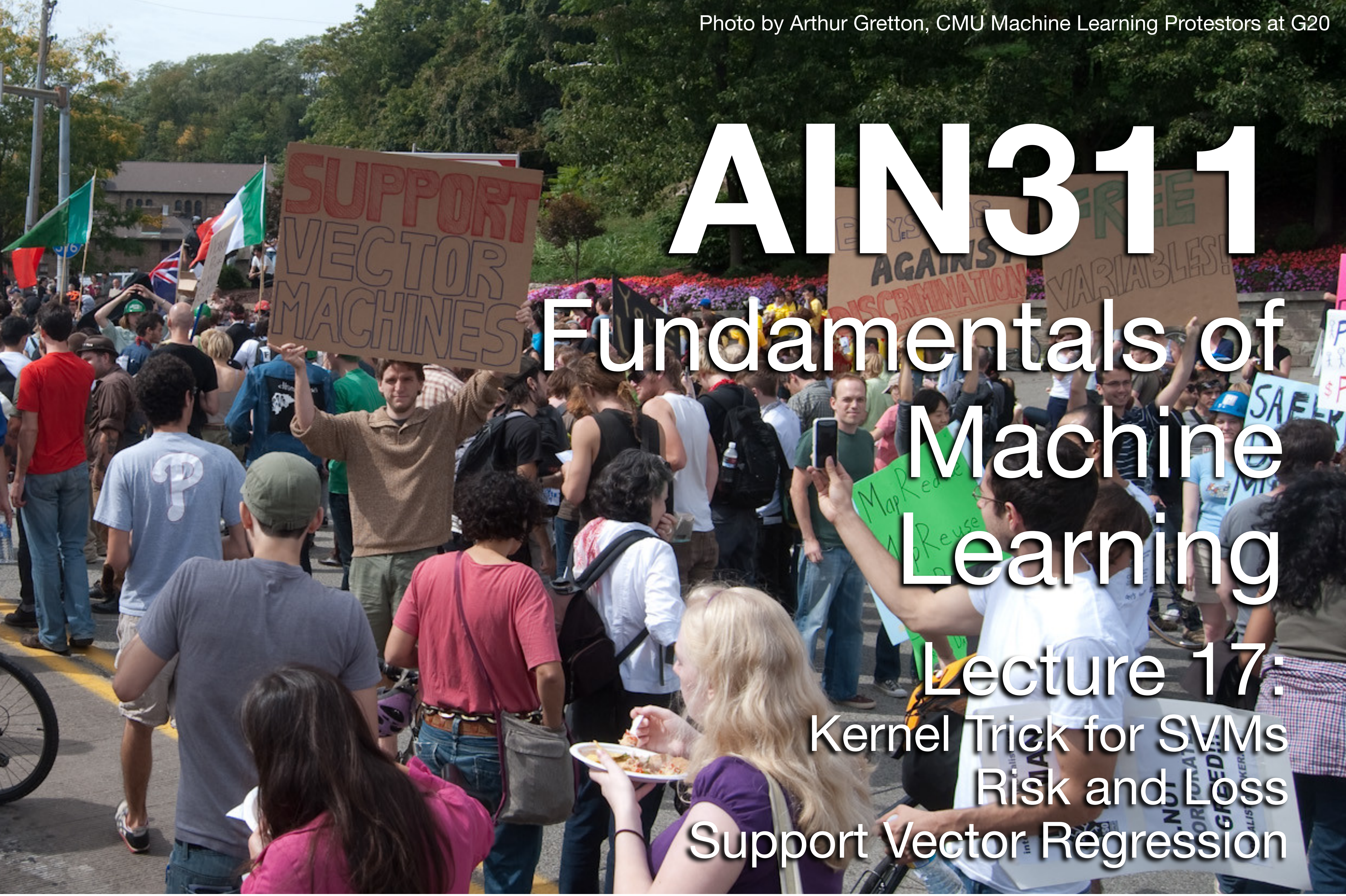


Photo by Arthur Gretton, CMU Machine Learning Protestors at G20

AIN311 Fundamentals of Machine Learning

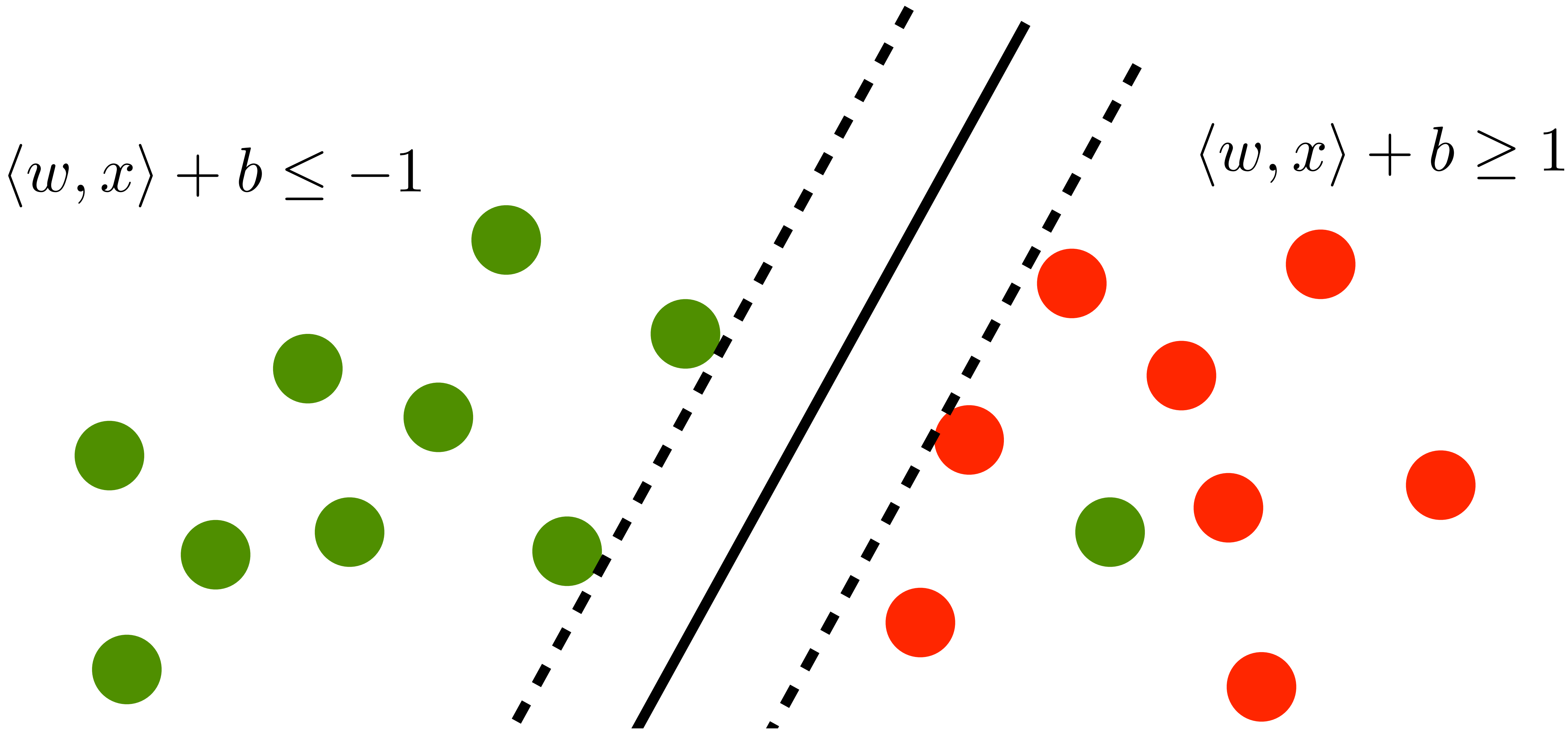
Lecture 17:

Kernel Trick for SVMs
Risk and Loss
Support Vector Regression

HACETTEPE UNIVERSITY COMPUTER VISION LAB

Erkut Erdem // Hacettepe University // Fall 2021

Last time… **Soft-margin Classifier**



minimum error separator
is impossible

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

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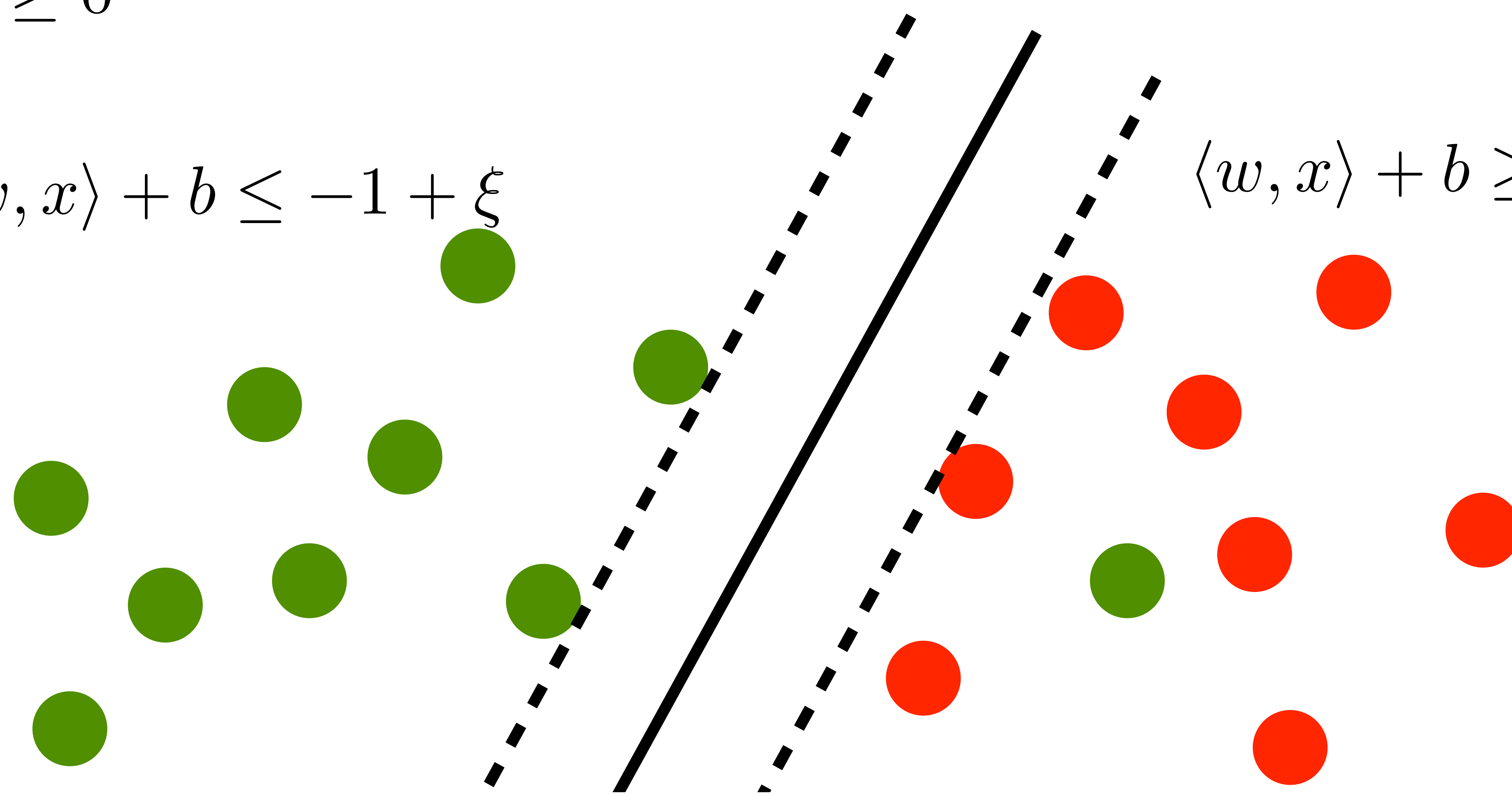
Last time... **Adding Slack Variables**

$$\xi_i \geq 0$$

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

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



minimize amount of slack

Convex optimization problem

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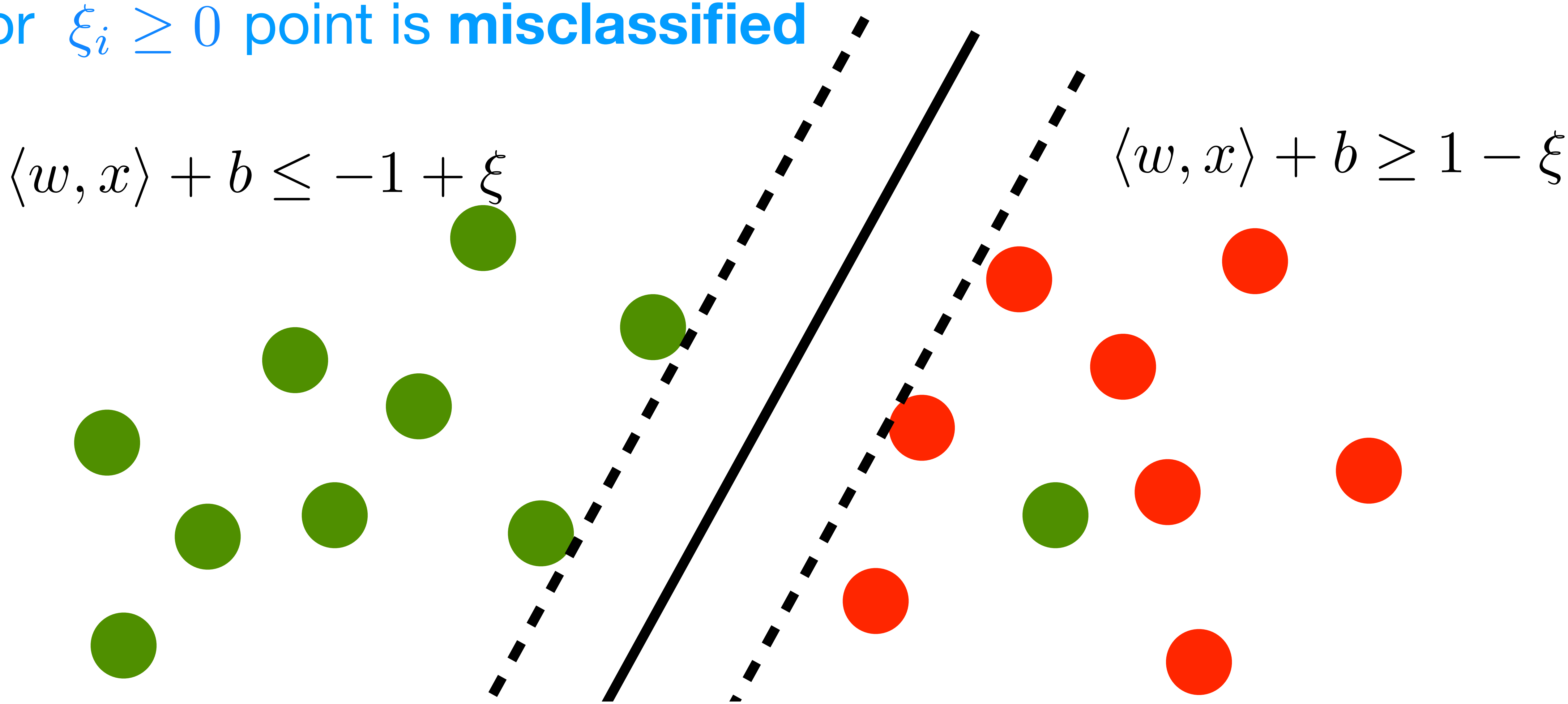
Last time... **Adding Slack Variables**

- for $0 < \xi \leq 1$ point is between the margin and **correctly classified**
- for $\xi_i \geq 0$ point is **misclassified**



minimize amount of slack

Convex optimization problem

adopted from Andrew Zisserman

Last time... **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)

slide by Alex Smola

Soft-margin classifier

- Optimization problem:

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

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

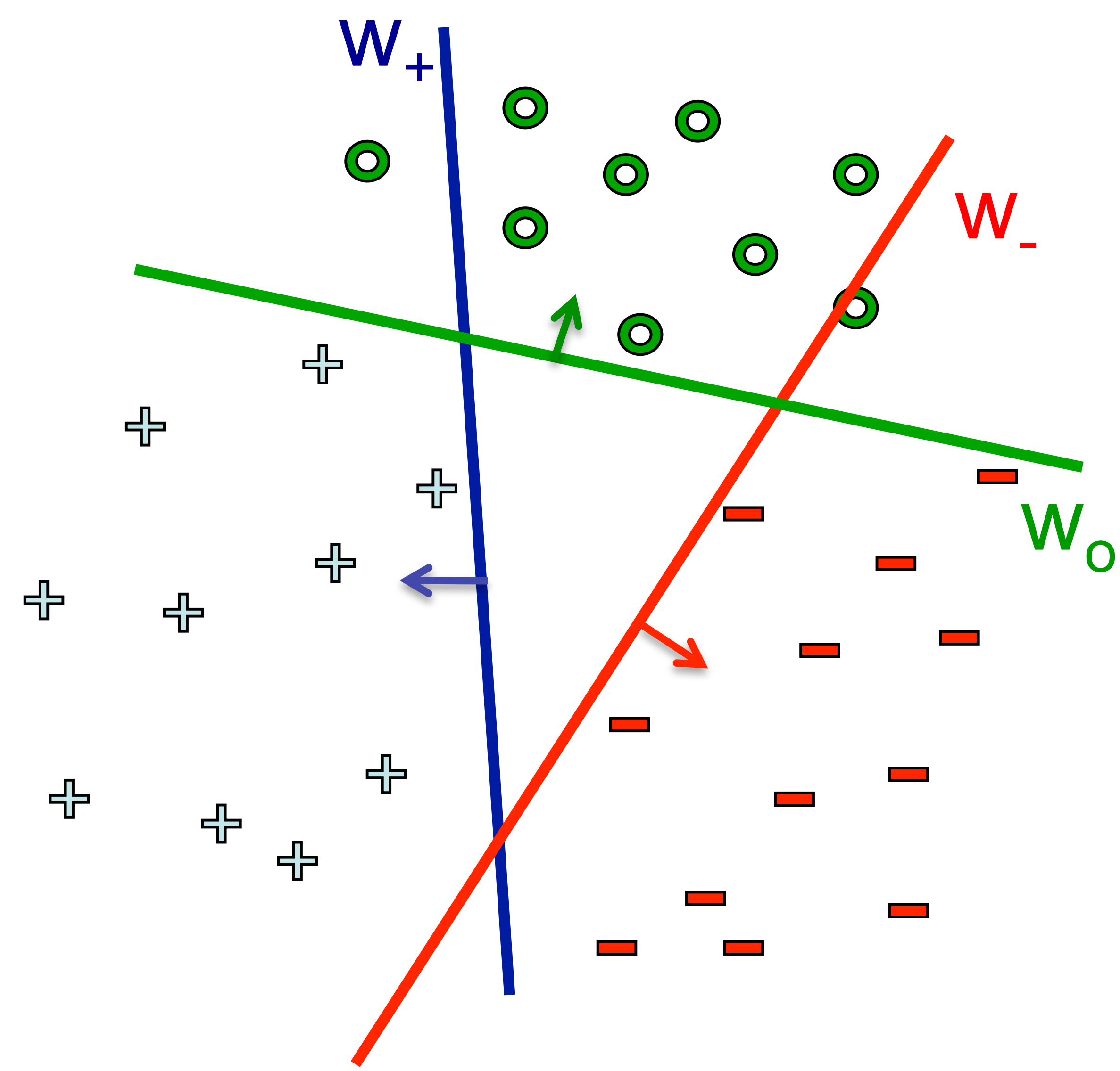
C is a **regularization** parameter:

- small C allows constraints to be easily ignored $\rightarrow$ **large margin**
- large C makes constraints hard to ignore $\rightarrow$ **narrow margin**
- $C = \infty$ enforces all constraints: **hard margin**

adopted from Andrew Zisserman

Last time… 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:

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

slide by Eric Xing

Last time… **Multi-class SVM**

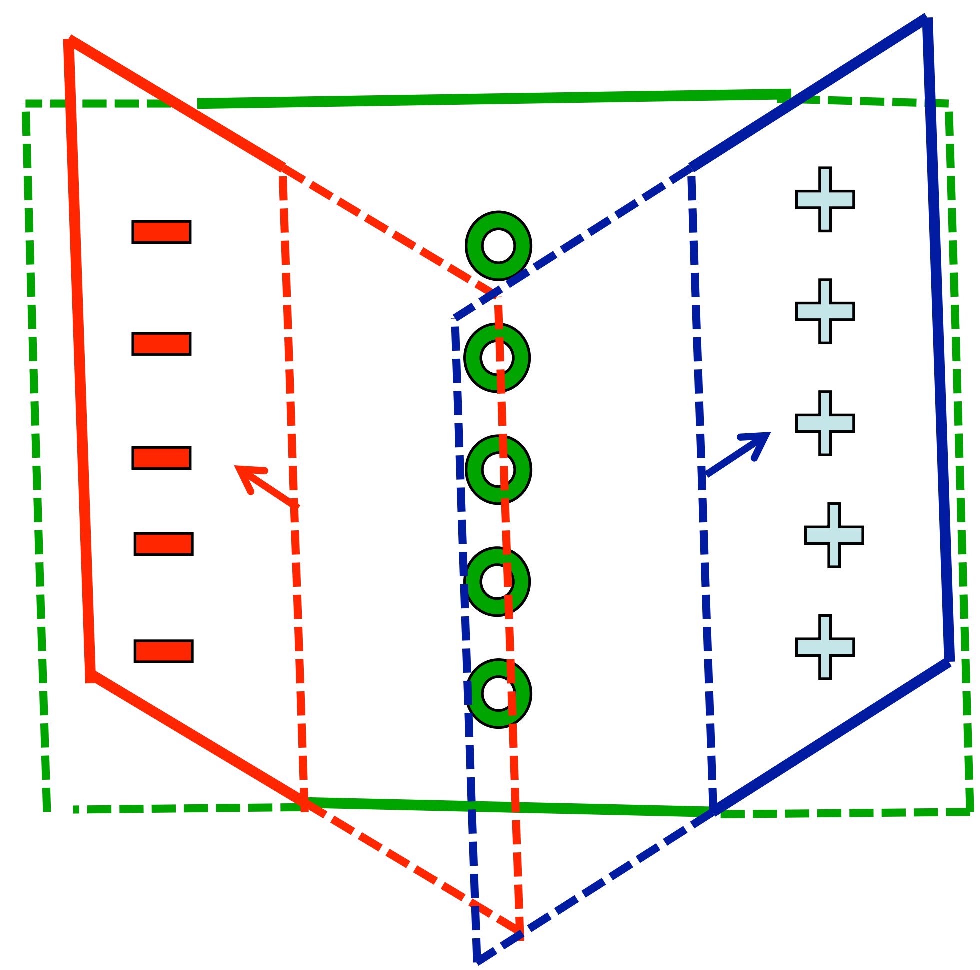
- As for the SVM, we introduce slack variables and maximize margin:

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

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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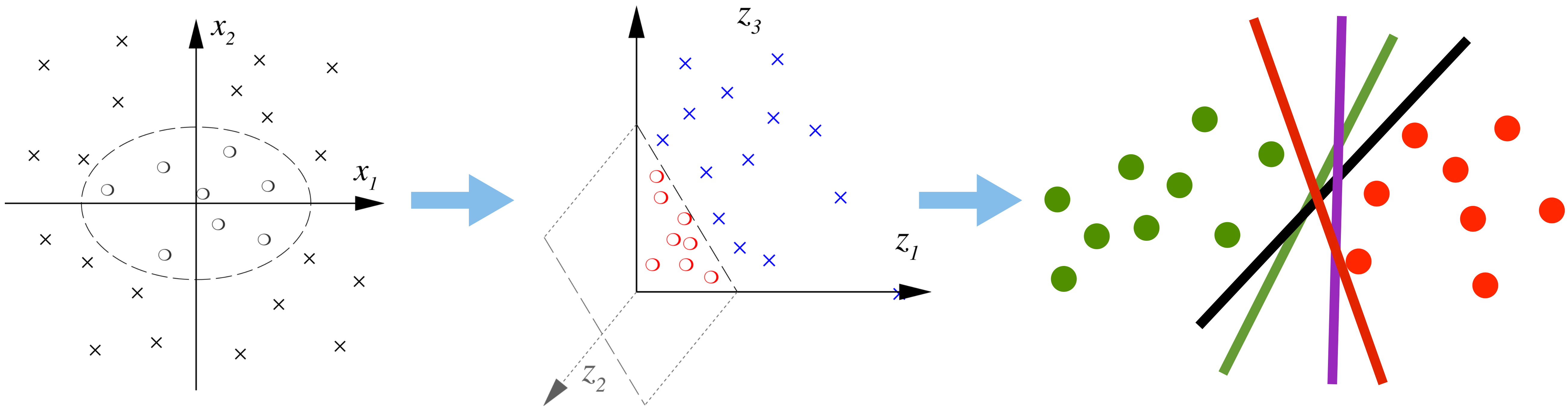
Last time… Kernels



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

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Last time… **Quadratic Features**

