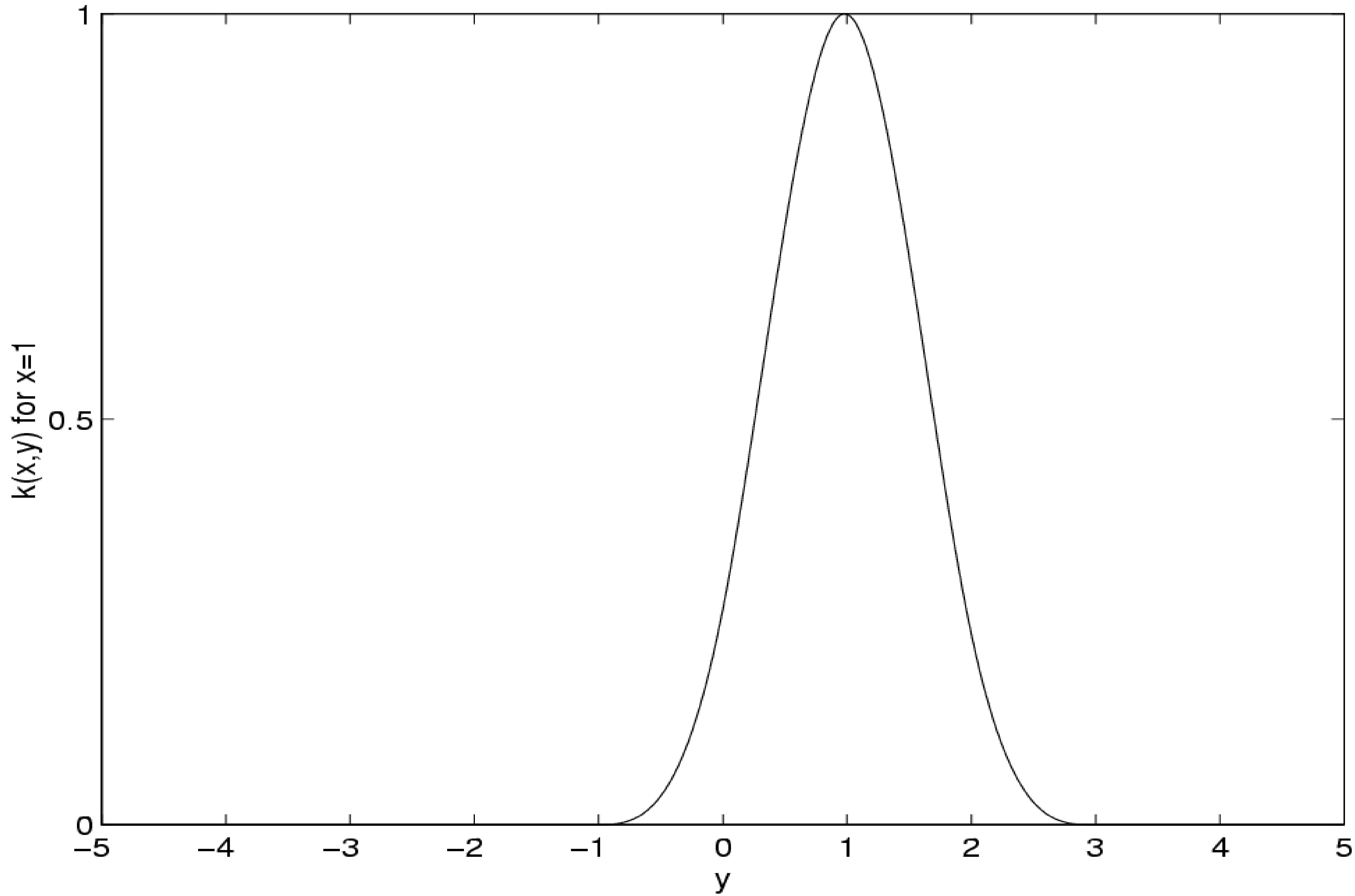
B_3 Spline Kernel



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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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