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

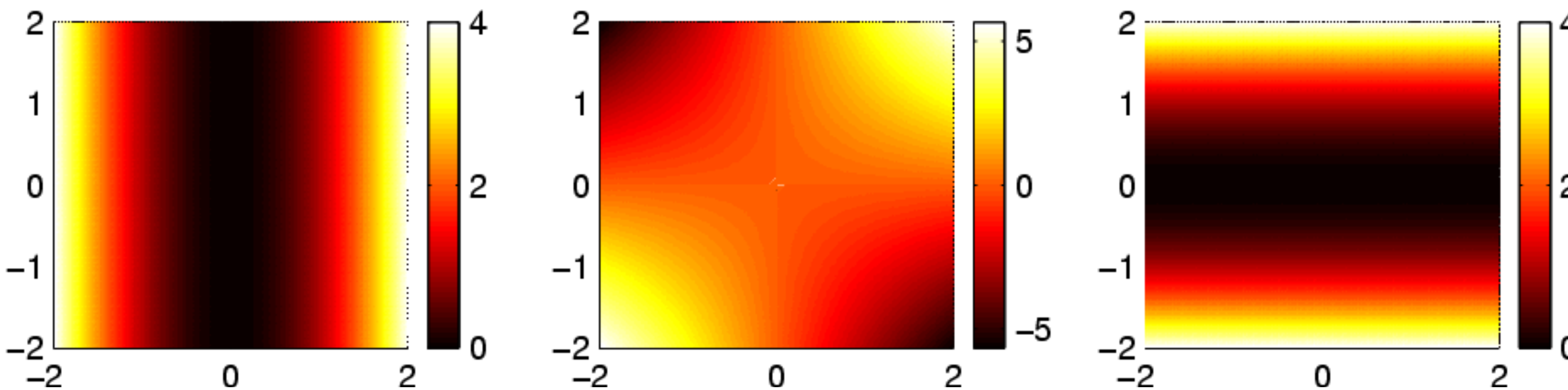
$$\Phi(x) := \left(x_1^2, \sqrt{2}x_1x_2, x_2^2\right)$$

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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Last time.. **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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Last time.. **Example kernels**

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	$\left(\langle x, x' \rangle + c \rangle\right)^d, c \geq 0, \ d \in \mathbb{N}$
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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Today

- The Kernel Trick for SVMs
- Risk and Loss
- Support Vector Regression

The Kernel Trick for SVMs

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The Kernel Trick for SVMs

- 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

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

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The Kernel Trick for SVMs

- 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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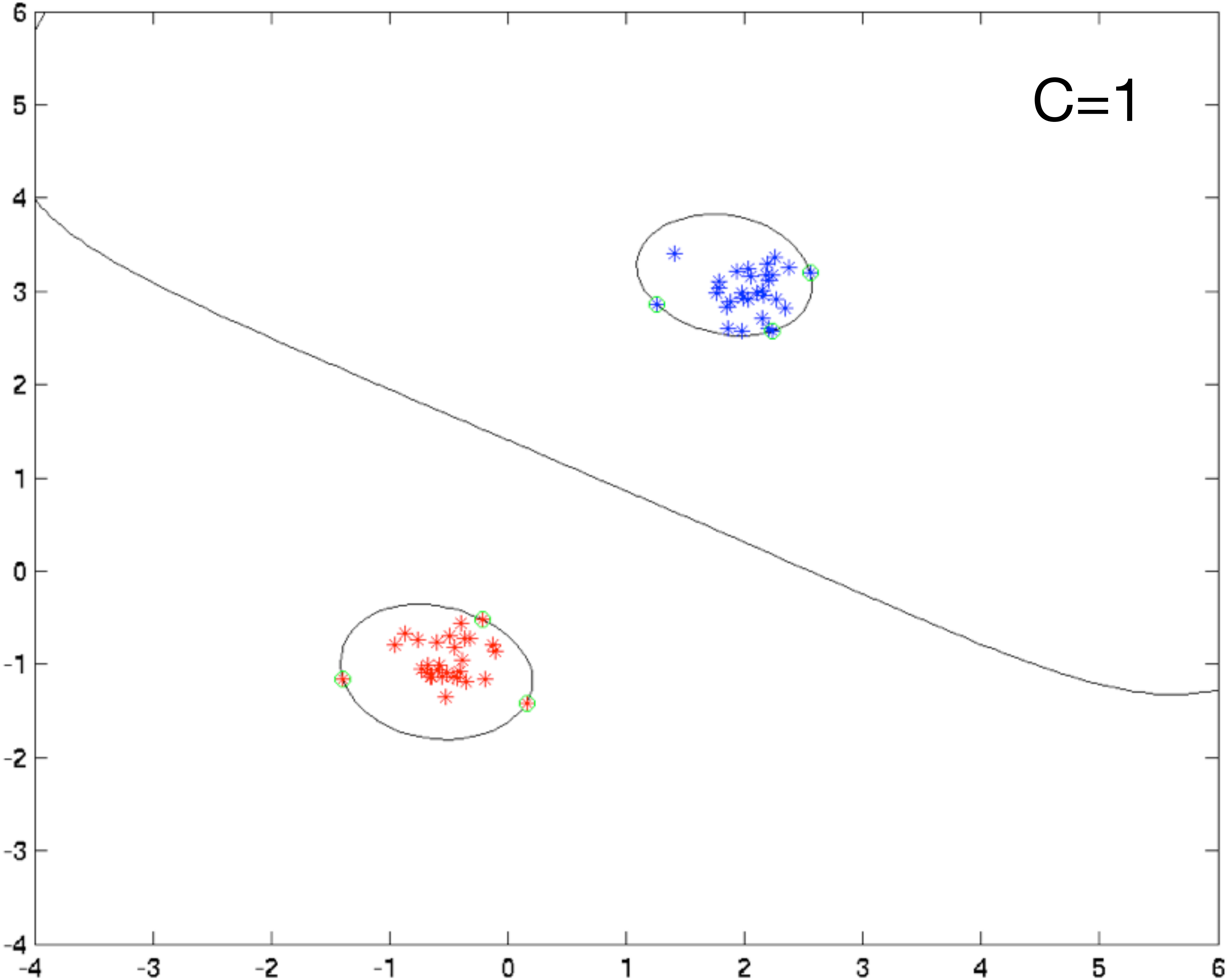

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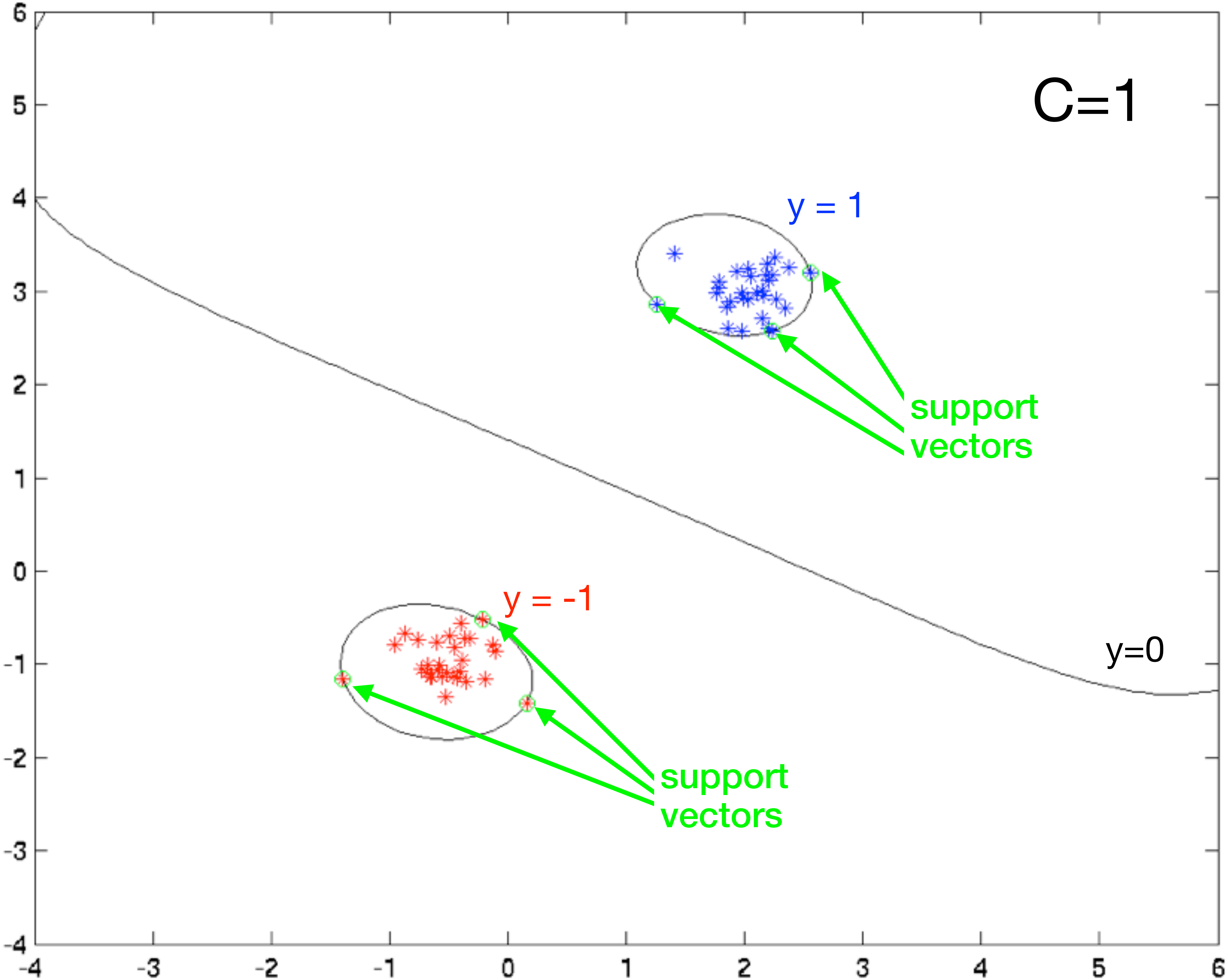

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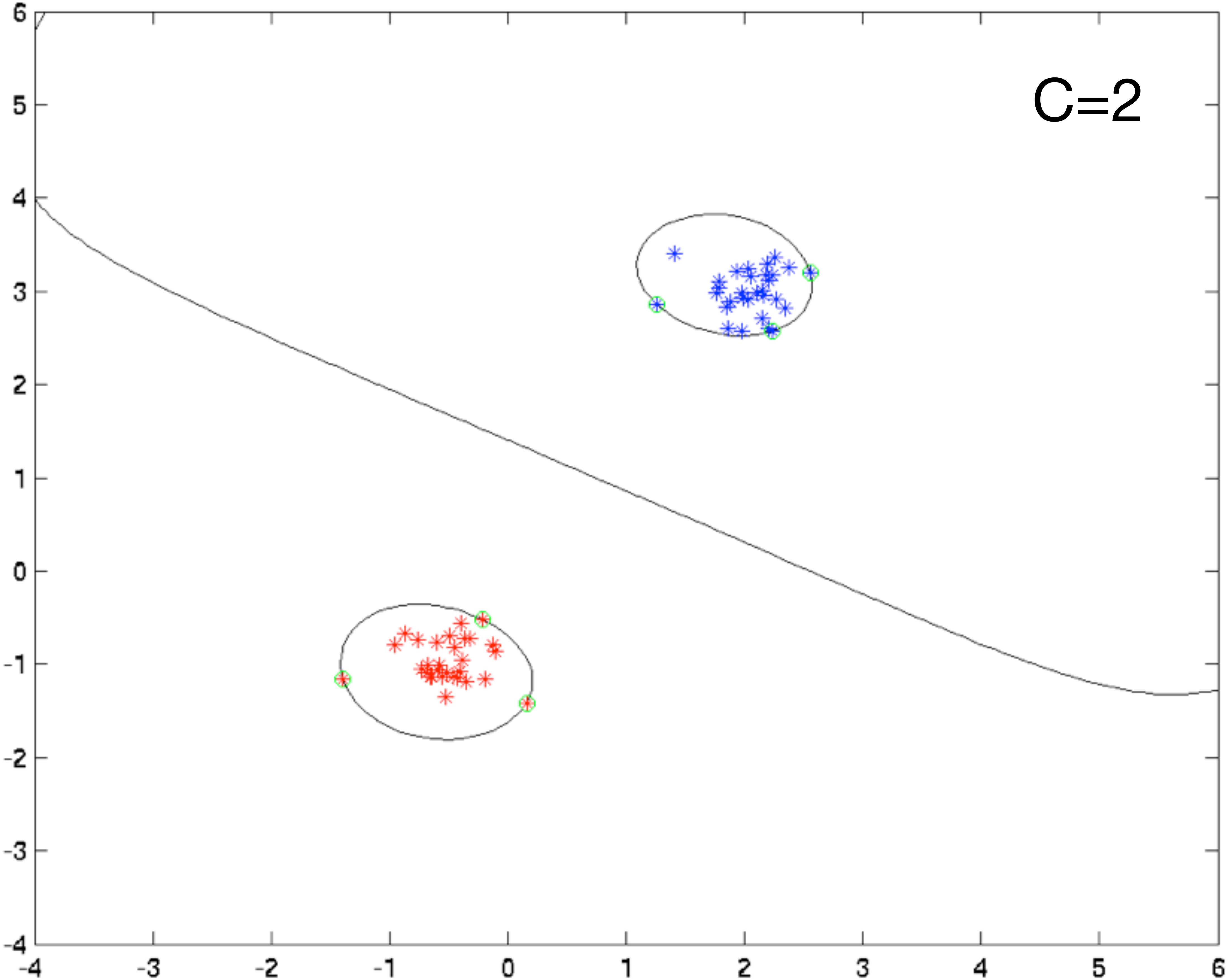

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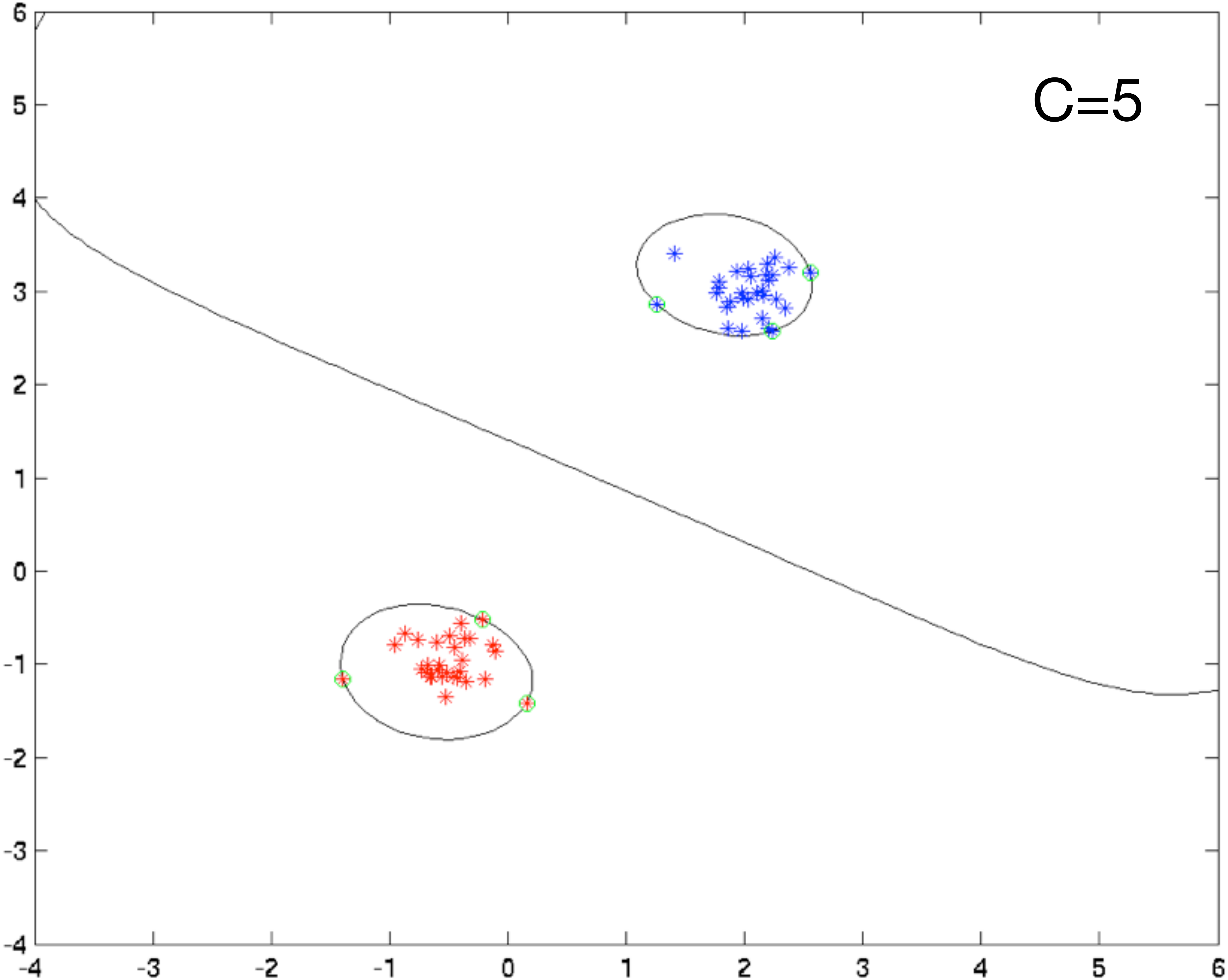

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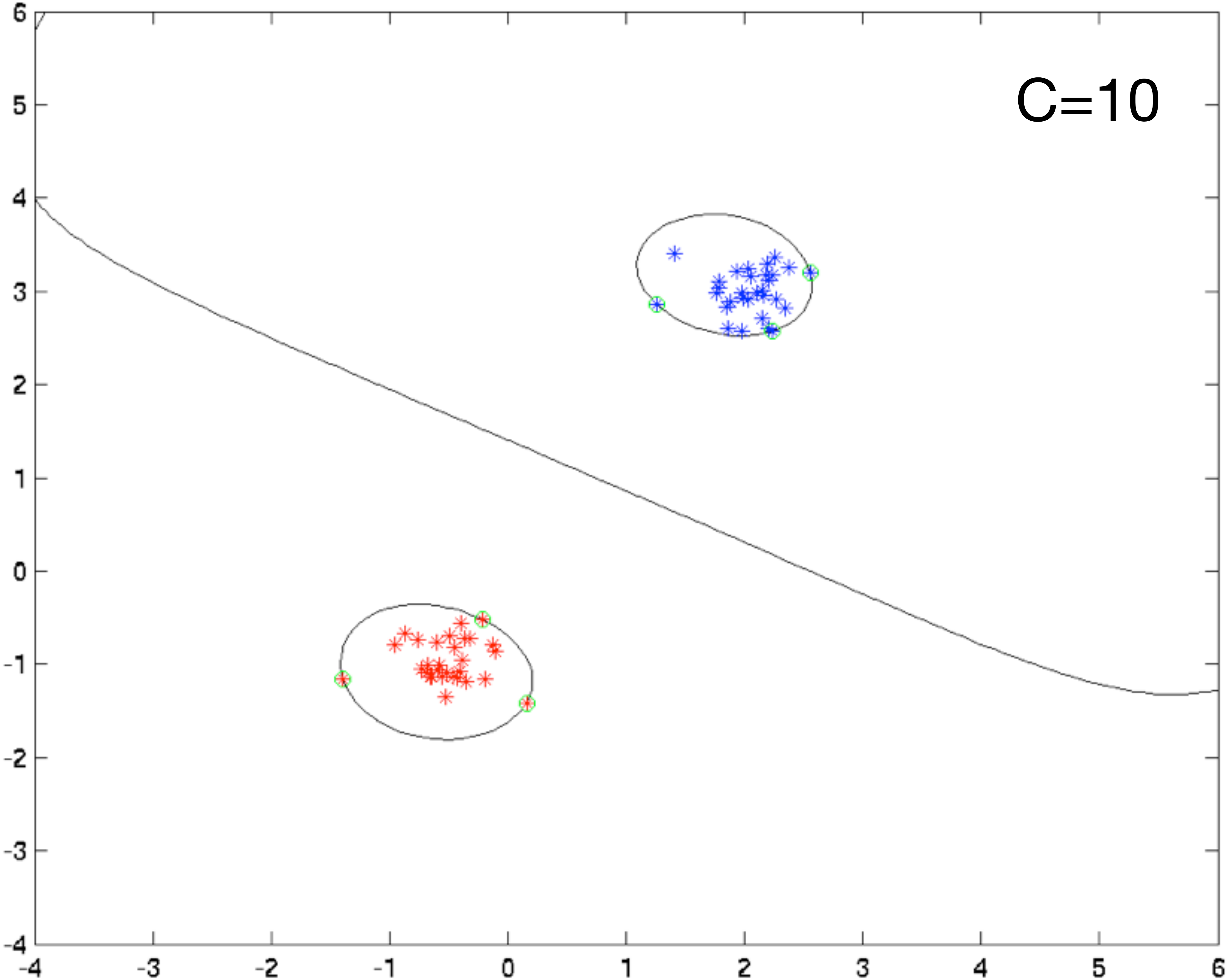

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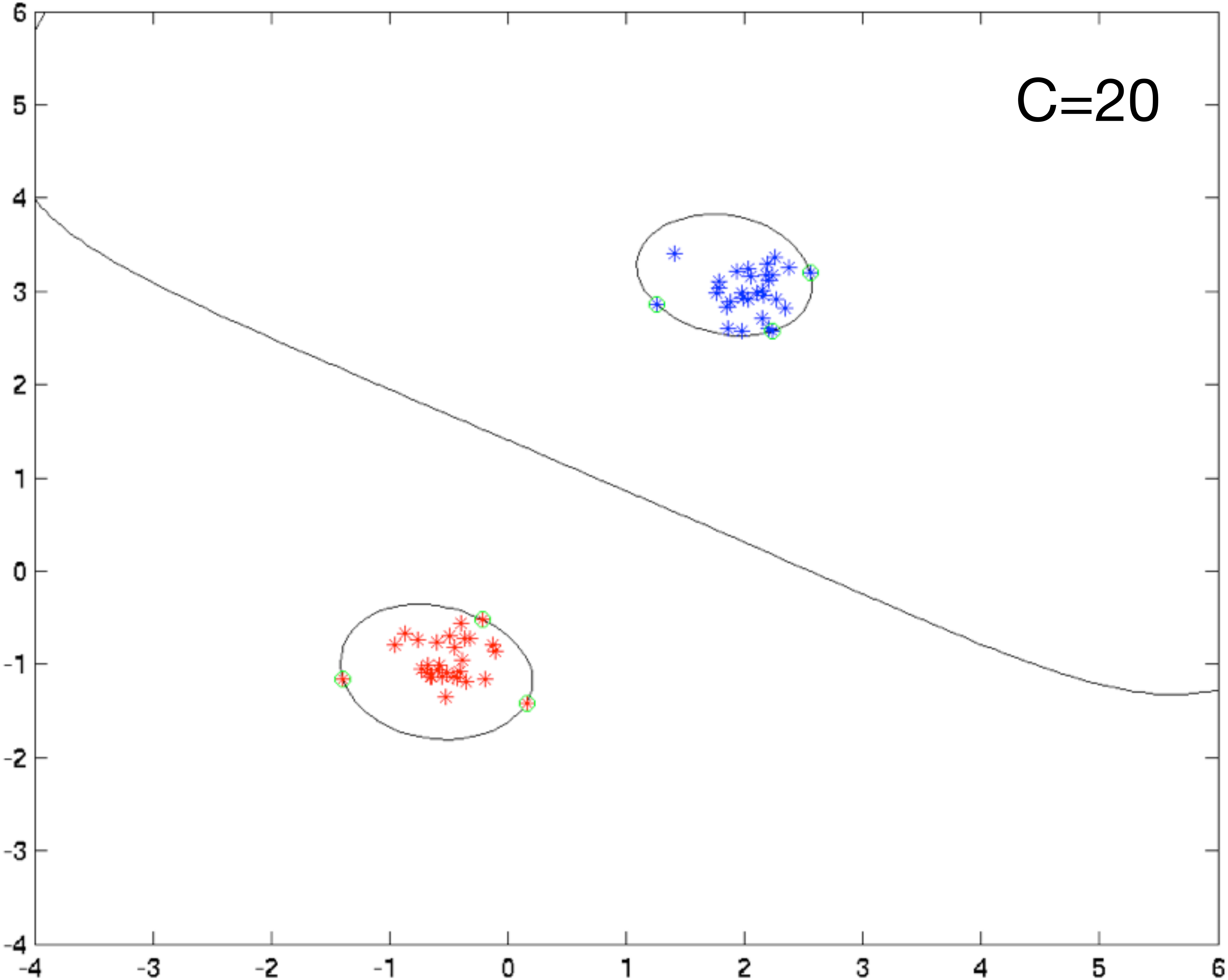

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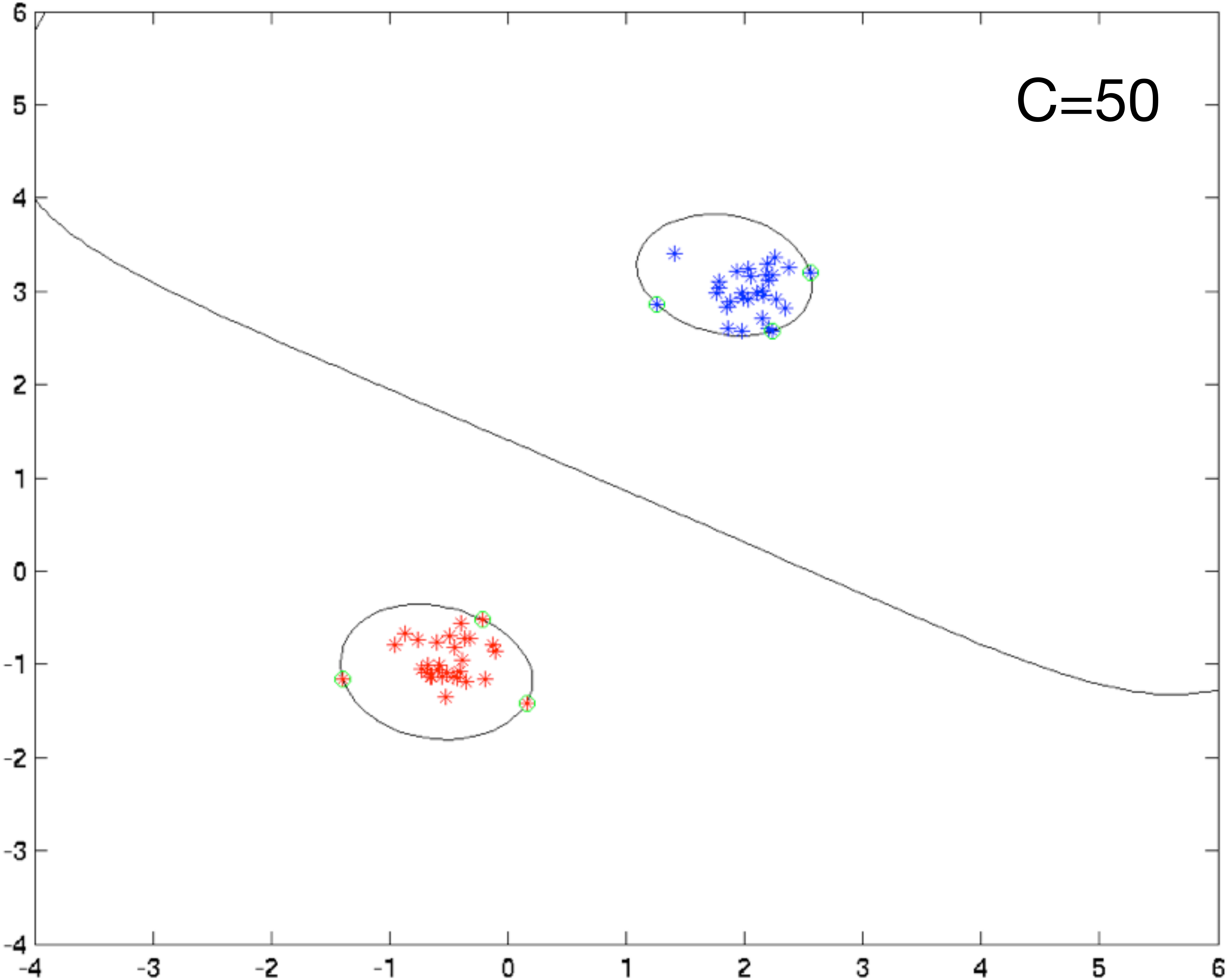

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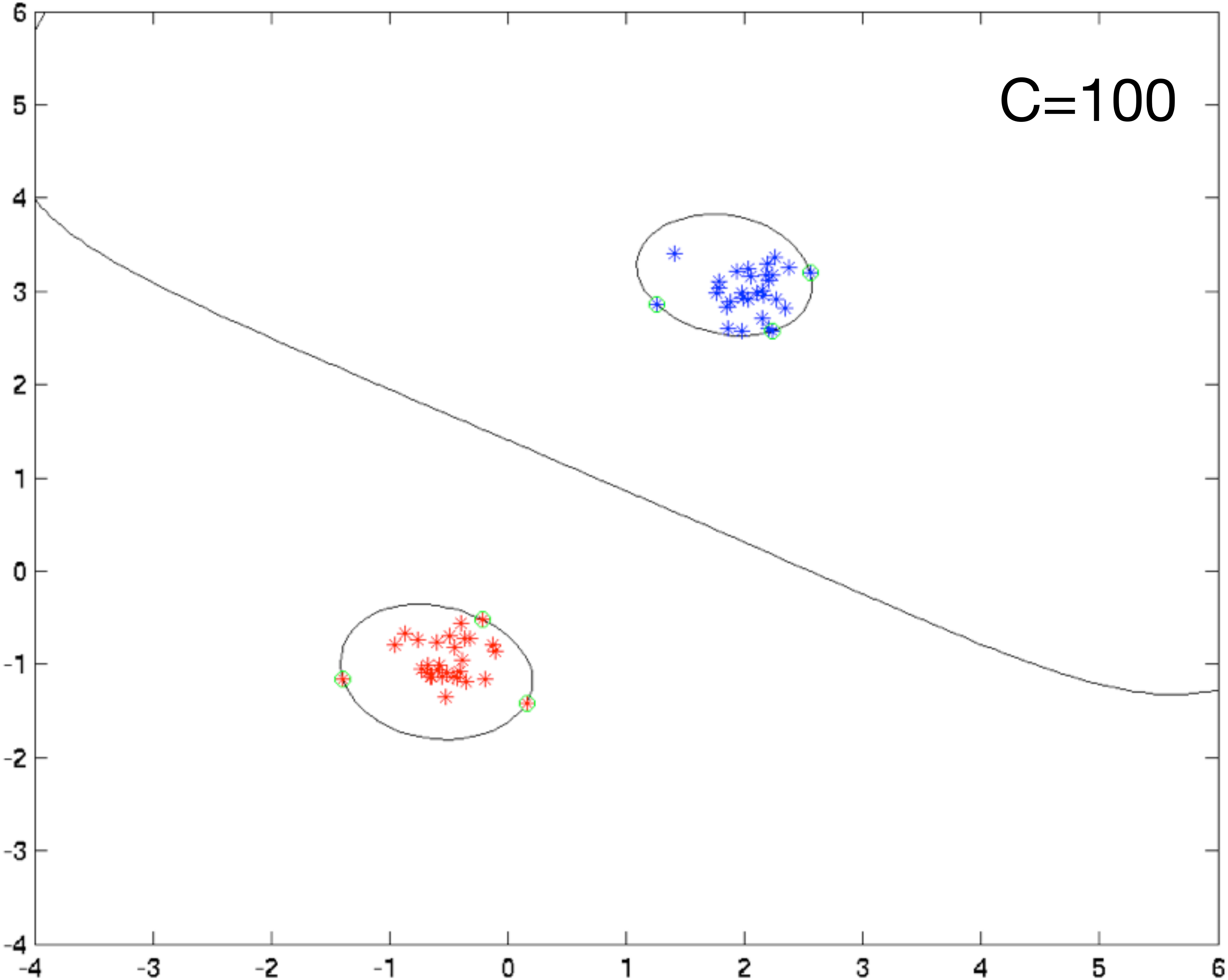

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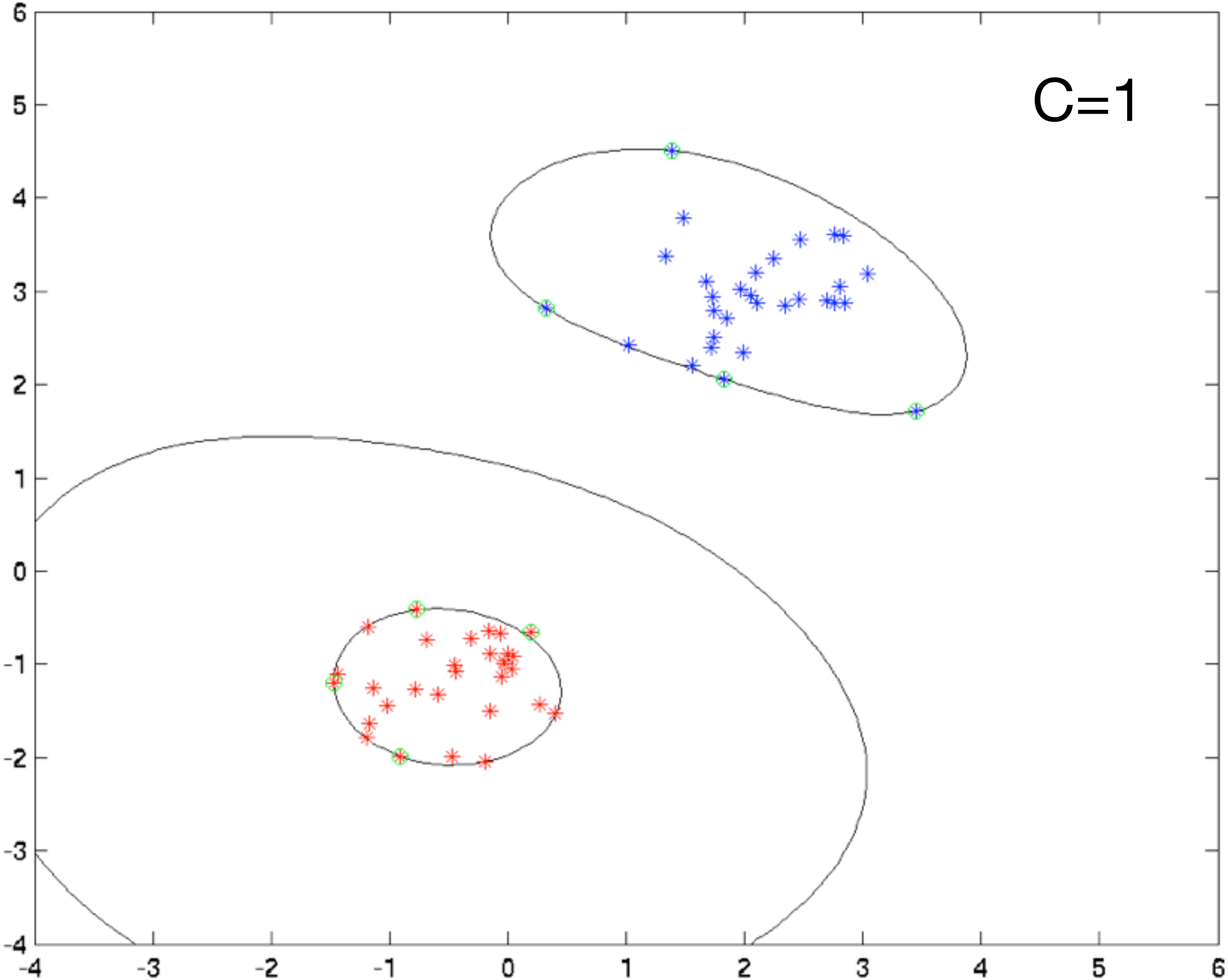

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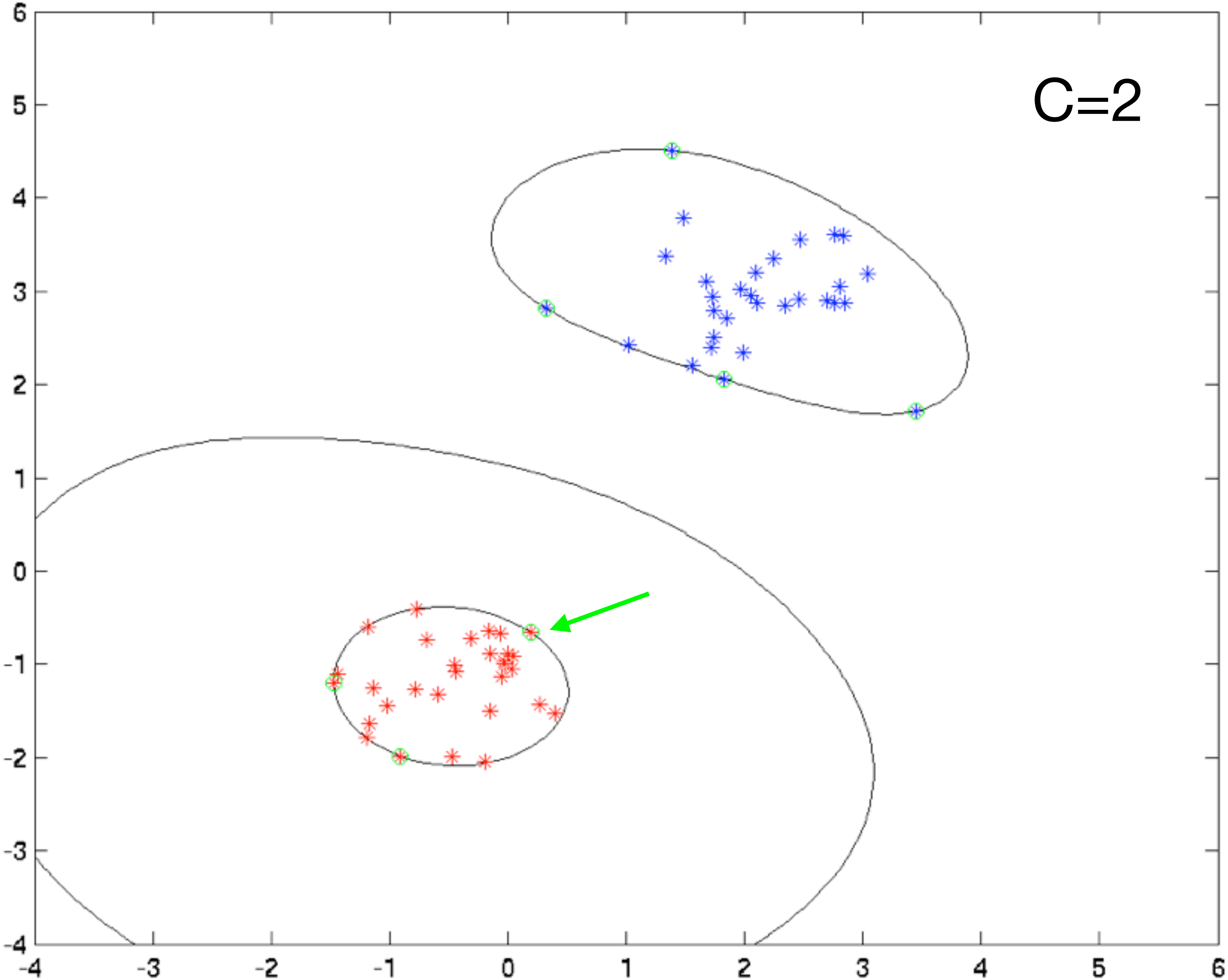

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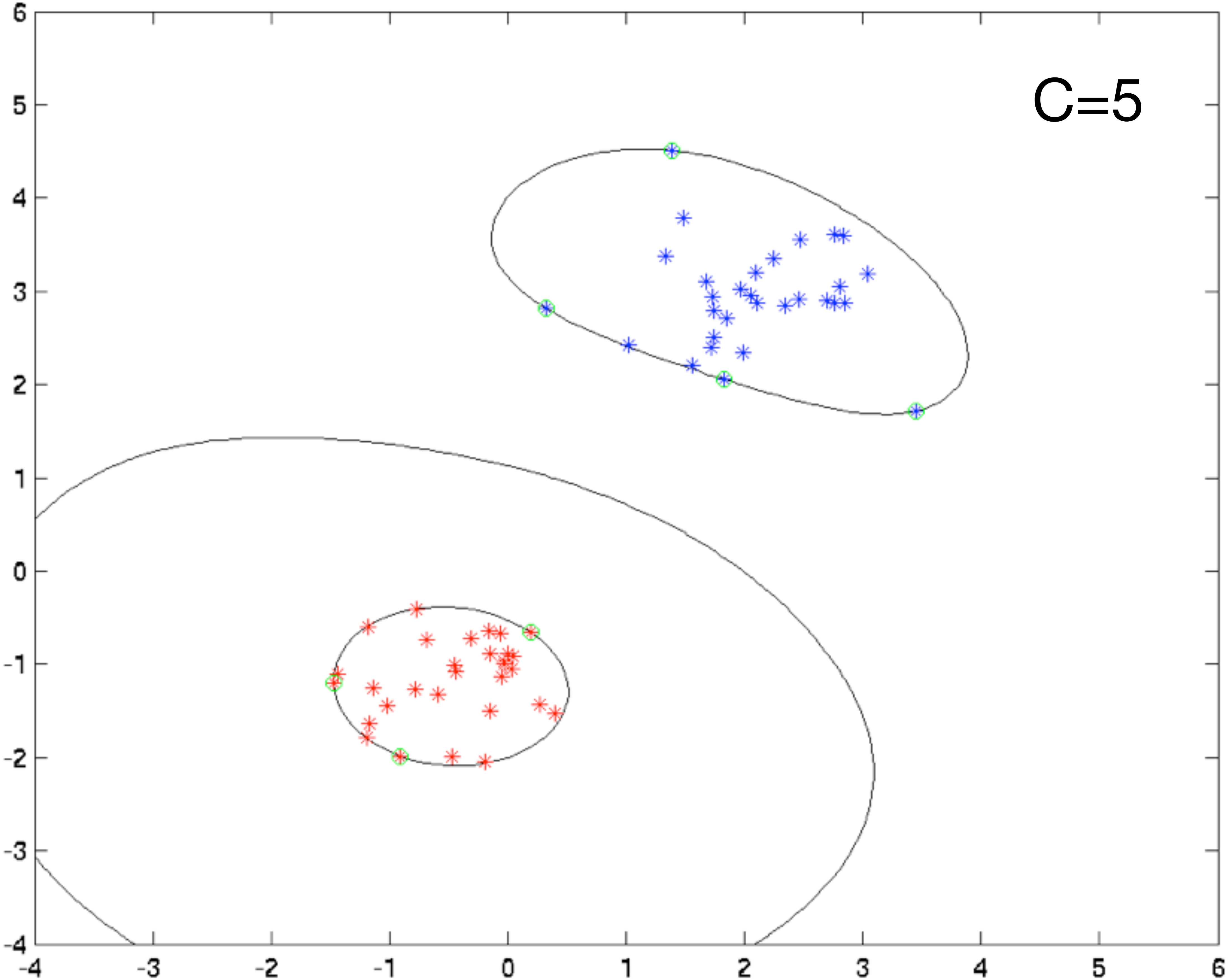

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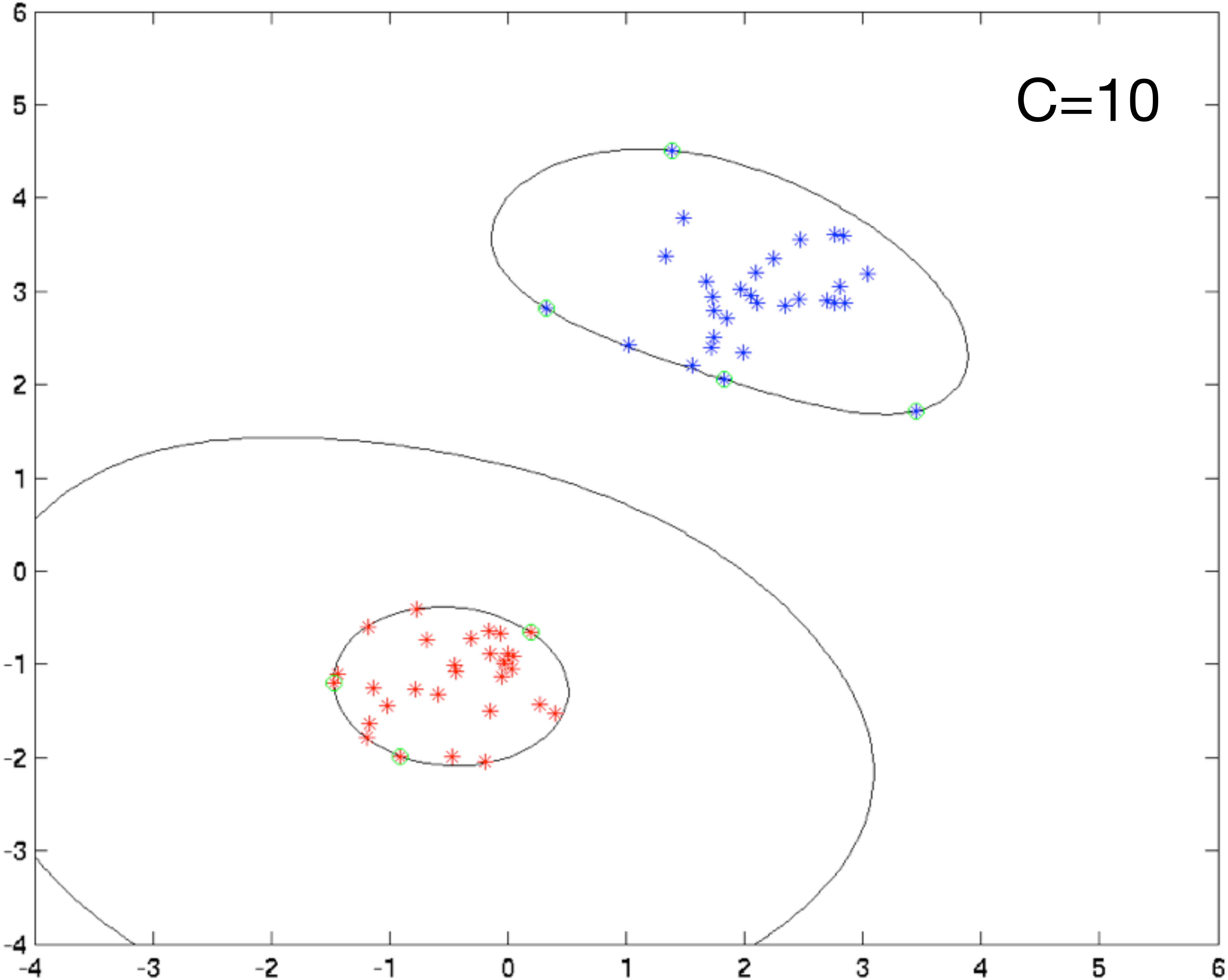

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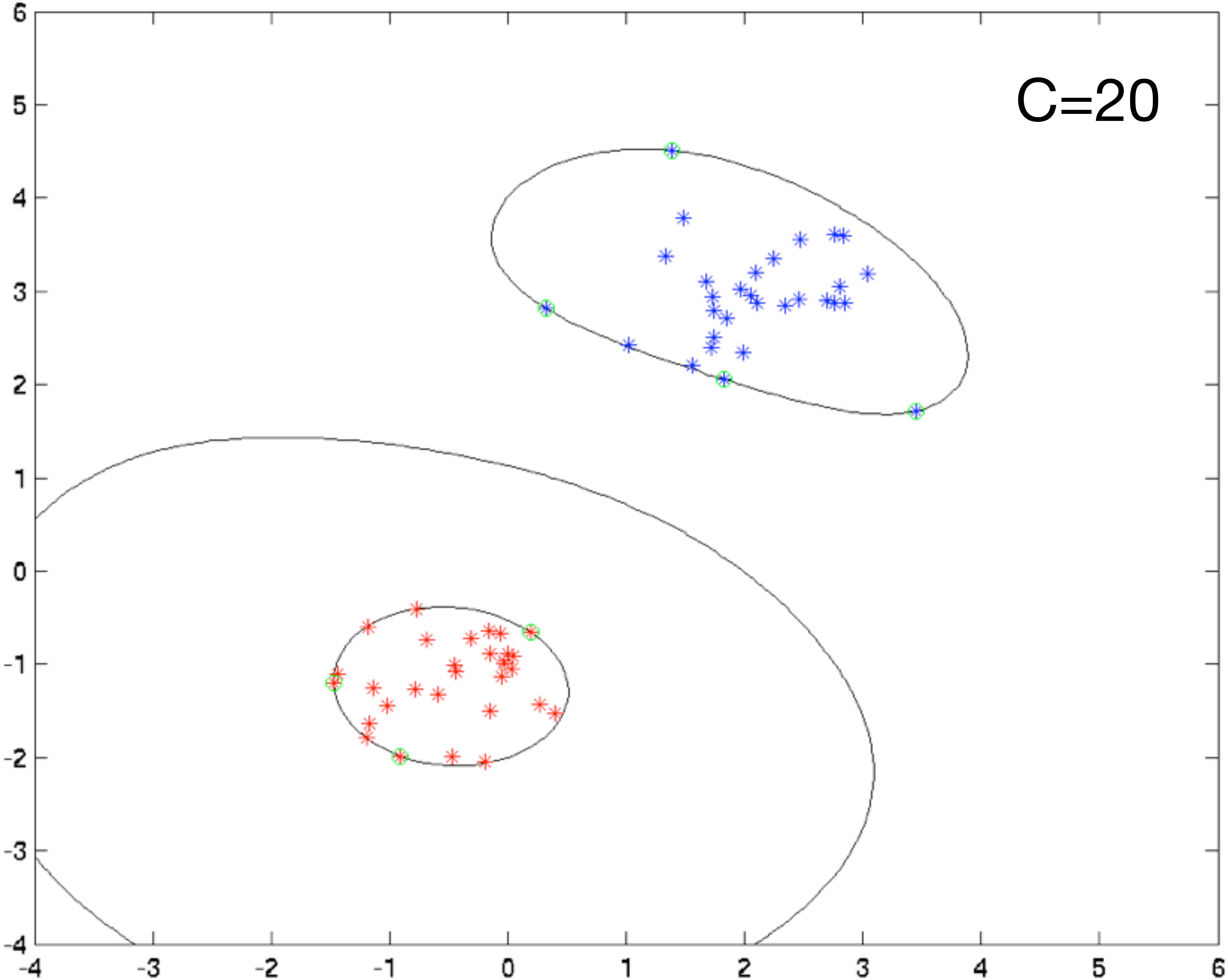