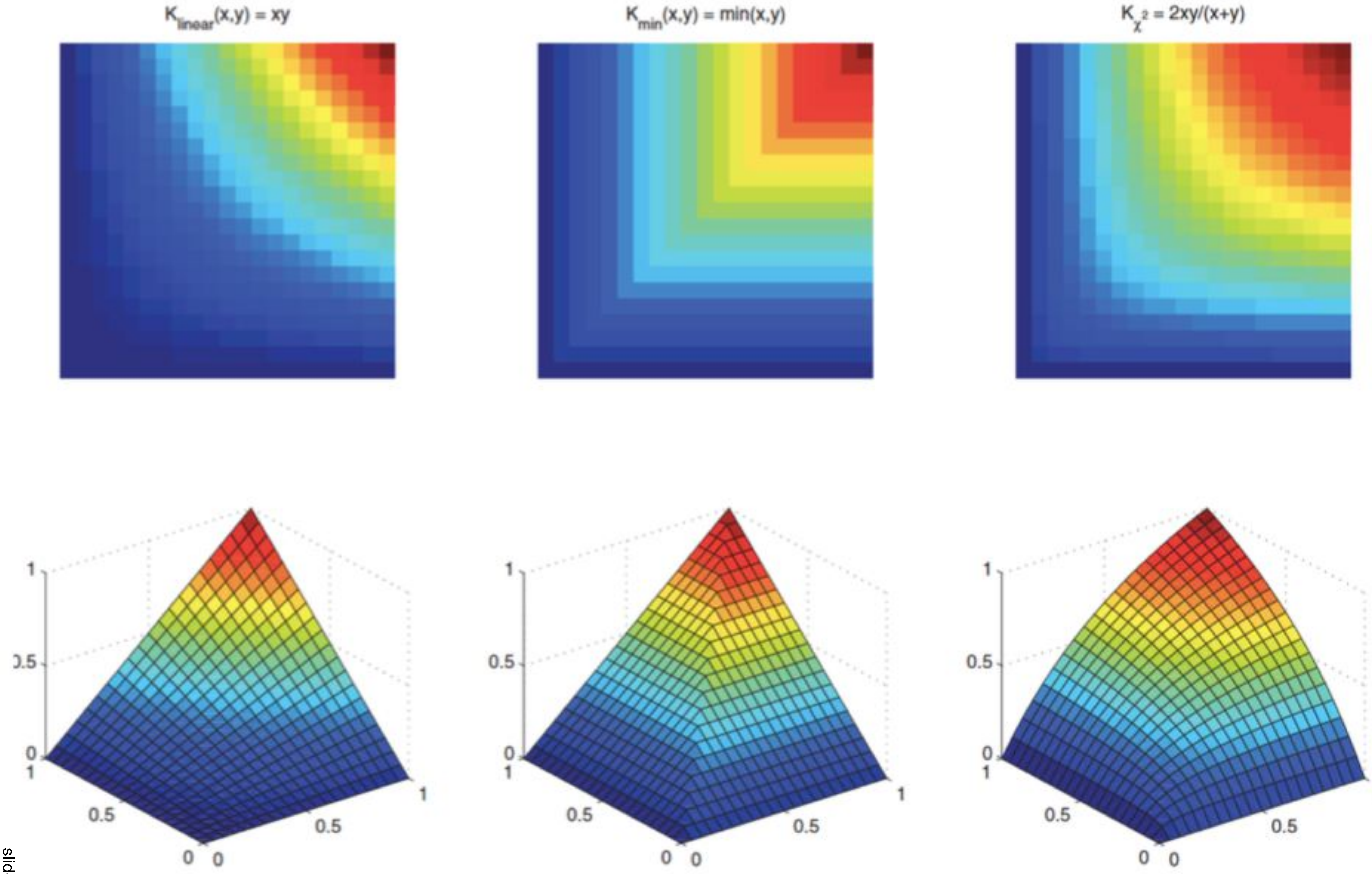

Image credit: Subhransu Maji

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Next Lecture:

Kernel Trick for SVMs,
Support Vector Regression