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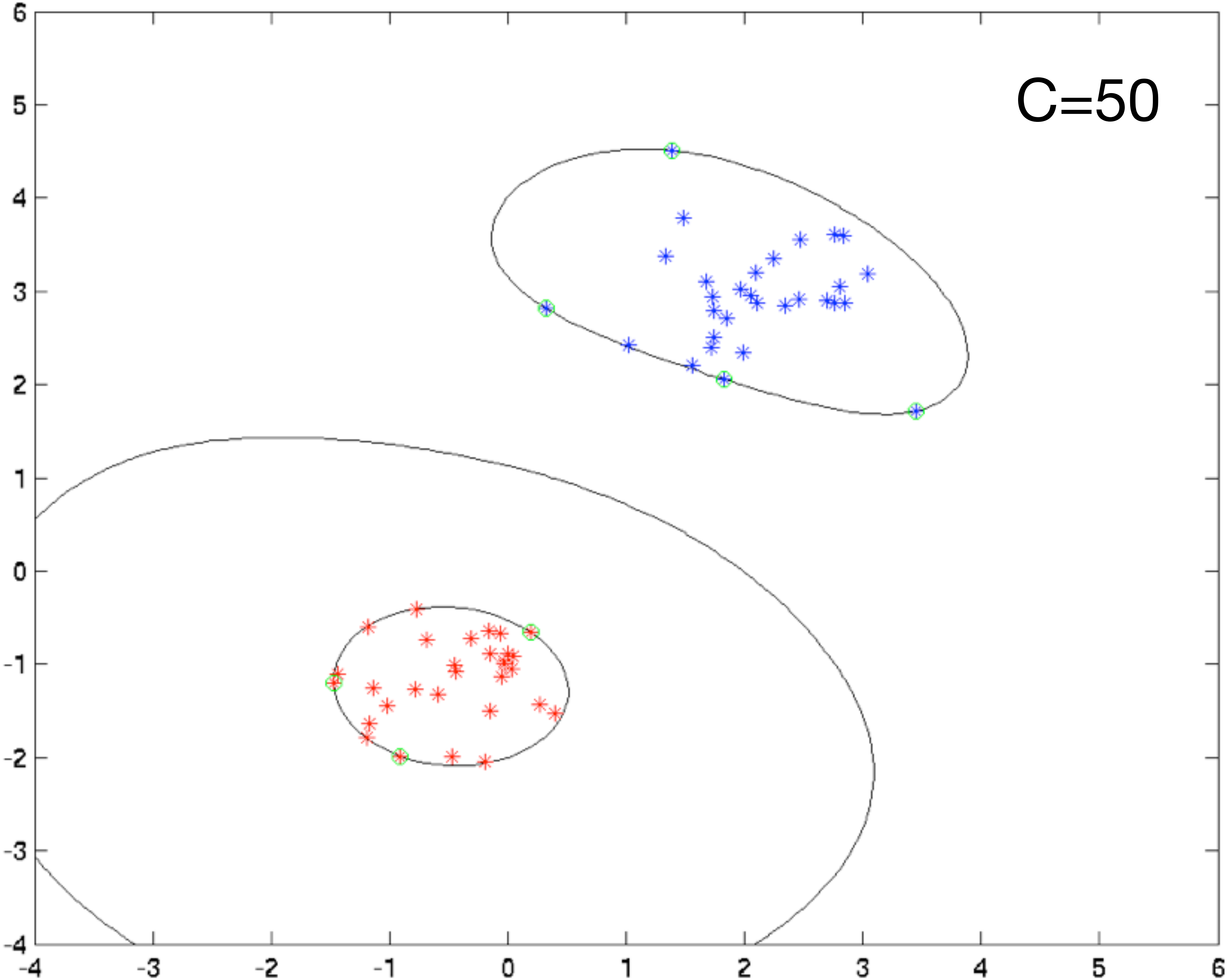

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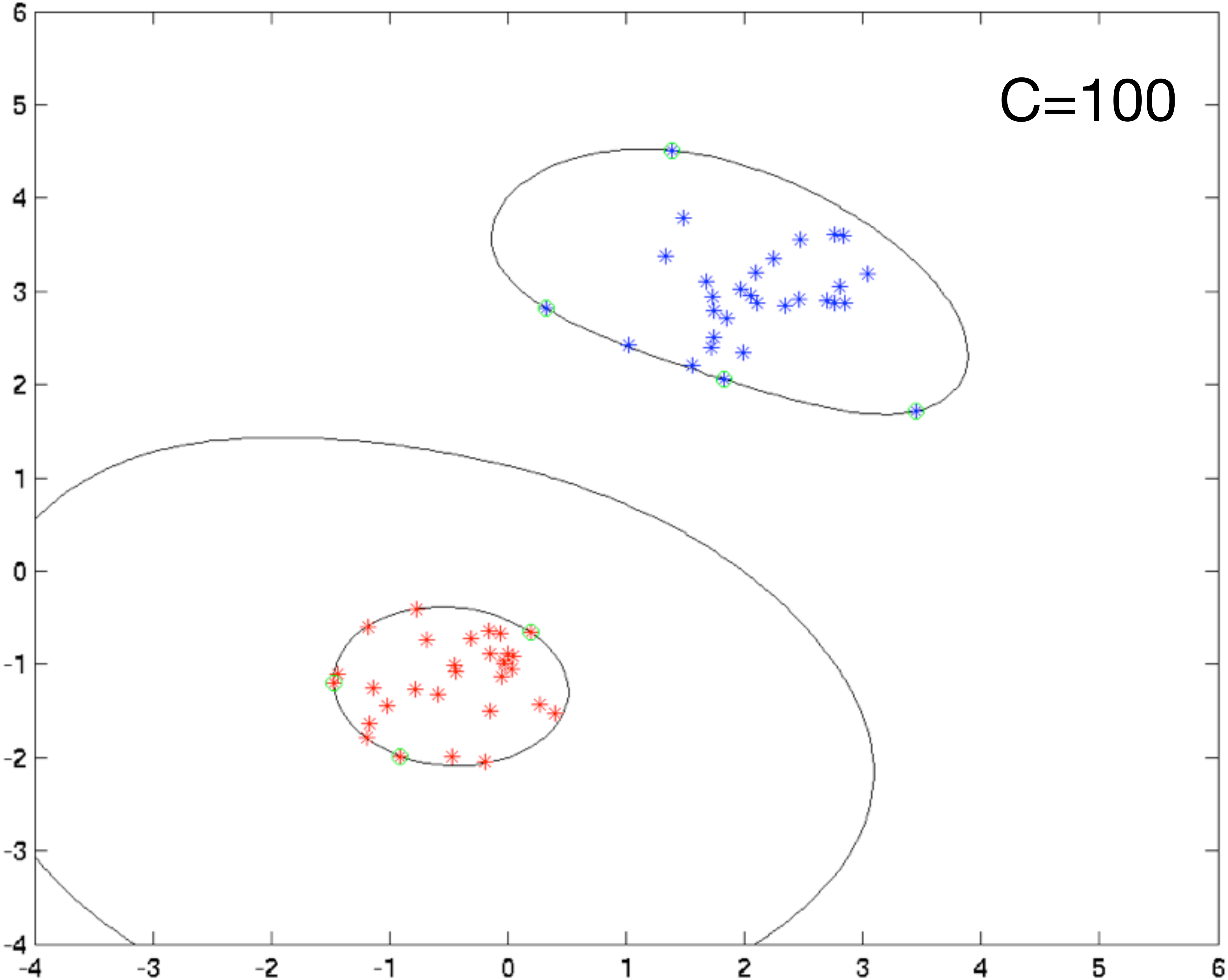

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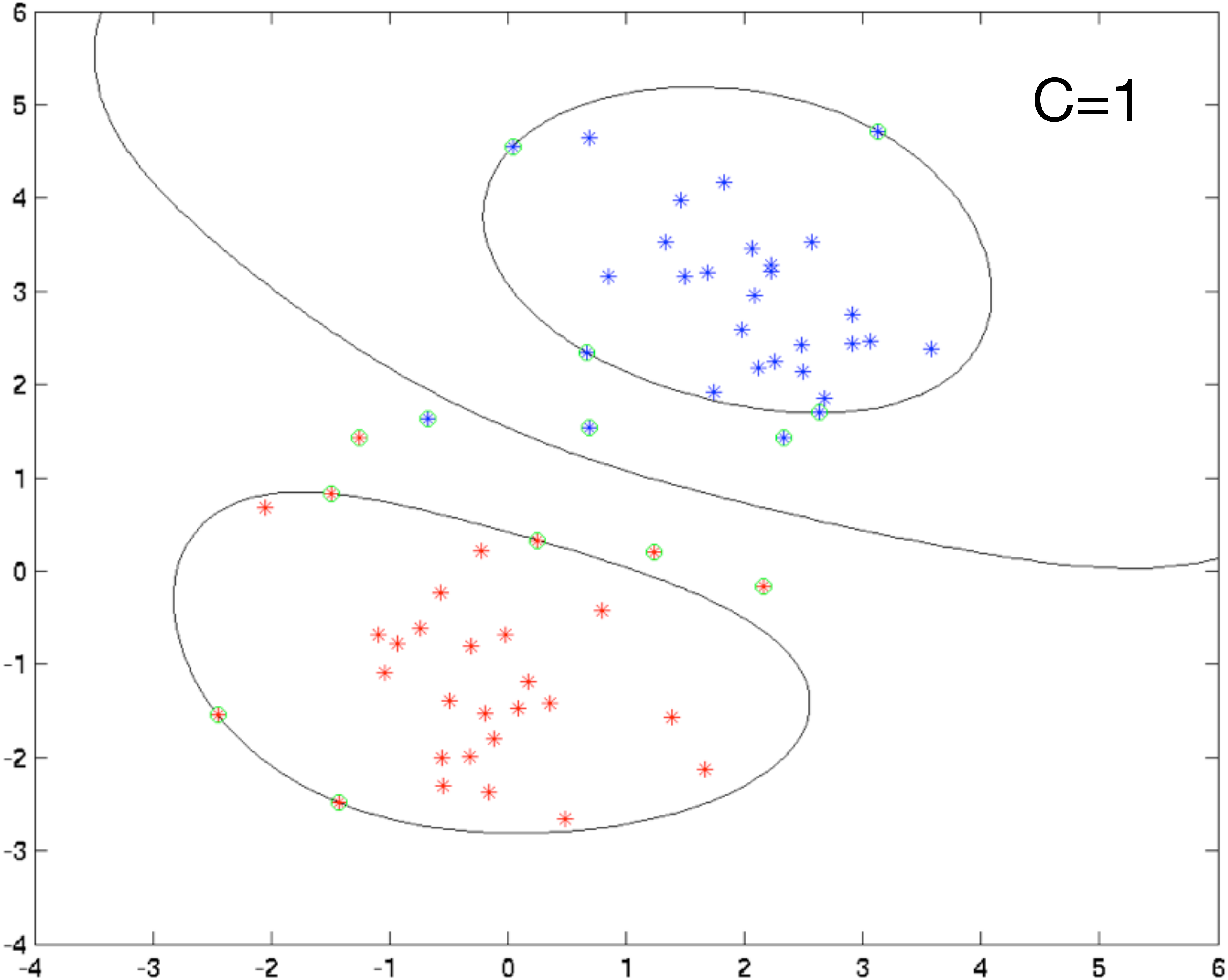

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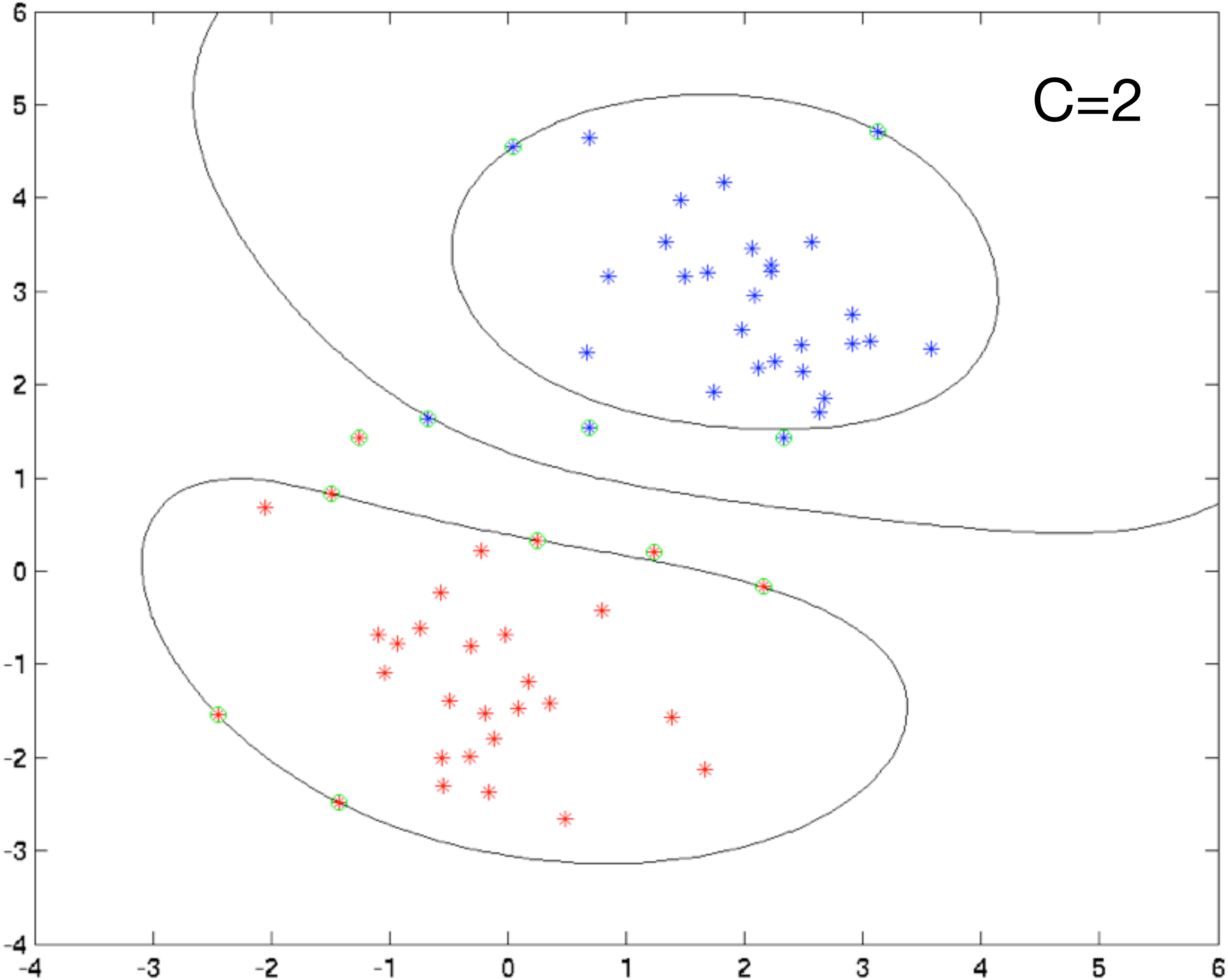

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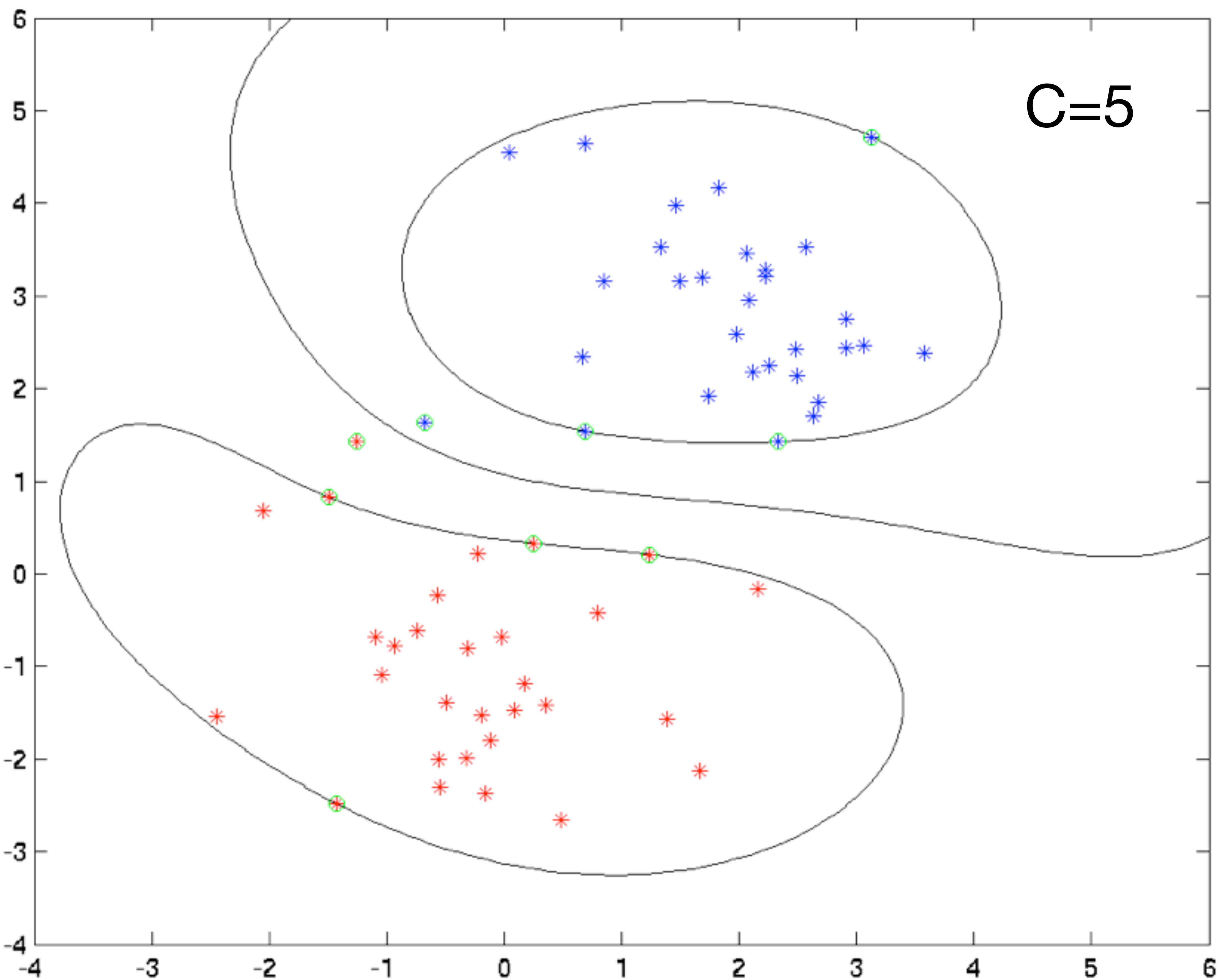

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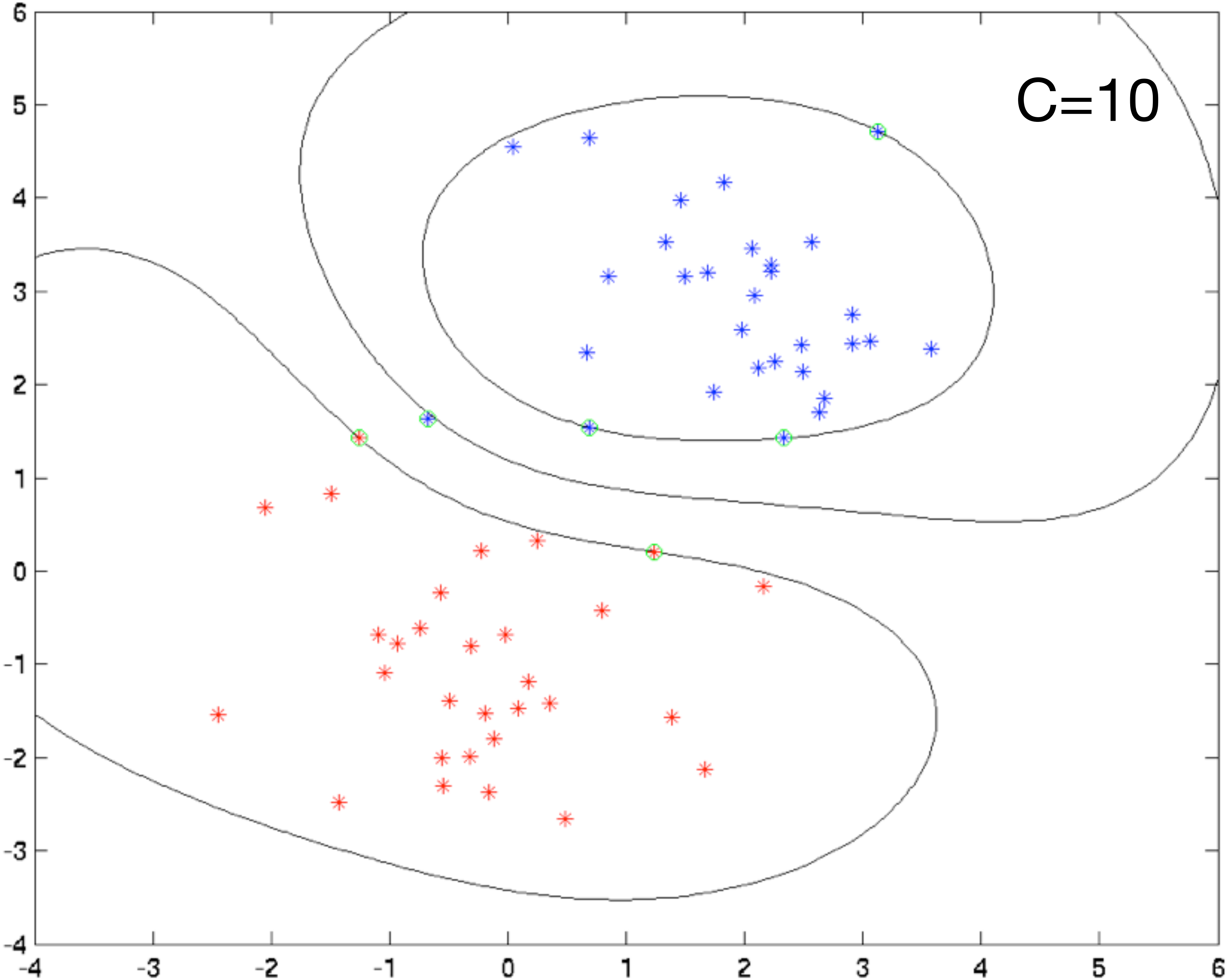

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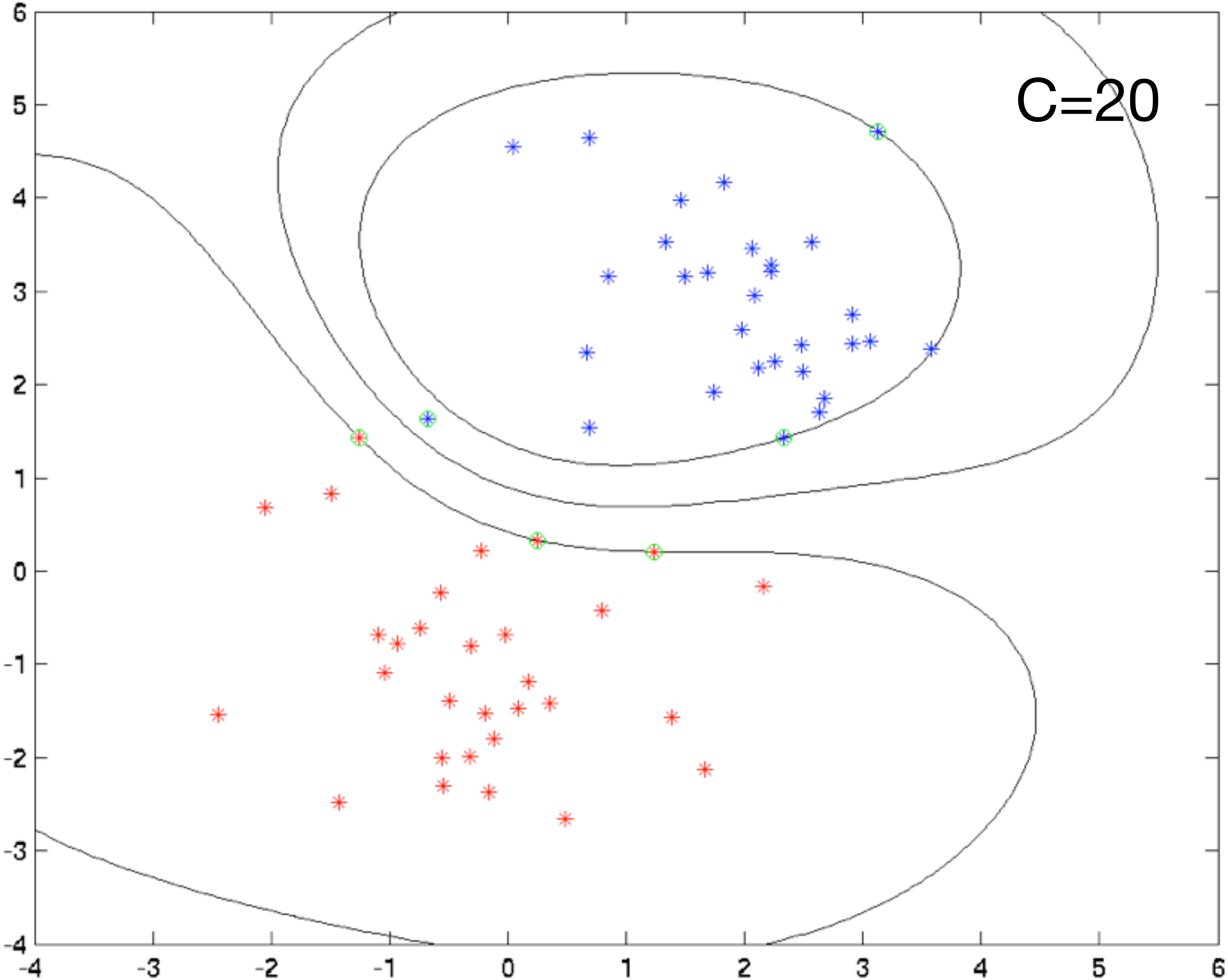

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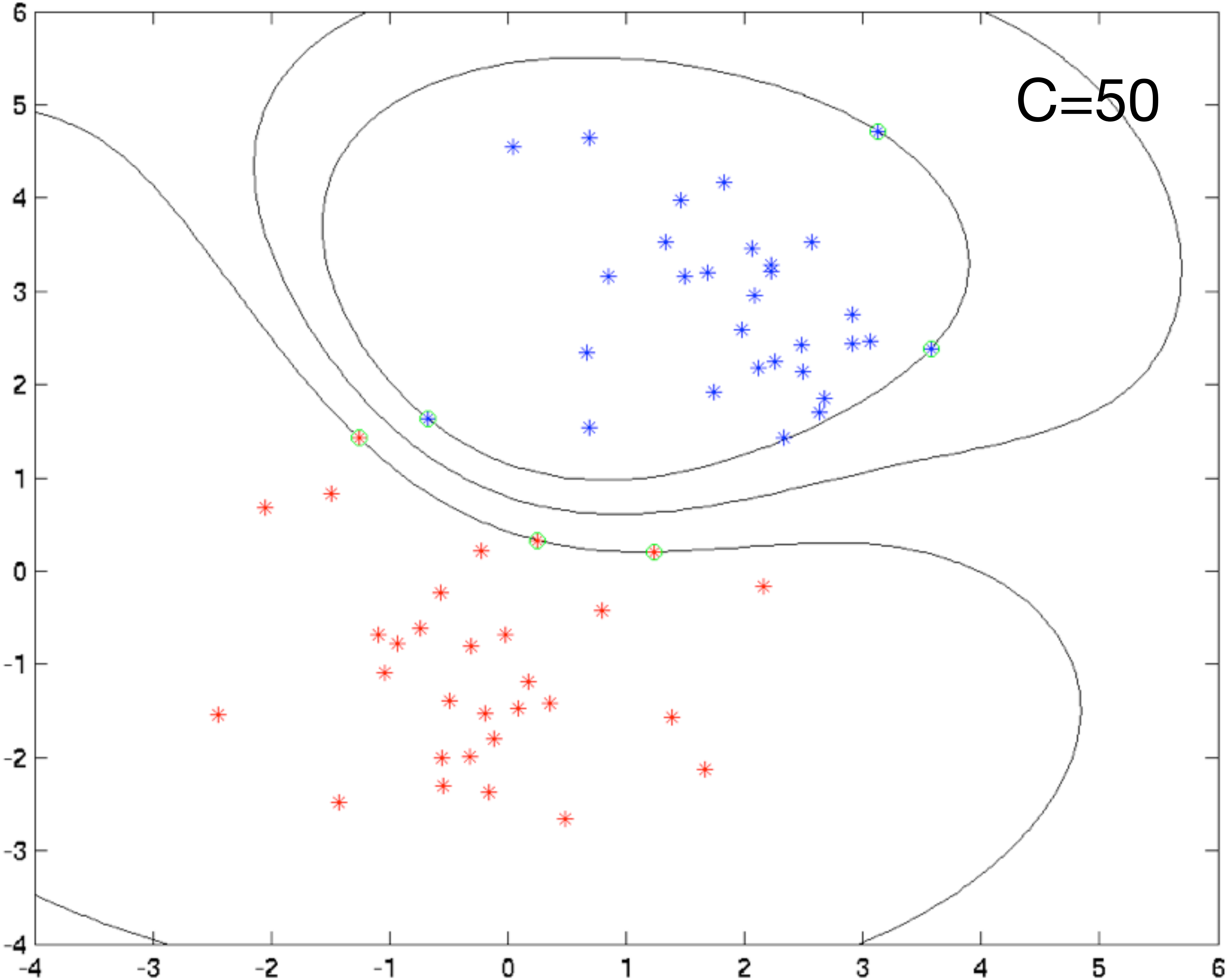

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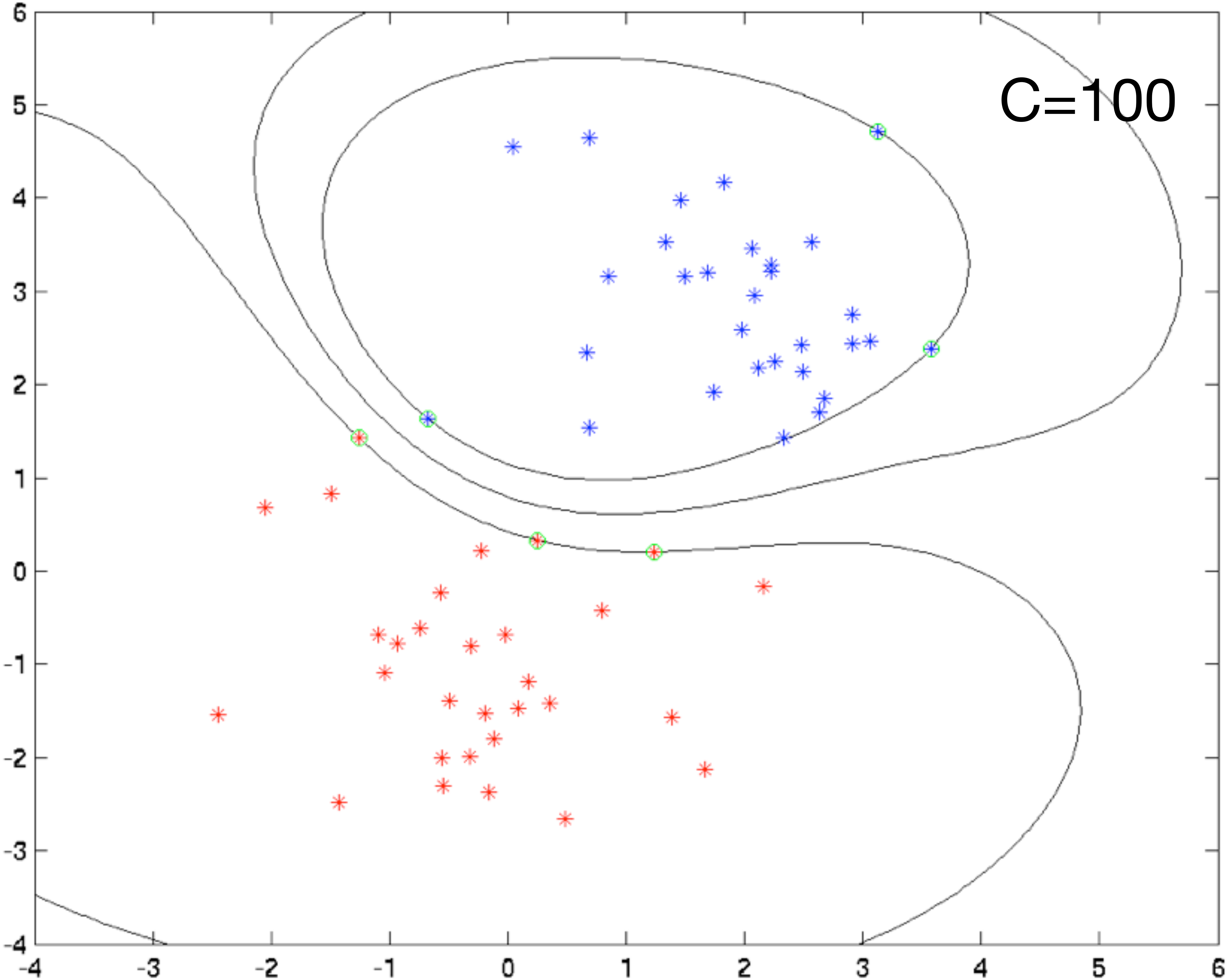

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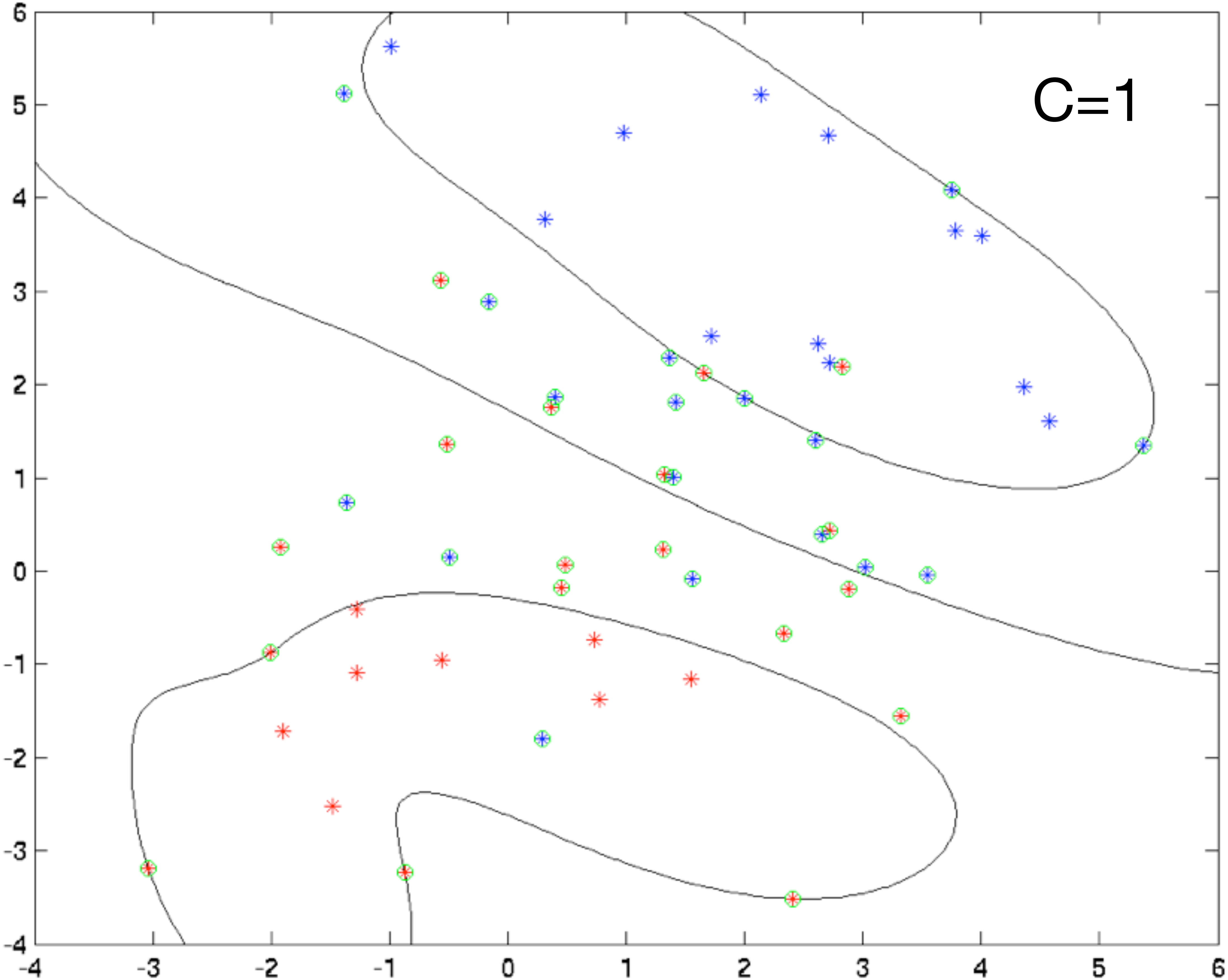

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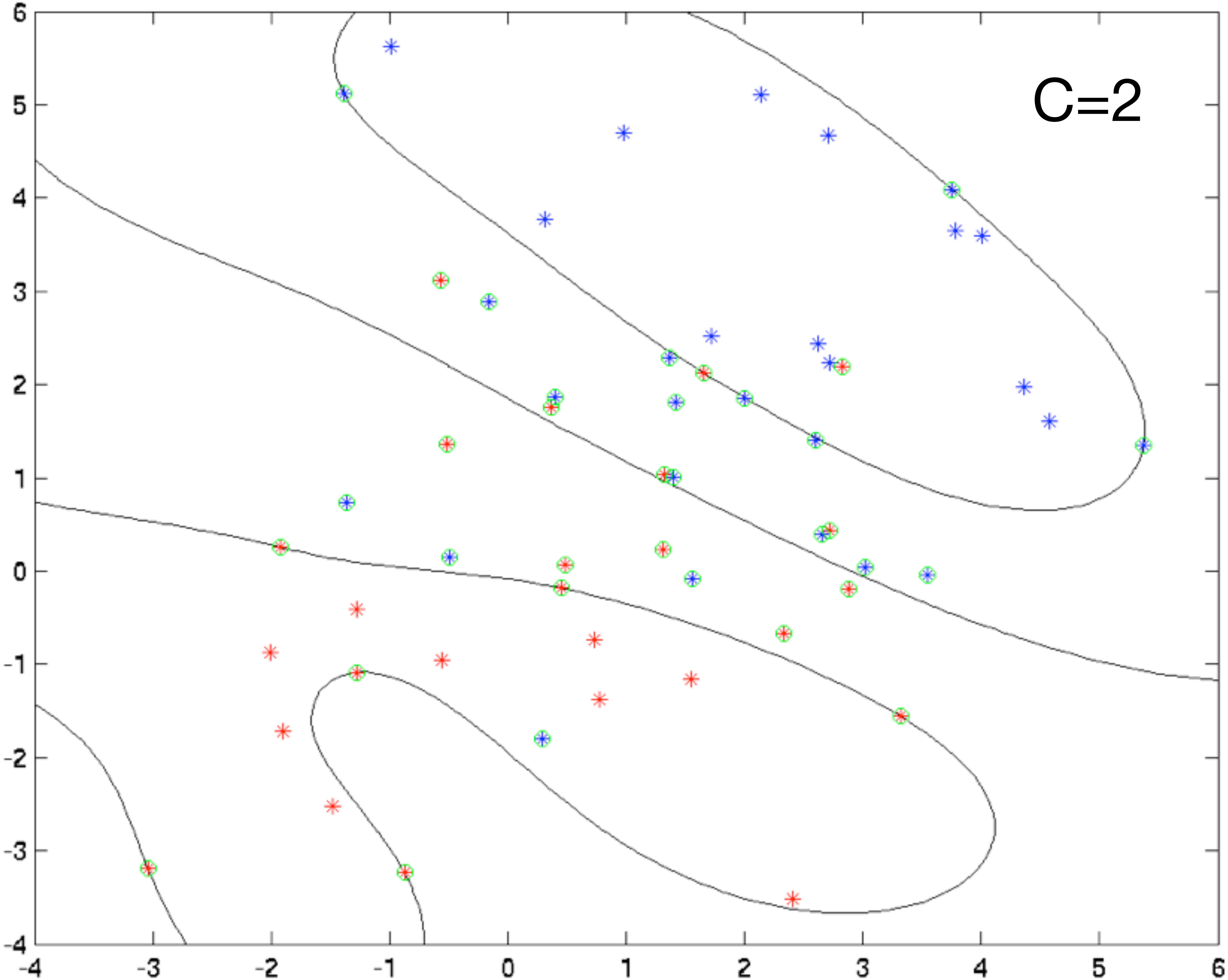

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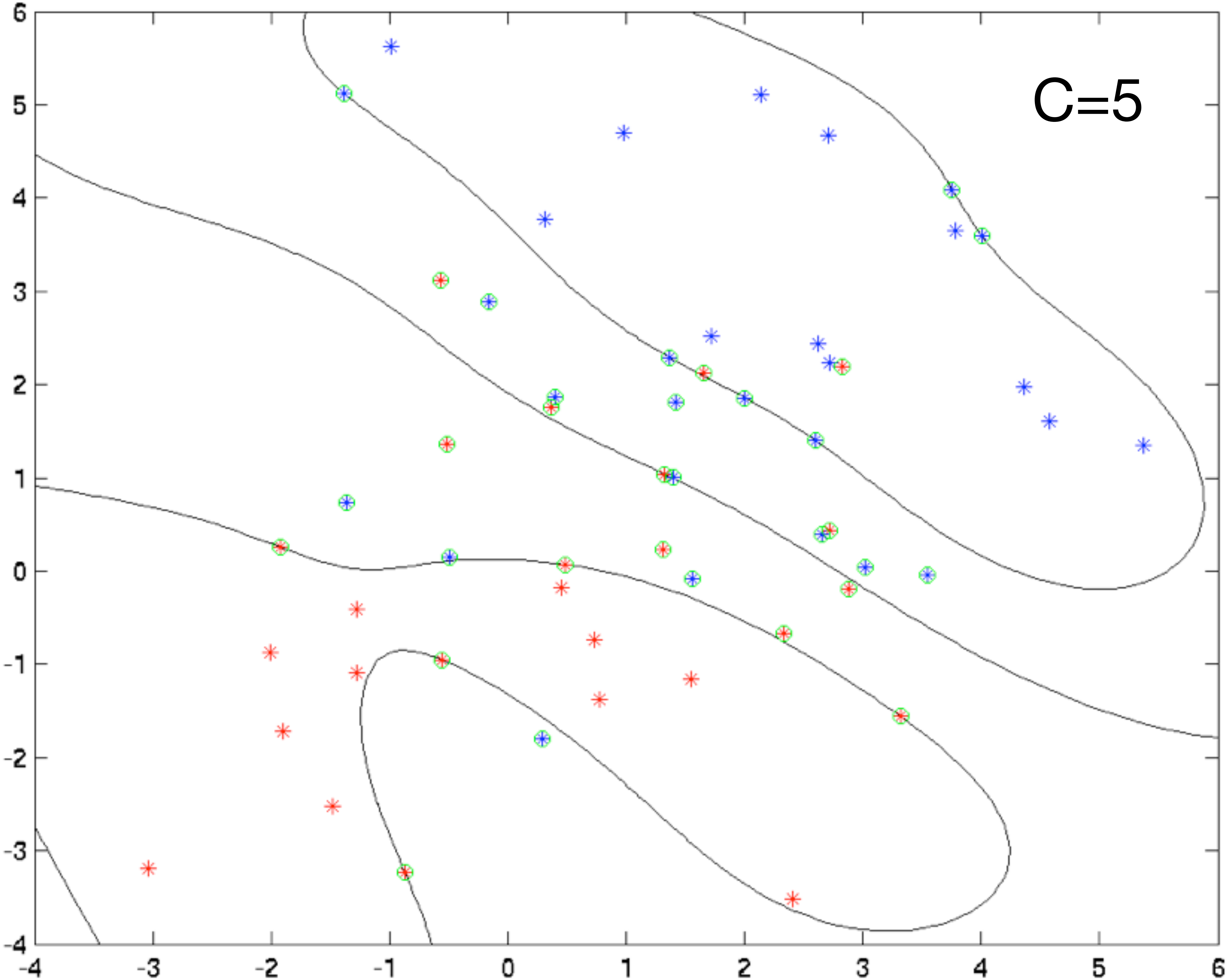

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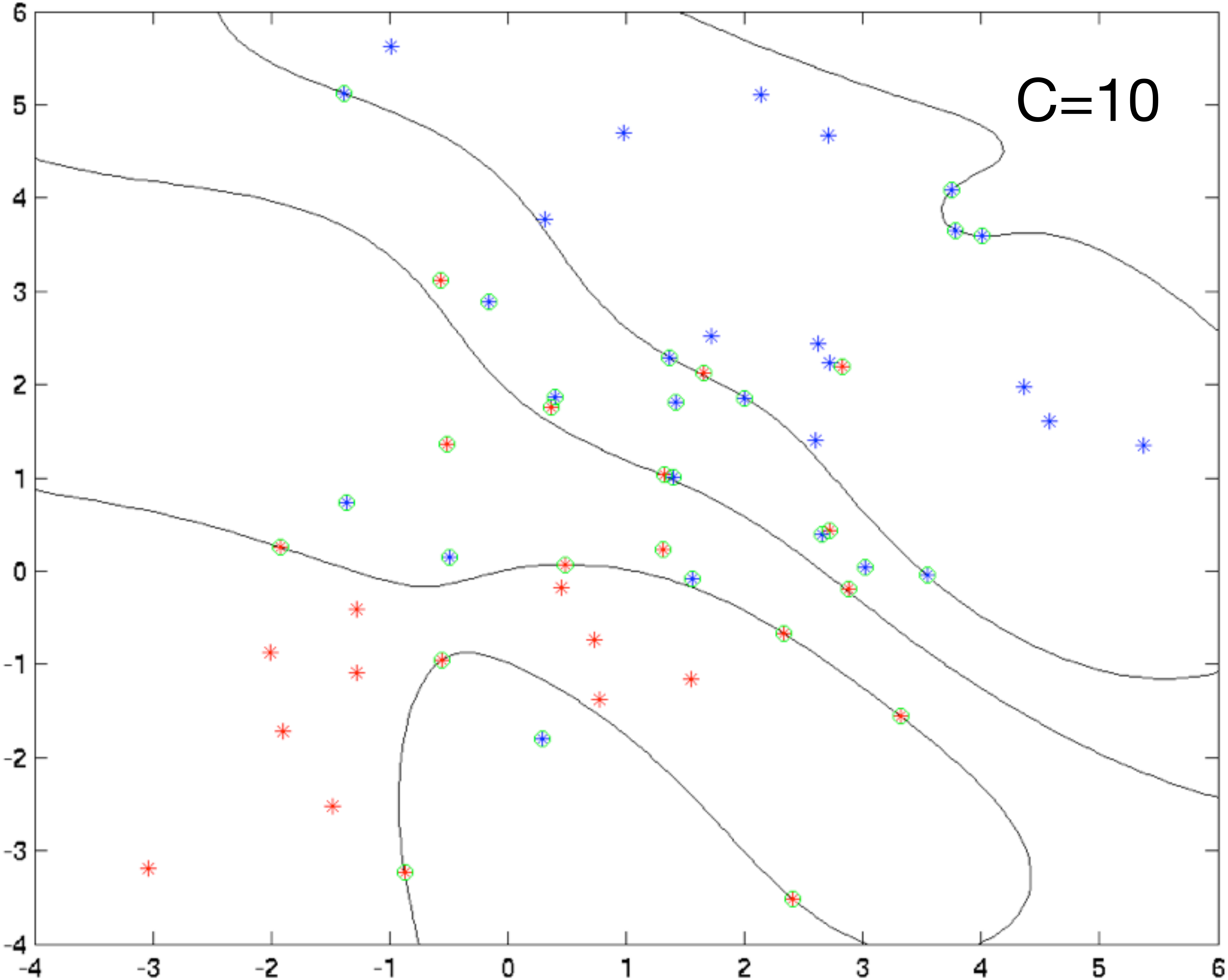

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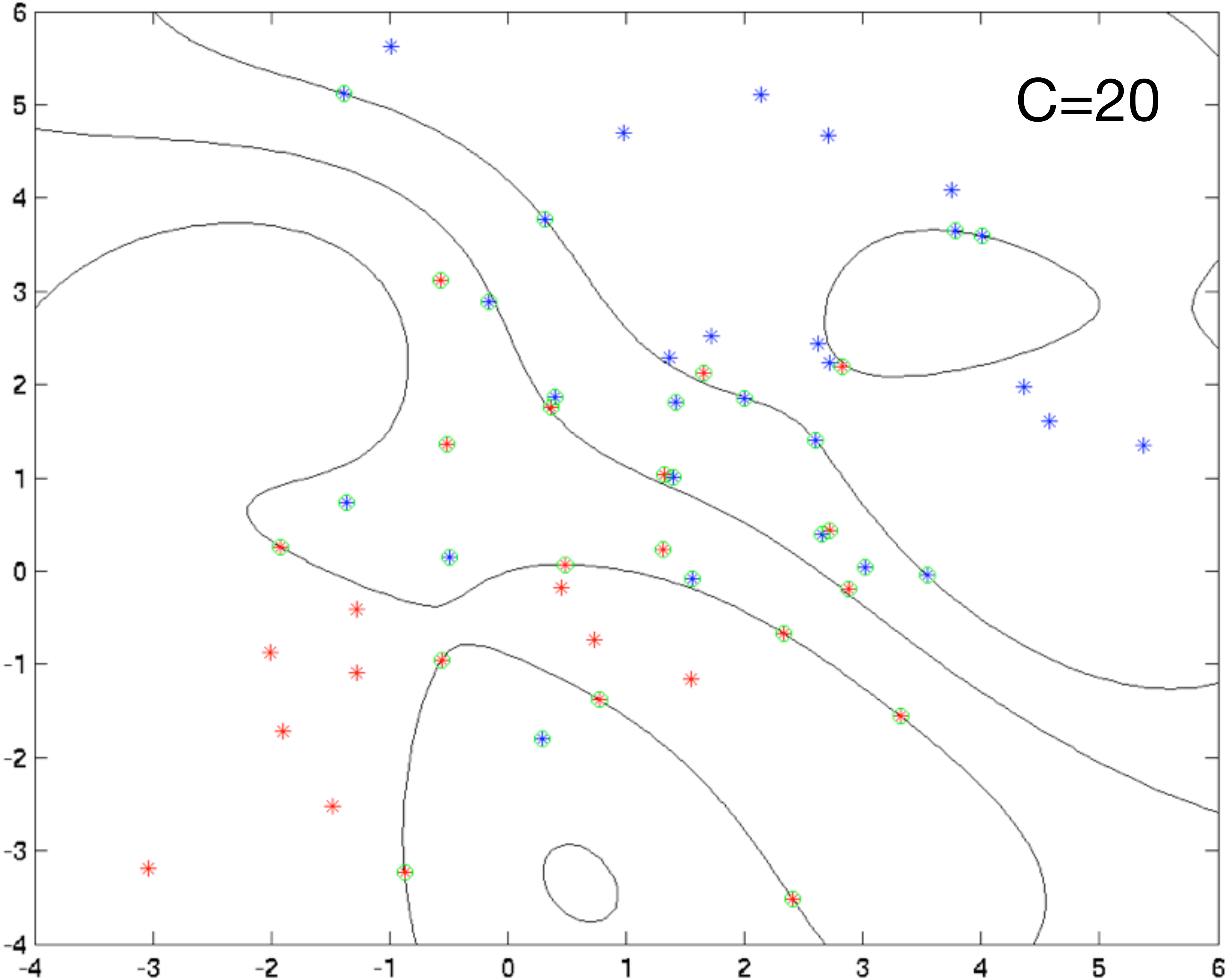

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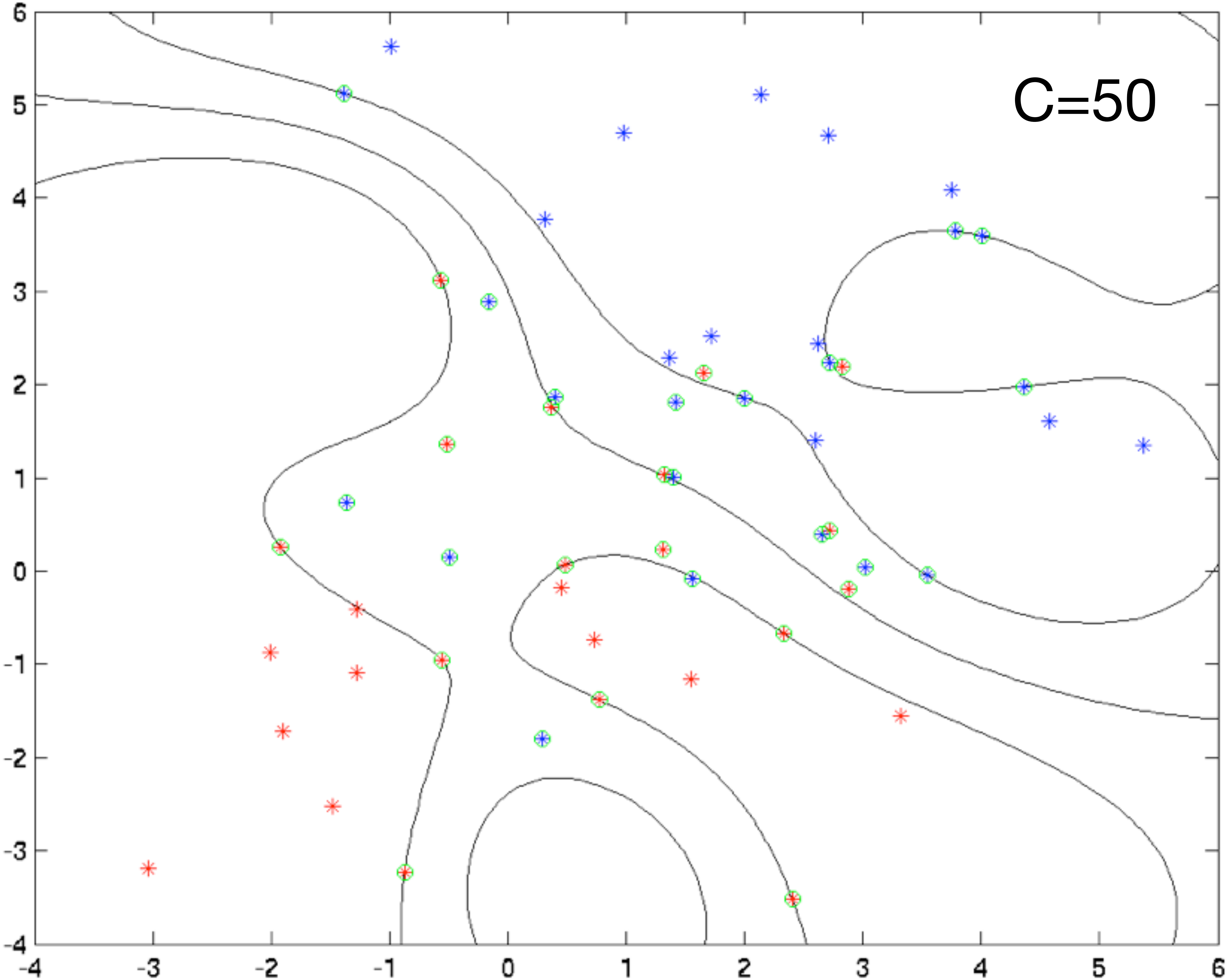

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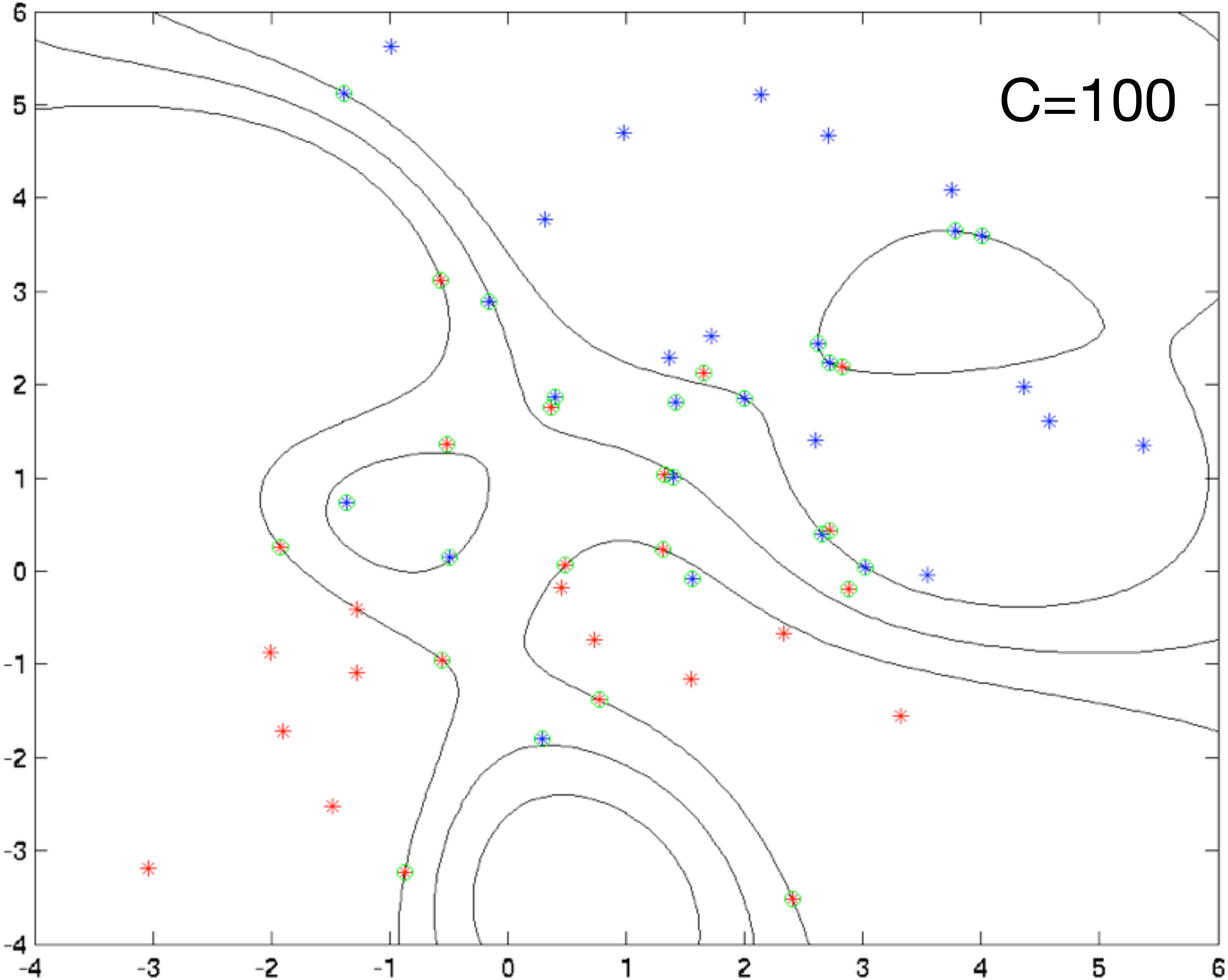

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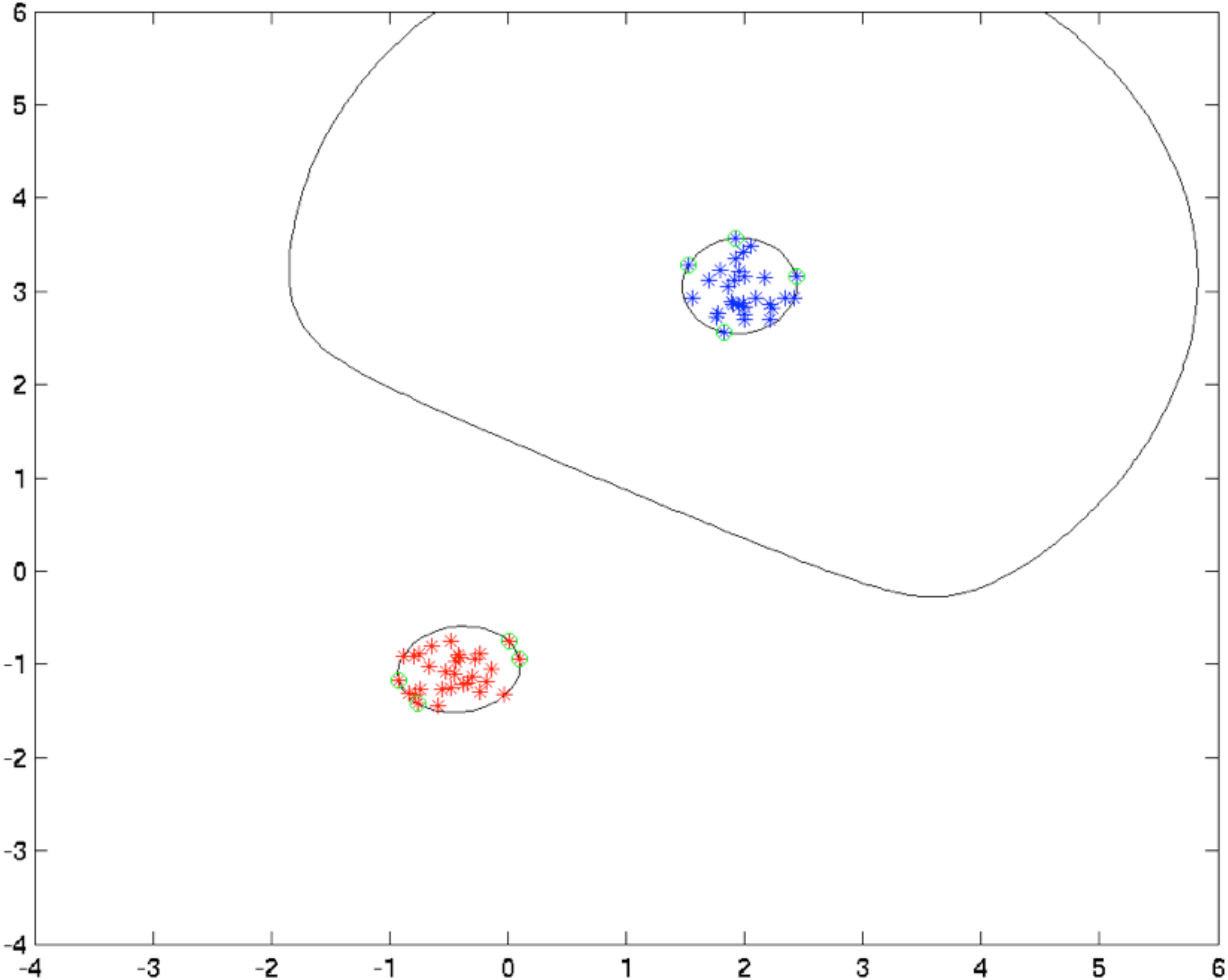
And now with a narrower kernel



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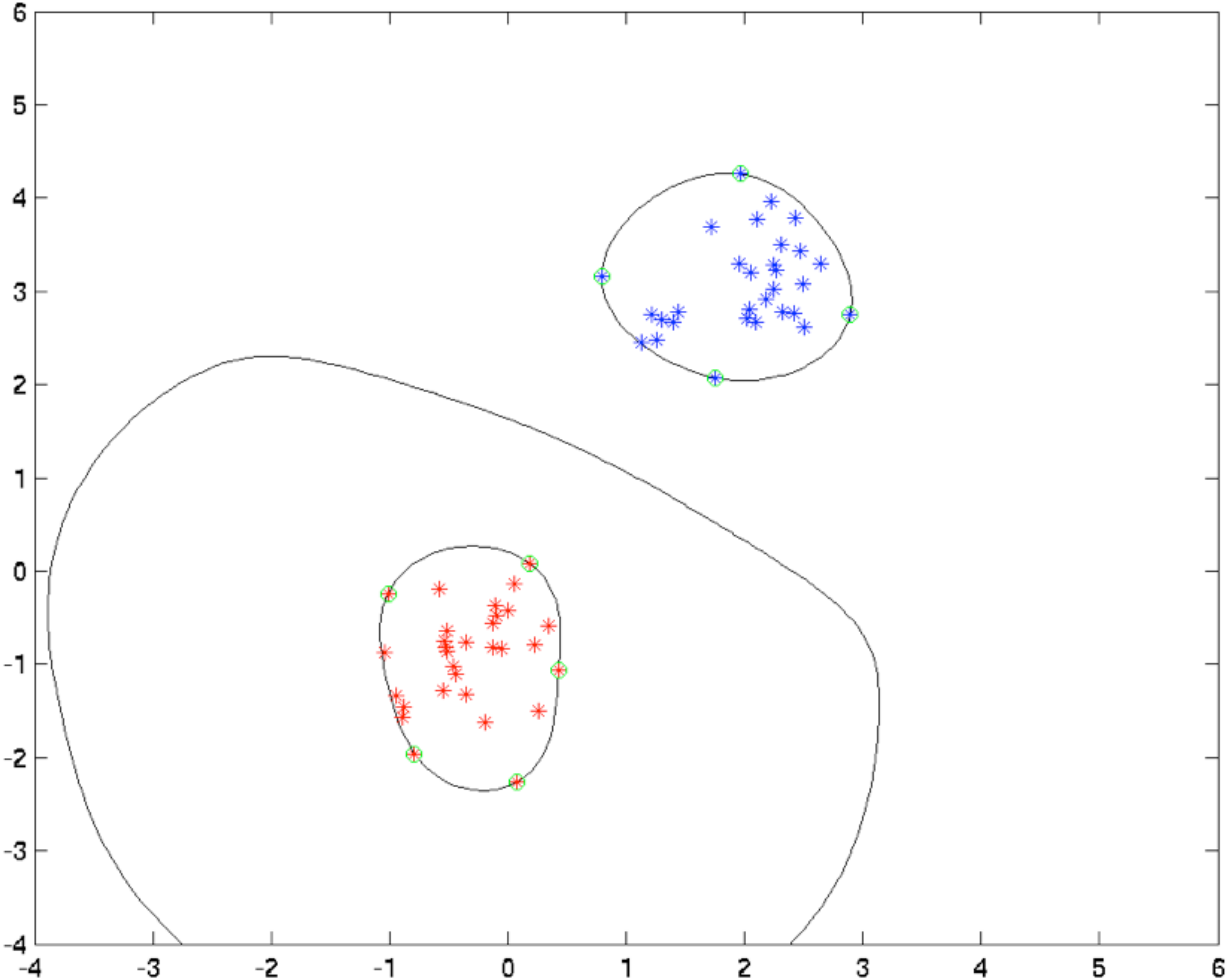

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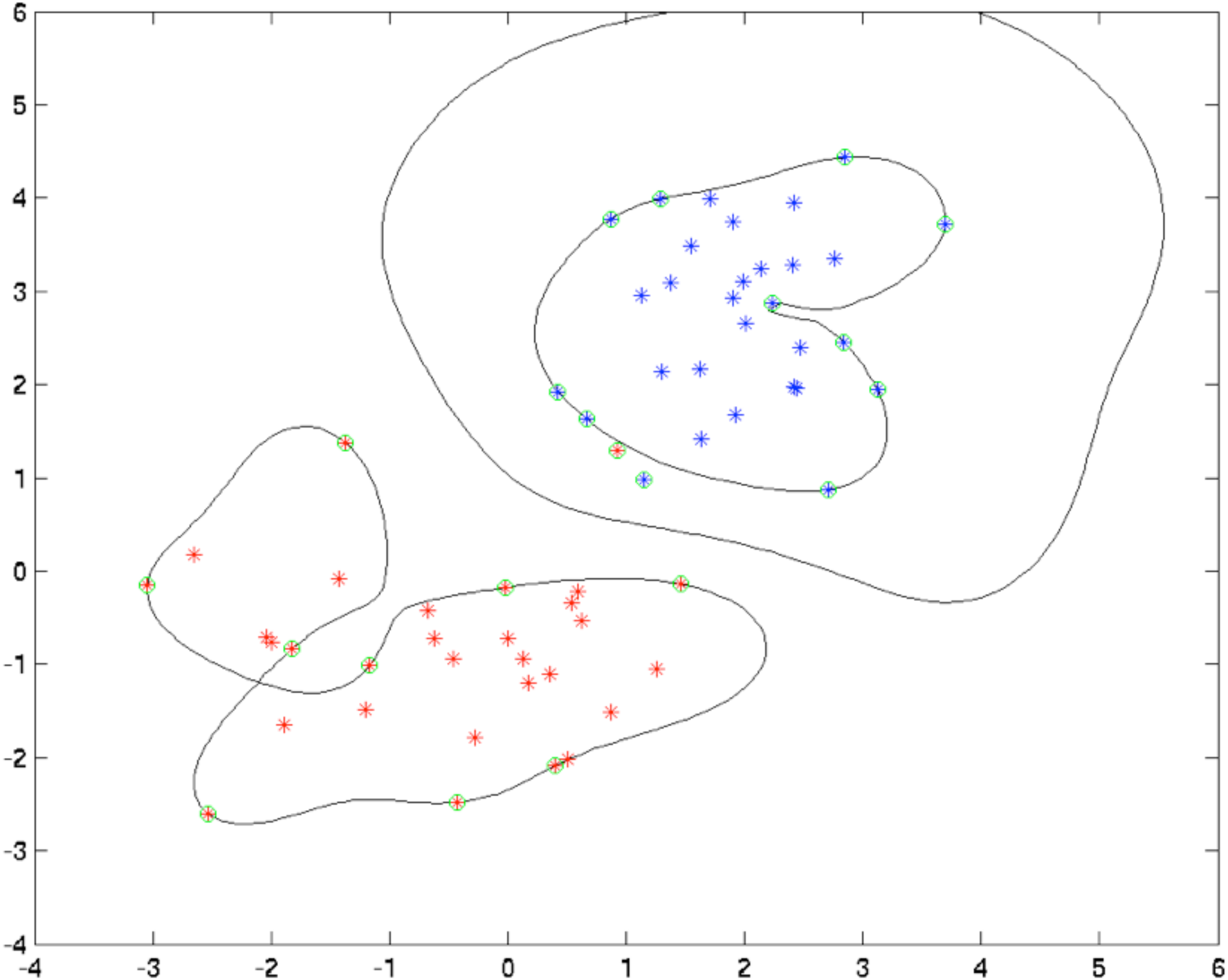

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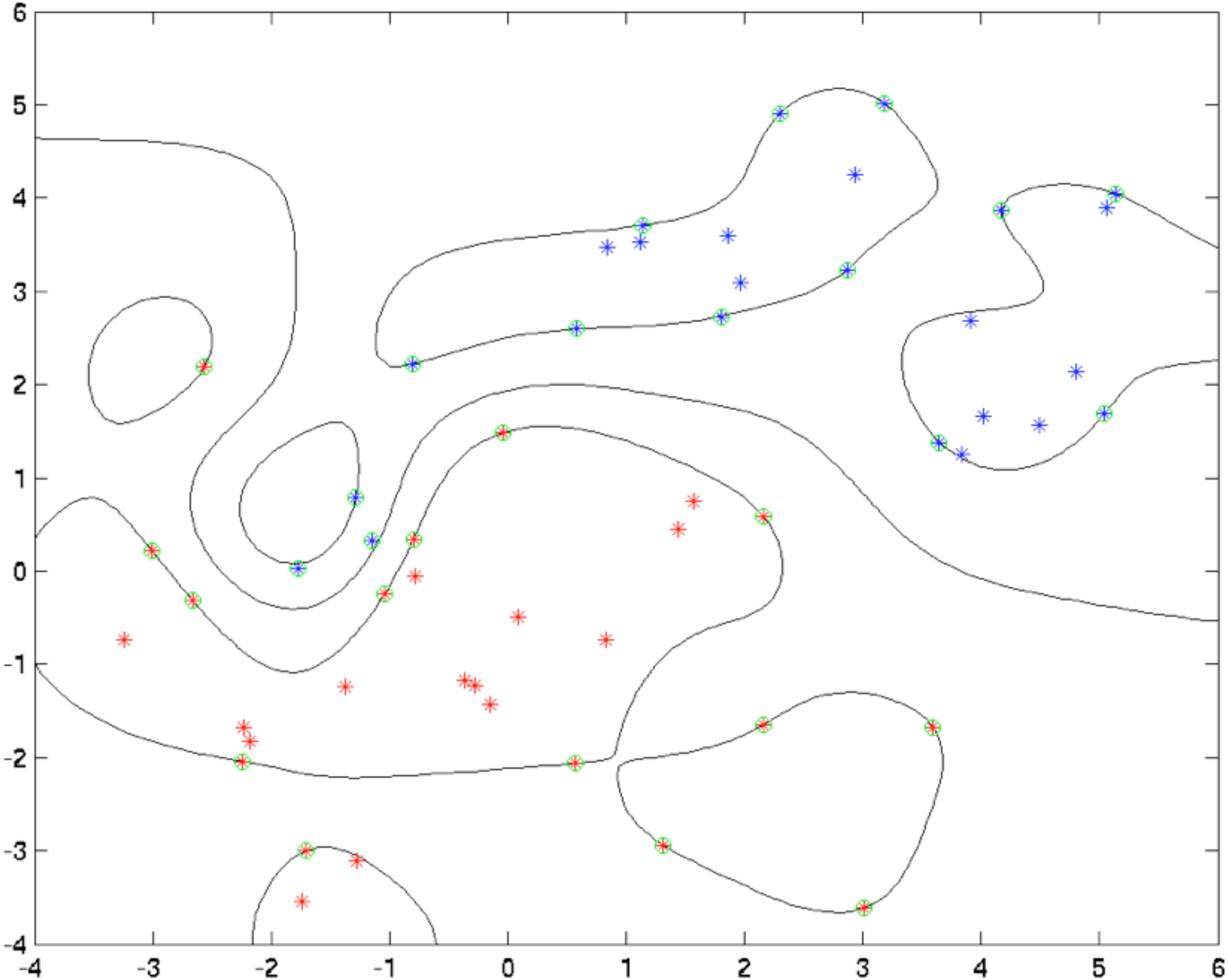

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And now with a very wide kernel

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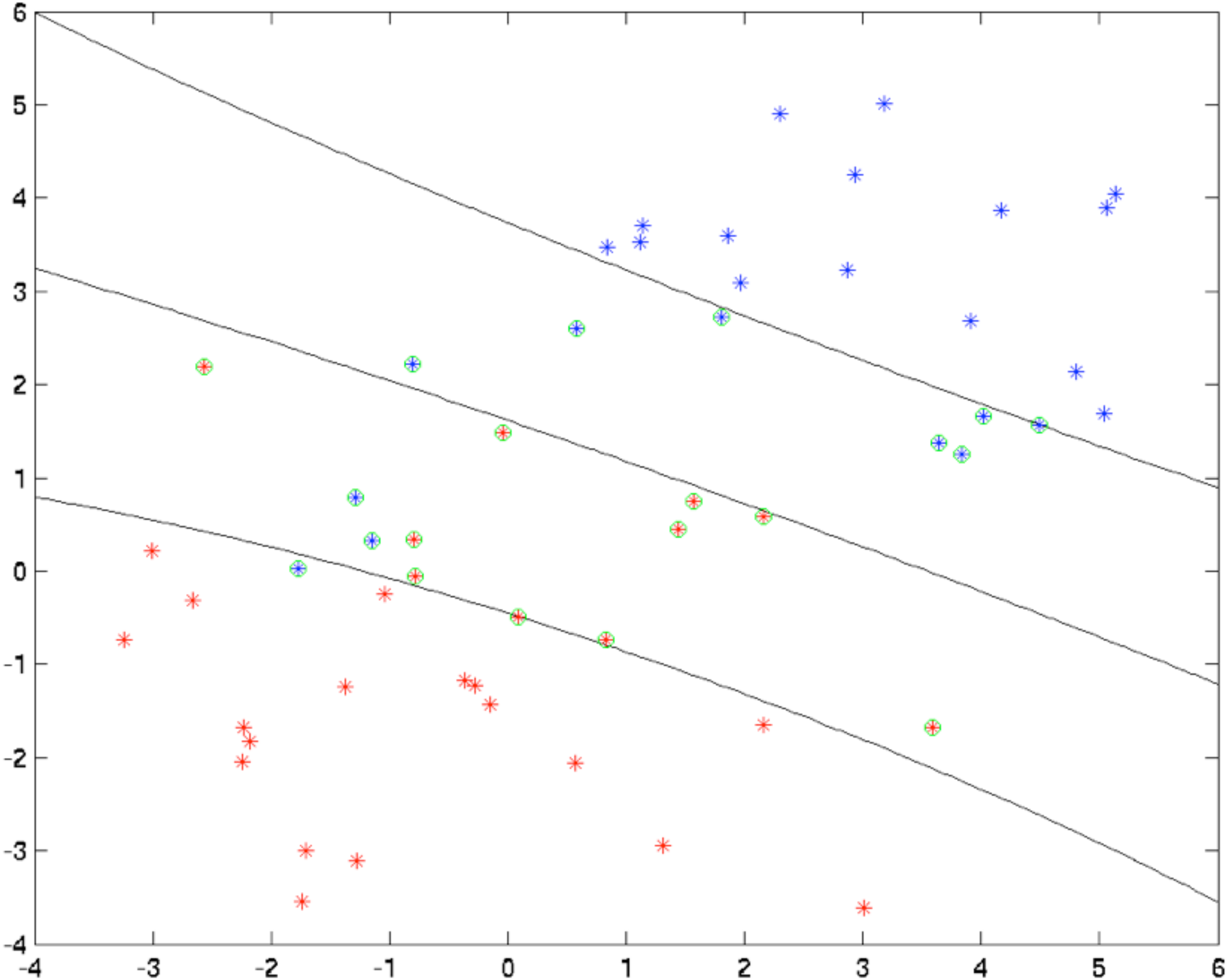

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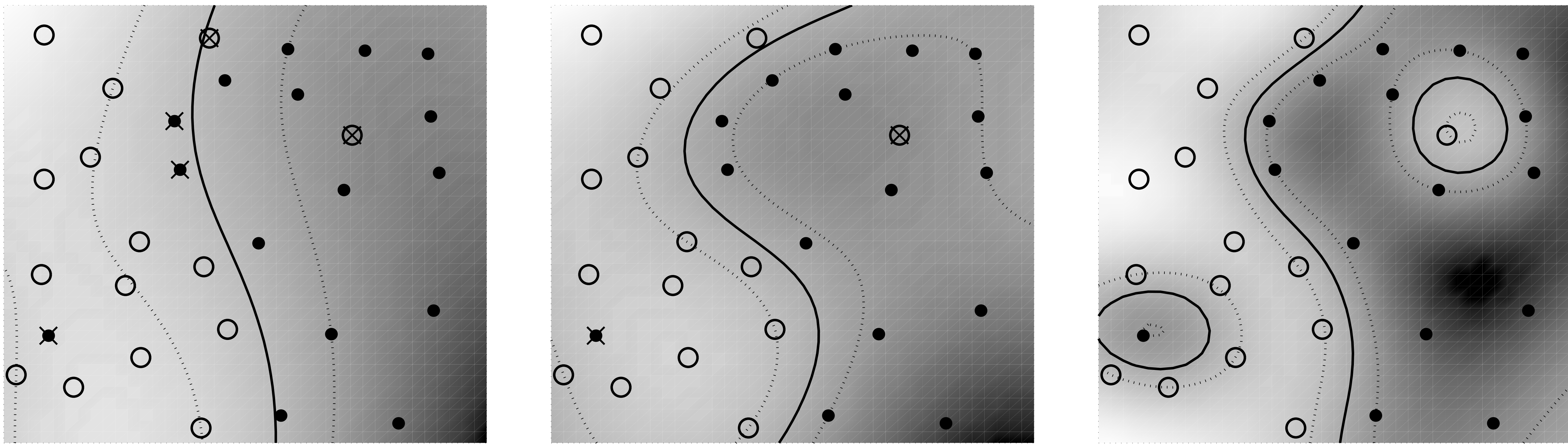
Nonlinear Separation



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

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Overfitting?

- **Huge feature space with kernels: should we worry about overfitting?**
- SVM objective seeks a solution with large margin
  - Theory says that large margin leads to good generalization (we will see this in a couple of lectures)
- **But everything overfits sometimes!!!**
- Can control by:
  - Setting C
  - Choosing a better Kernel
  - Varying parameters of the Kernel (width of Gaussian, etc.)

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Risk and Loss

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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.

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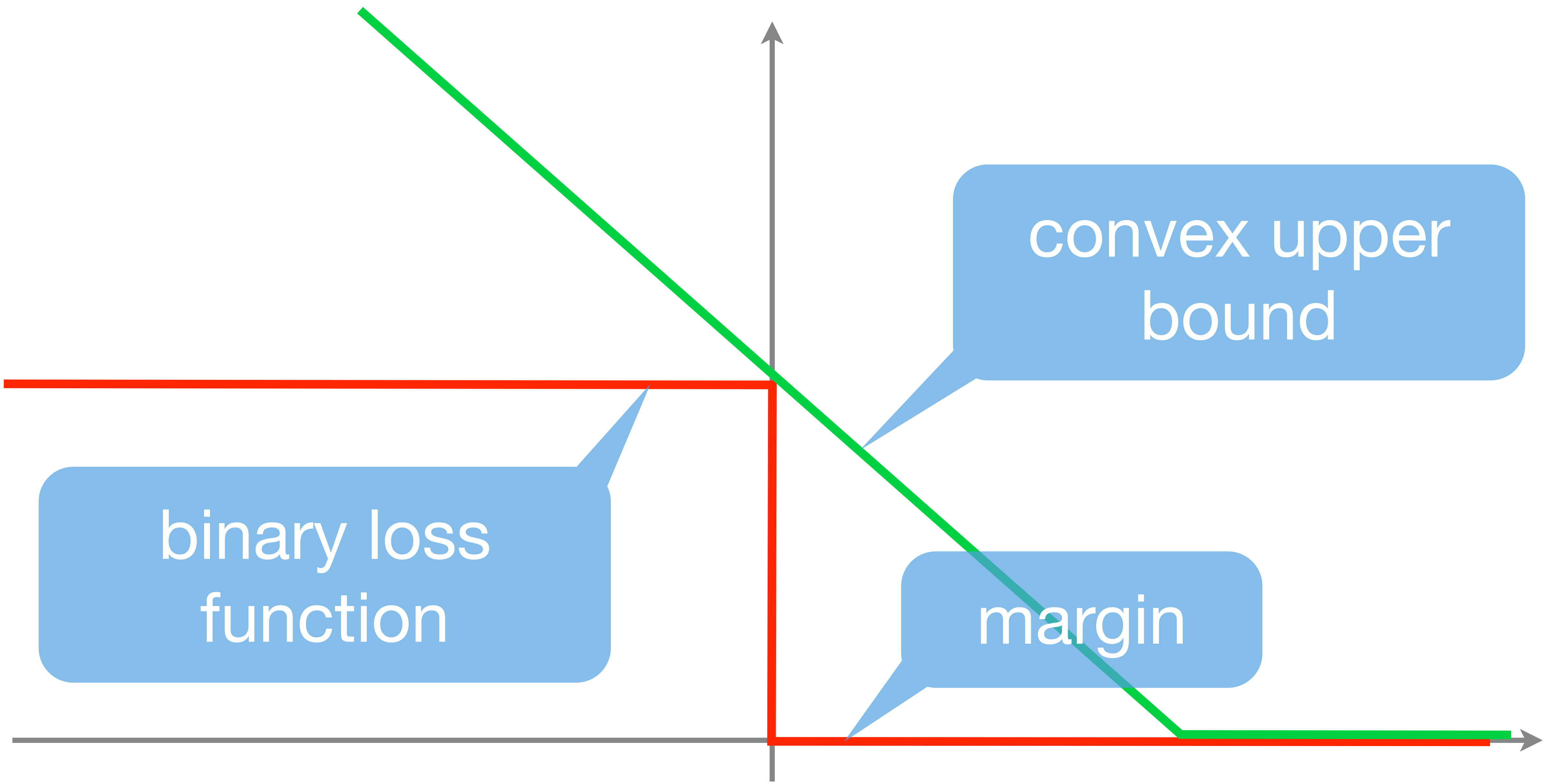
Soft margin as proxy for binary

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



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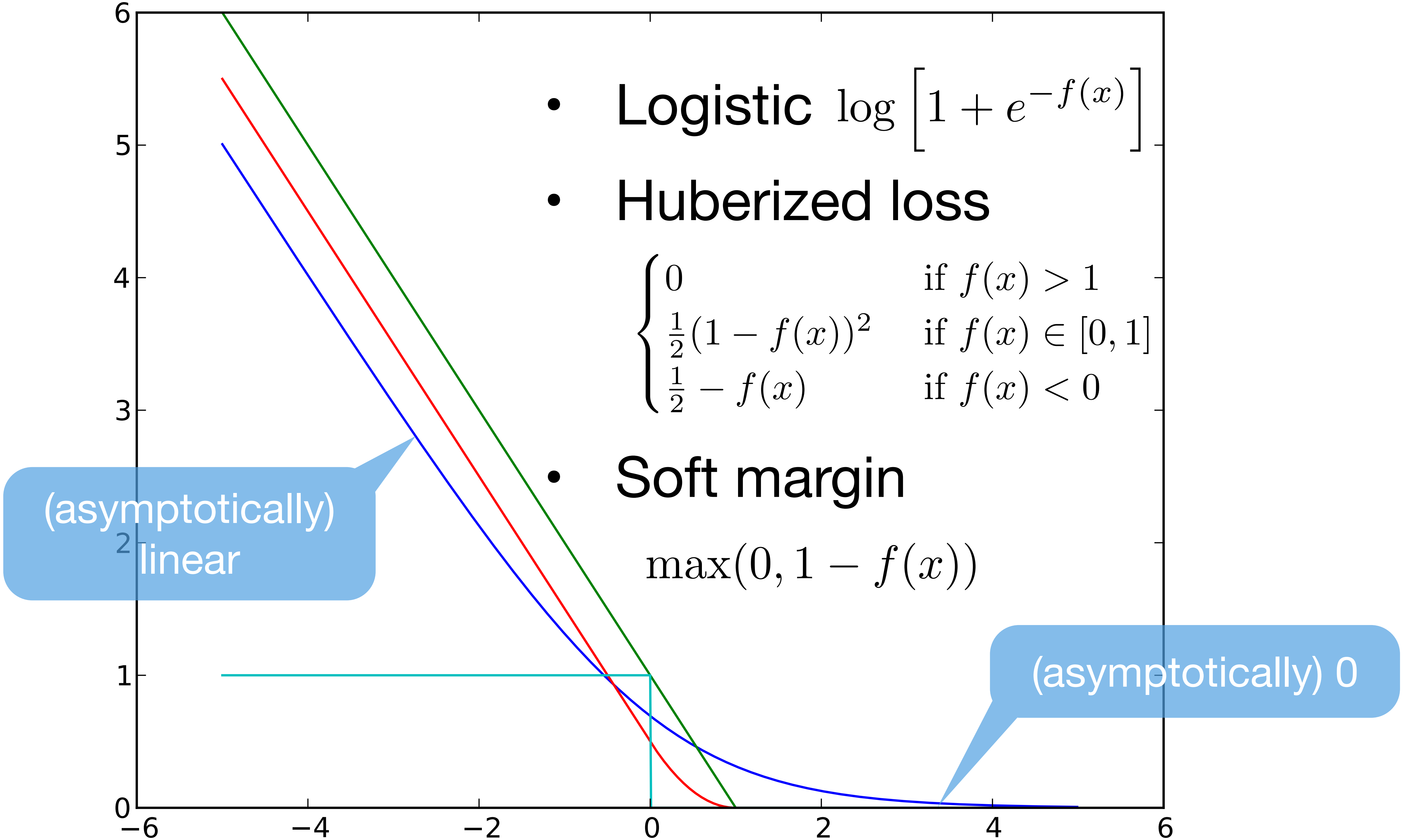
More loss functions



- 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

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

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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

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Support Vector Regression

Regression Estimation

- Find function f minimizing regression error

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

- Compute empirical average

$$R_{\mathrm{emp}}[f] := \frac{1}{m} \sum_{i=1}^{m} l(y_i, f(x_i))$$

Overfitting as we minimize empirical error

- Add regularization for capacity control

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

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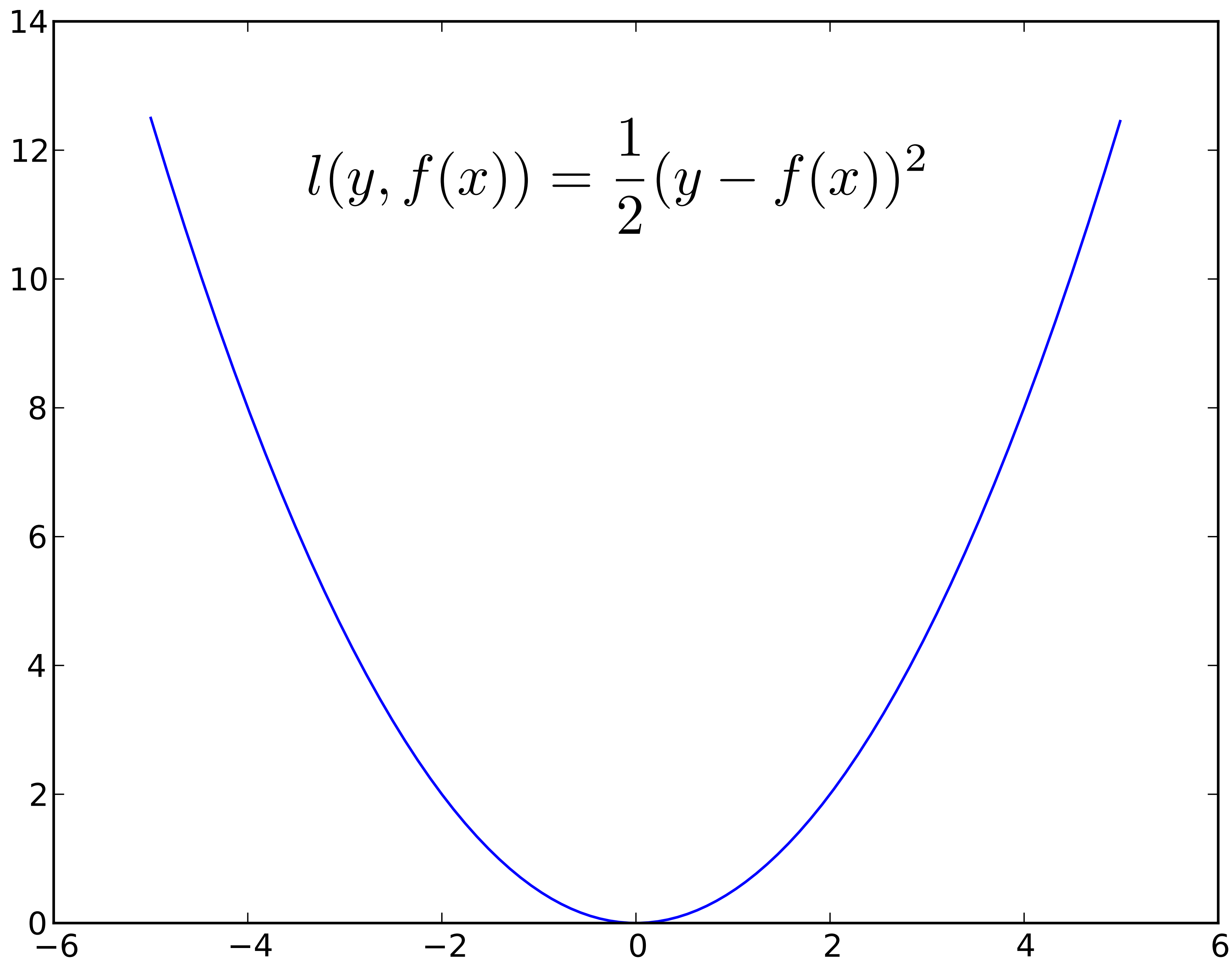
Squared loss



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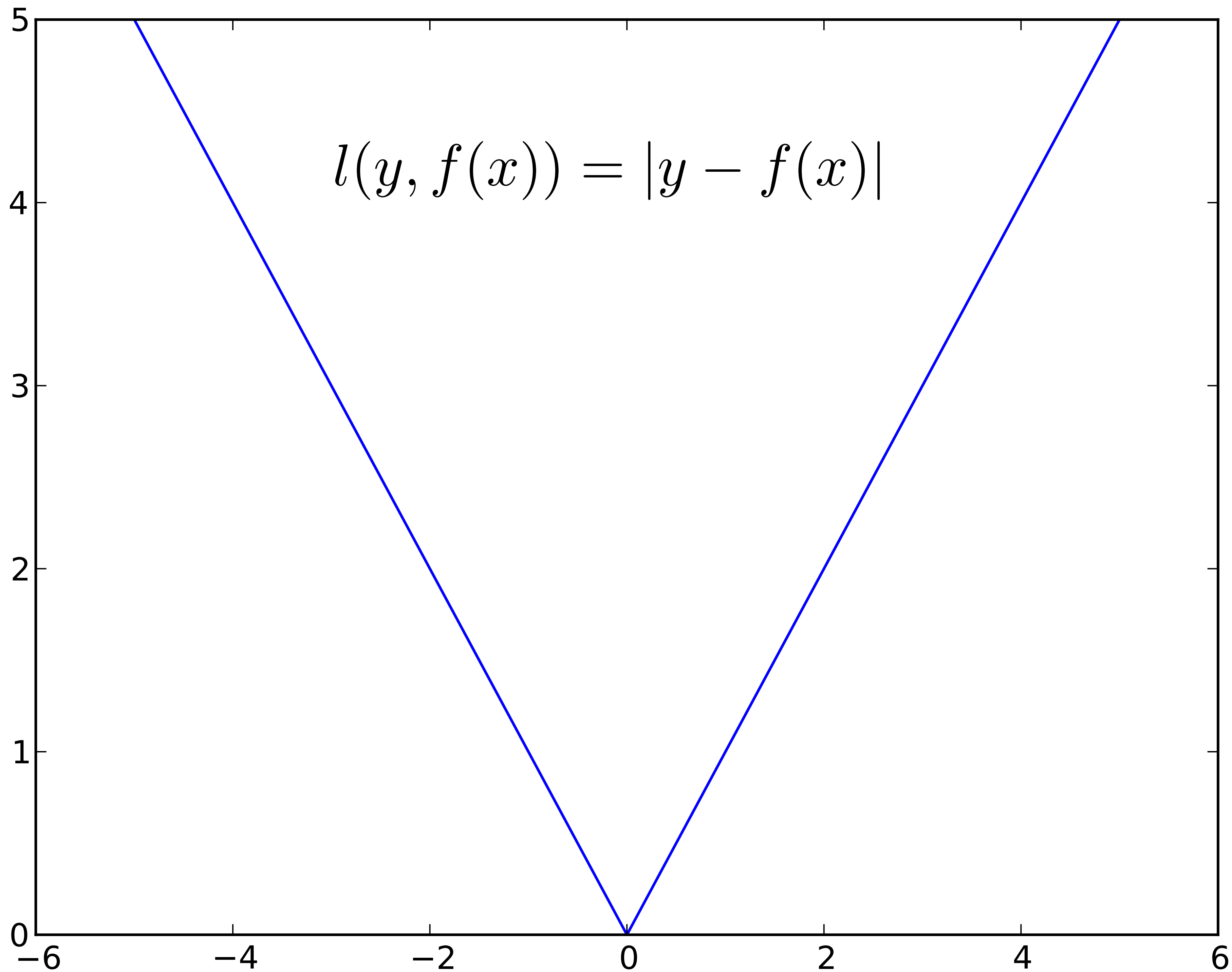
l1 loss



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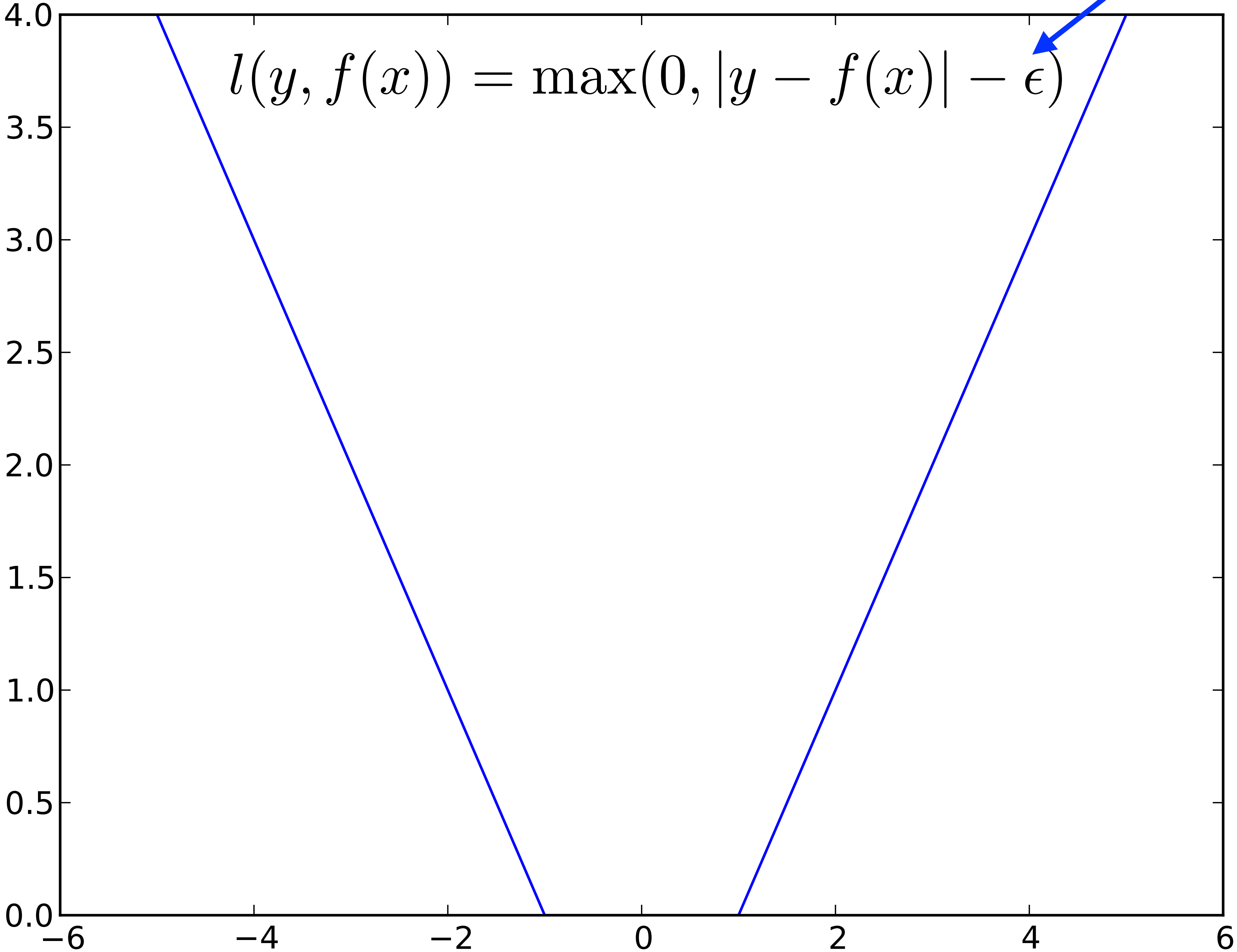
ε-insensitive Loss

allow some deviation
without a penalty



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Penalized least mean squares

- Optimization problem

$$\underset{w}{\text{minimize}} \frac{1}{2m} \sum_{i=1}^{m} (y_i - \langle x_i, w \rangle)^2 + \frac{\lambda}{2} \|w\|^2$$

- Solution

$$\partial_w [\ldots] = \frac{1}{m} \sum_{i=1}^{m} \left[x_i x_i^\top w - x_i y_i \right] + \lambda w$$

$$= \left[\frac{1}{m} X X^\top + \lambda \mathbf{1} \right] w - \frac{1}{m} X y = 0$$

$$\text{hence } w = \left[X X^\top + \lambda m \mathbf{1} \right]^{-1} X y$$

Outer product matrix in X

Conjugate Gradient
Sherman Morrison Woodbury

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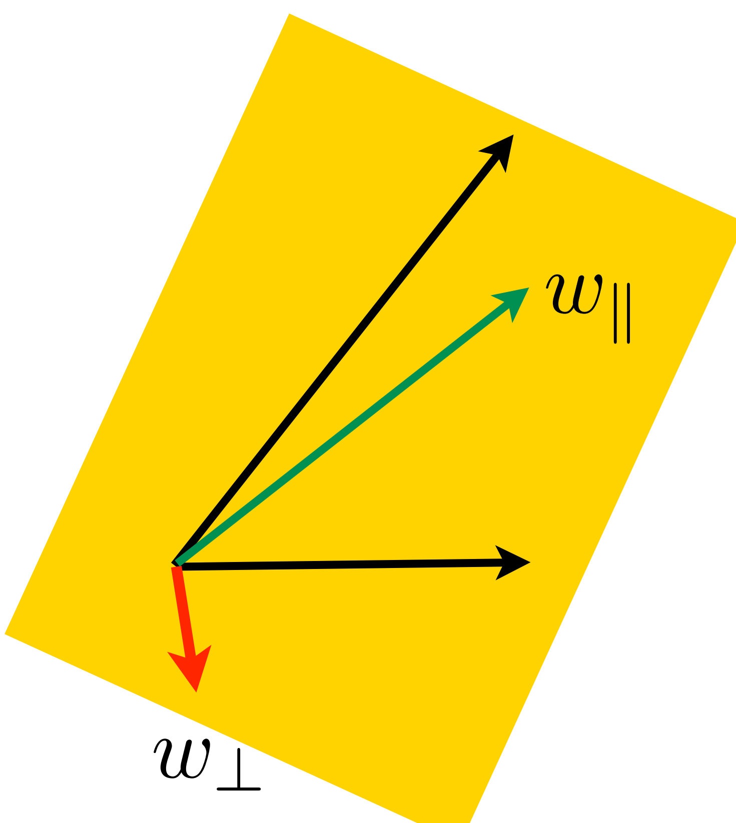
Penalized least mean squares ... now with kernels

- Optimization problem

$$\underset{w}{\text{minimize}} \; \frac{1}{2m} \sum_{i=1}^{m} (y_i - \langle \phi(x_i), w \rangle)^2 + \frac{\lambda}{2} \|w\|^2$$

- Representer Theorem (Kimeldorf & Wahba, 1971)



$$\|w\|^2 = \|w_{\|}\|^2 + \|w_{\perp}\|^2$$

empirical risk dependent

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Penalized least mean squares ... now with kernels

- Optimization problem

$$\underset{w}{\text{minimize}} \frac{1}{2m}\sum_{i=1}^{m}(y_i - \langle \phi(x_i), w\rangle)^2 + \frac{\lambda}{2}\|w\|^2$$

- Representer Theorem (Kimeldorf & Wahba, 1971)
  - Optimal solution is in span of data $w = \sum_i \alpha_i \phi(x_i)$
  - Proof - risk term only depends on data via $\phi(x_i)$
  - Regularization ensures that orthogonal part is 0
- Optimization problem in terms of w

$$\underset{\alpha}{\text{minimize}} \frac{1}{2m}\sum_{i=1}^{m}\Big(y_i - \sum_j K_{ij}\alpha_j\Big)^2 + \frac{\lambda}{2}\sum_{i,j}\alpha_i\alpha_j K_{ij}$$

solve for $\alpha = (K + m\lambda\mathbf{1})^{-1}y$ as linear system

Penalized least mean squares ... now with kernels

- Optimization problem

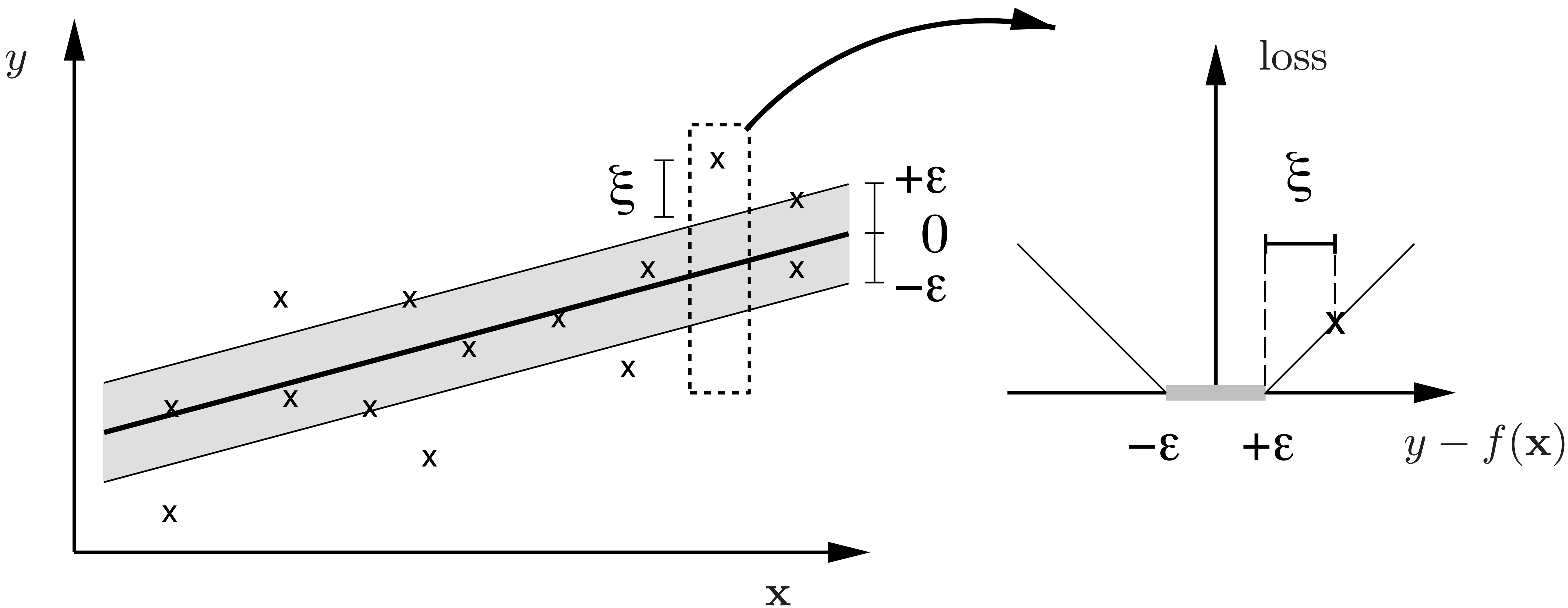
$$\underset{w}{\text{minimize}} \frac{1}{2m} \sum_{i=1}^{m} (y_i - \langle \phi(x_i), w \rangle)^2 + \frac{\lambda}{2} \|w\|^2$$

- Representer Theorem (Kimeldorf & Wahba, 1971)
  - Optimal solution is in span of data $\boxed{w = \sum_i \alpha_i \phi(x_i)}$
  - Proof - risk term only depends on data via $\phi(x_i)$
  - Regularization ensures that orthogonal part is 0
- Optimization problem in terms of w

$$\underset{\alpha}{\text{minimize}} \frac{1}{2m} \sum_{i=1}^{m} \left(y_i - \sum_j K_{ij} \alpha_j \right)^2 + \frac{\lambda}{2} \sum_{i,j} \alpha_i \alpha_j K_{ij}$$

solve for $\alpha = (K + m\lambda \mathbf{1})^{-1} y$ as linear system

SVM Regression (ϵ-insensitive loss)



don’t care about deviations within the tube

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SVM Regression (ϵ-insensitive loss)

- Optimization Problem (as constrained QP)

$$\underset{w,b}{\text{minimize}} \ \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{m}[\xi_i + \xi_i^*]$$

$$\text{subject to } \ \langle w, x_i \rangle + b \leq y_i + \epsilon + \xi_i \ \text{ and } \xi_i \geq 0$$

$$\langle w, x_i \rangle + b \geq y_i - \epsilon - \xi_i^* \ \text{ and } \xi_i^* \geq 0$$

- Lagrange Function

$$L = \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{m}[\xi_i + \xi_i^*] - \sum_{i=1}^{m}[\eta_i\xi_i + \eta_i^*\xi_i^*] +$$

$$\sum_{i=1}^{m}\alpha_i\left[\langle w, x_i \rangle + b - y_i - \epsilon - \xi_i\right] + \sum_{i=1}^{m}\alpha_i^*\left[y_i - \epsilon - \xi_i^* - \langle w, x_i \rangle - b\right]$$

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SVM Regression (ϵ-insensitive loss)

- First order conditions

$$\partial_w L = 0 = w + \sum_i [\alpha_i - \alpha_i^*] x_i$$

$$\partial_b L = 0 = \sum_i [\alpha_i - \alpha_i^*]$$

$$\partial_{\xi_i} L = 0 = C - \eta_i - \alpha_i$$

$$\partial_{\xi_i^*} L = 0 = C - \eta_i^* - \alpha_i^*$$

- Dual problem

$$\underset{\alpha,\alpha^*}{\text{minimize}} \;\; \frac{1}{2}(\alpha - \alpha^*)^\top K(\alpha - \alpha^*) + \epsilon 1^\top(\alpha + \alpha^*) + y^\top(\alpha - \alpha^*)$$

$$\text{subject to } 1^\top(\alpha - \alpha^*) = 0 \text{ and } \alpha_i, \alpha_i^* \in [0, C]$$

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Properties

- Ignores 'typical' instances with small error
- Only upper or lower bound active at any time
- QP in 2n variables as cheap as SVM problem
- Robustness with respect to outliers
  - l_1 loss yields same problem without epsilon
  - Huber's robust loss yields similar problem but with added quadratic penalty on coefficients

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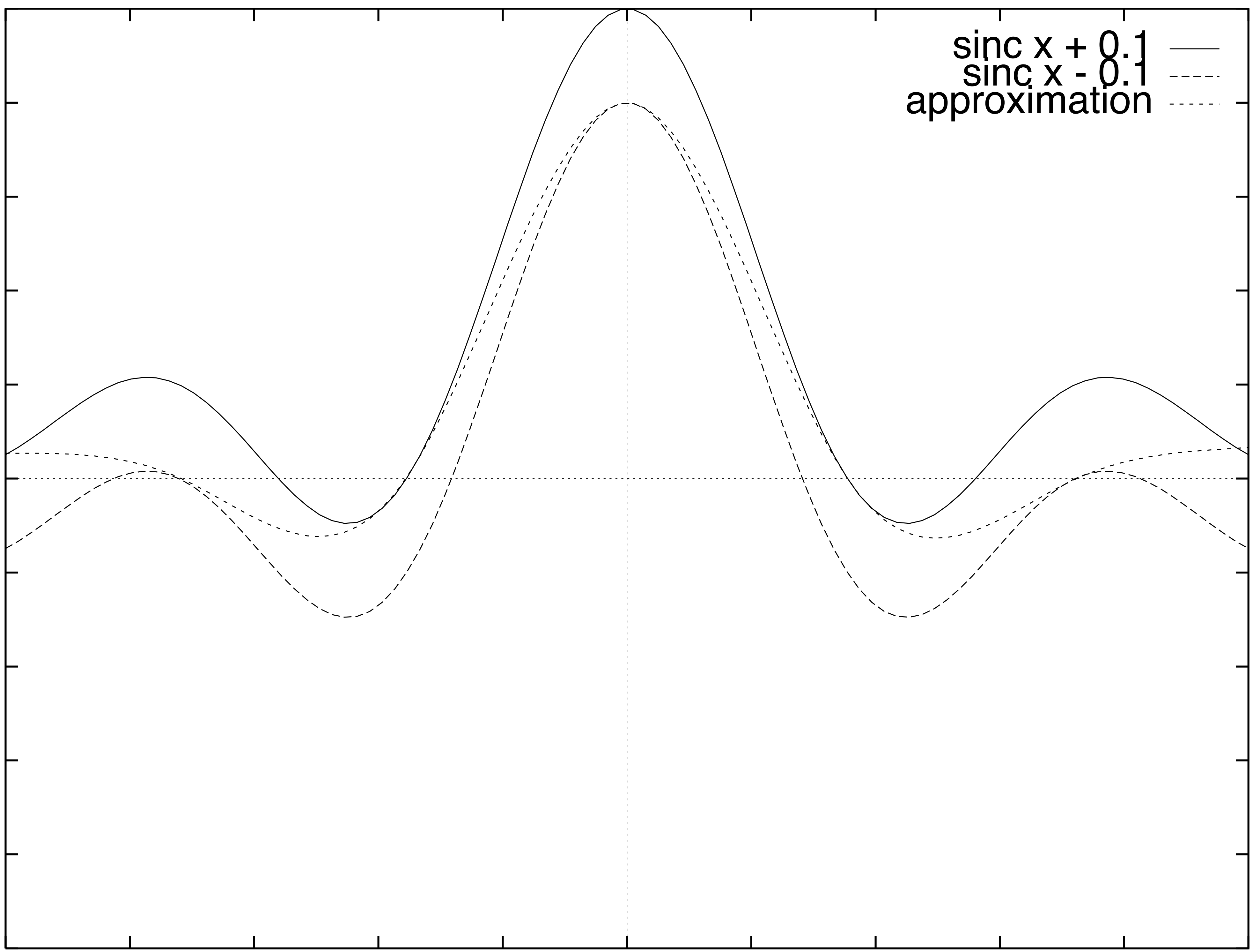
Regression example



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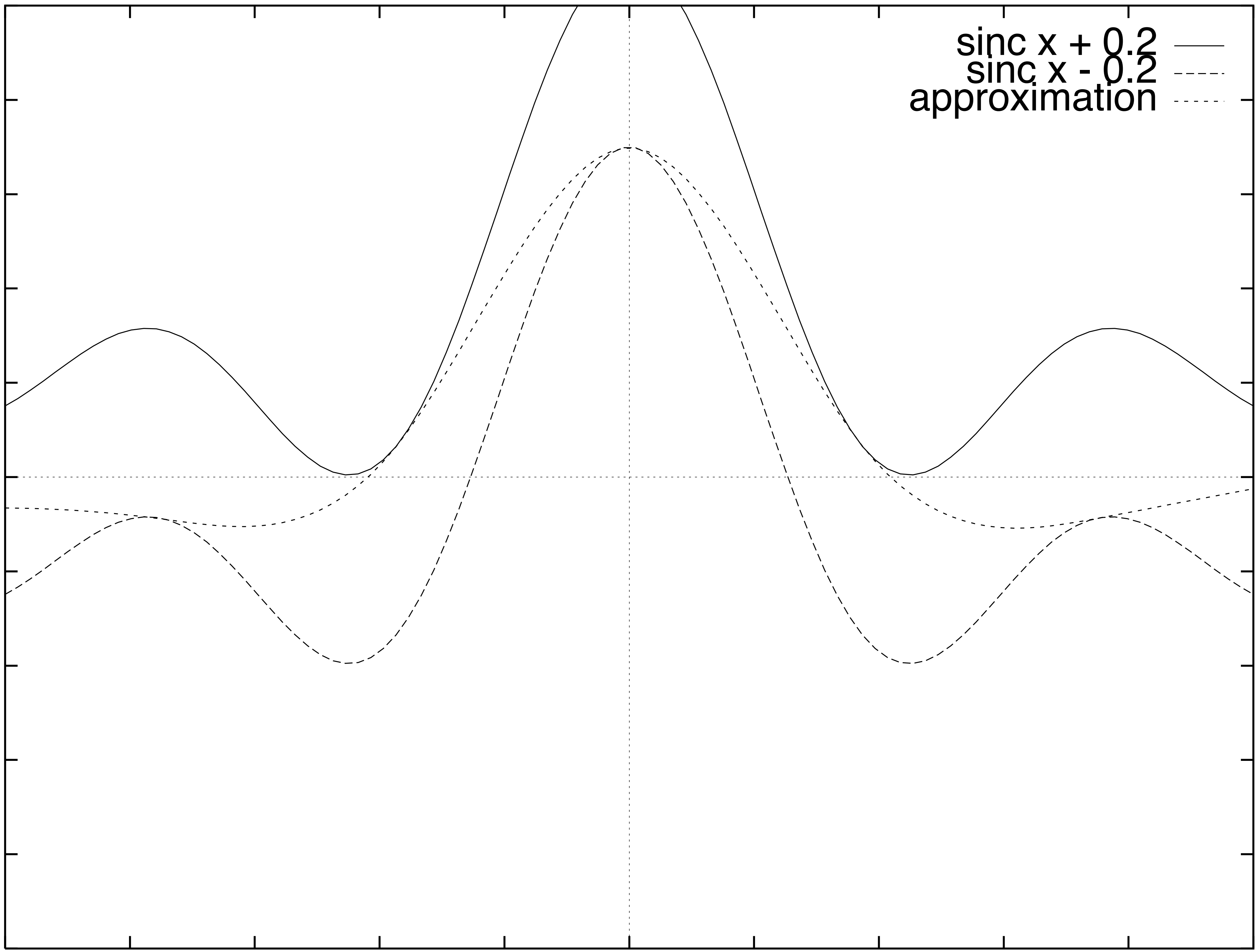
Regression example



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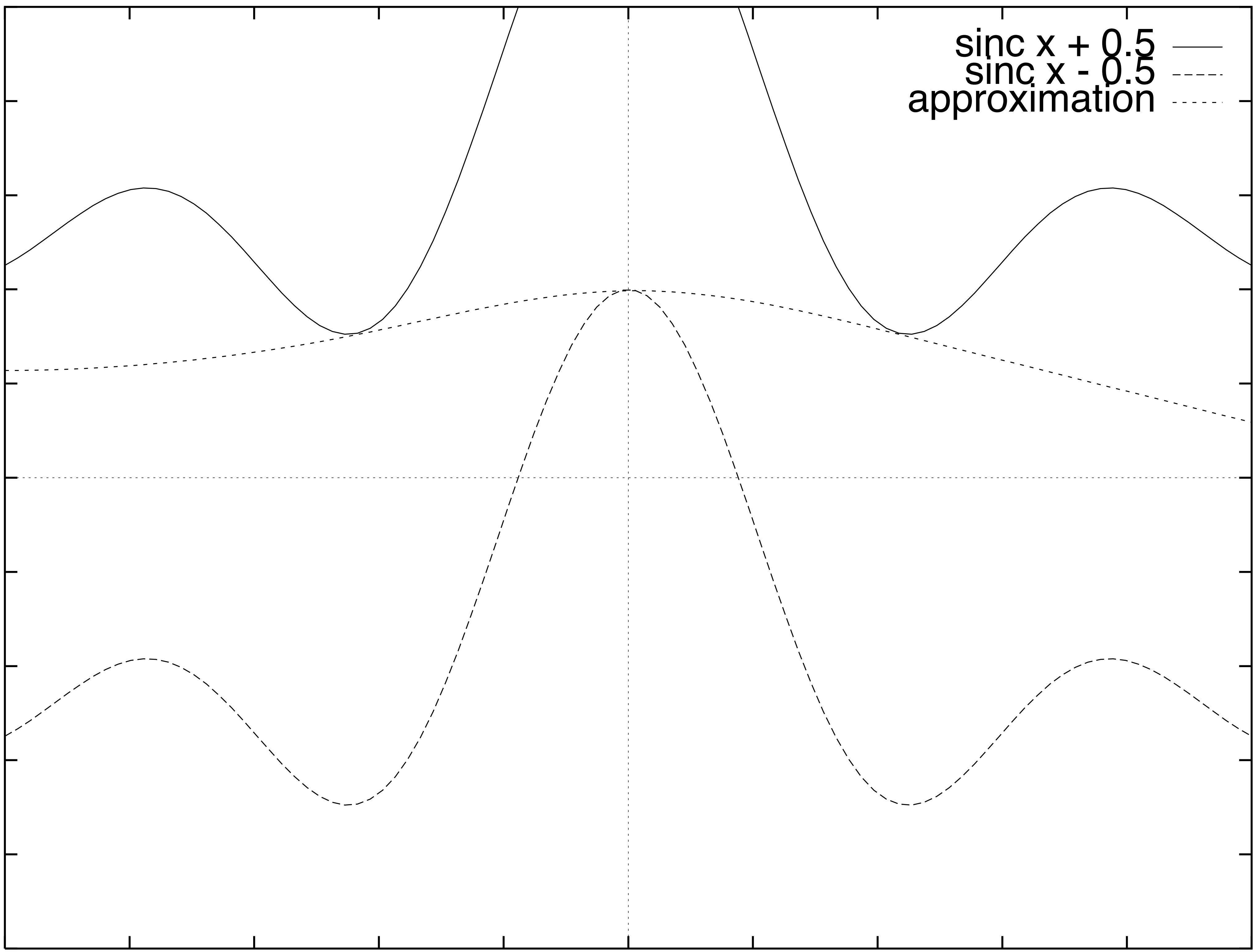
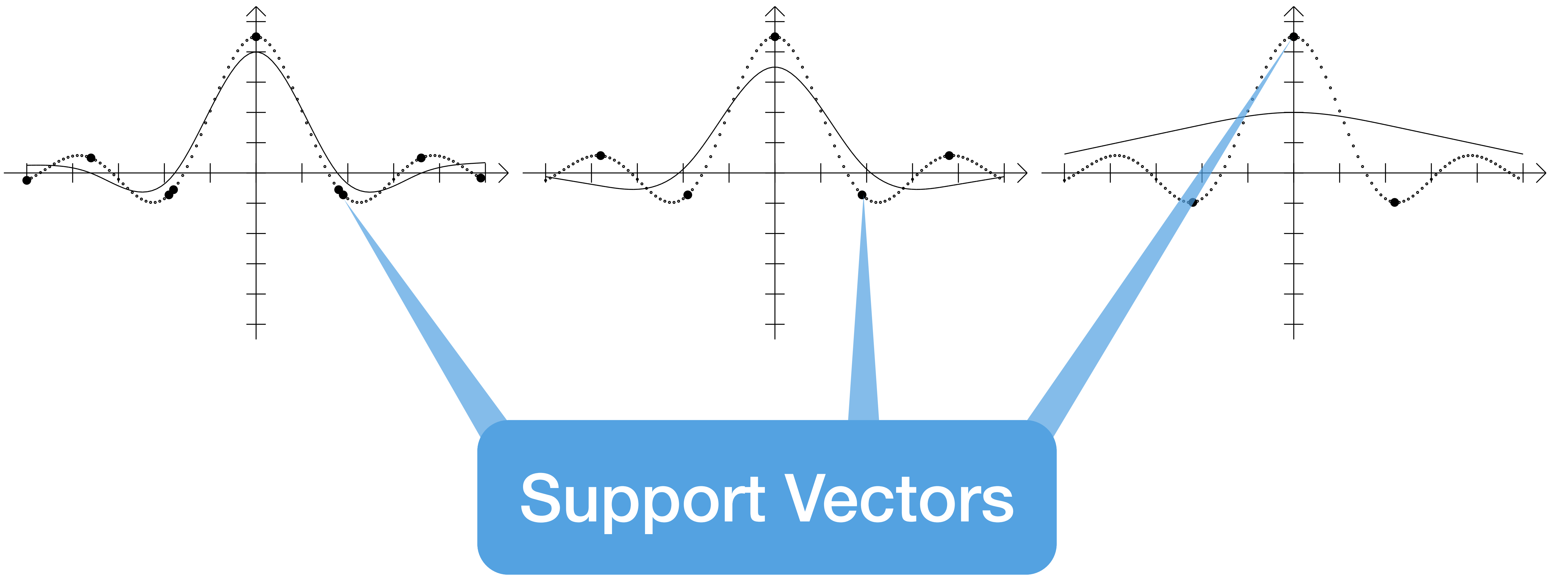
Regression example



Regression example



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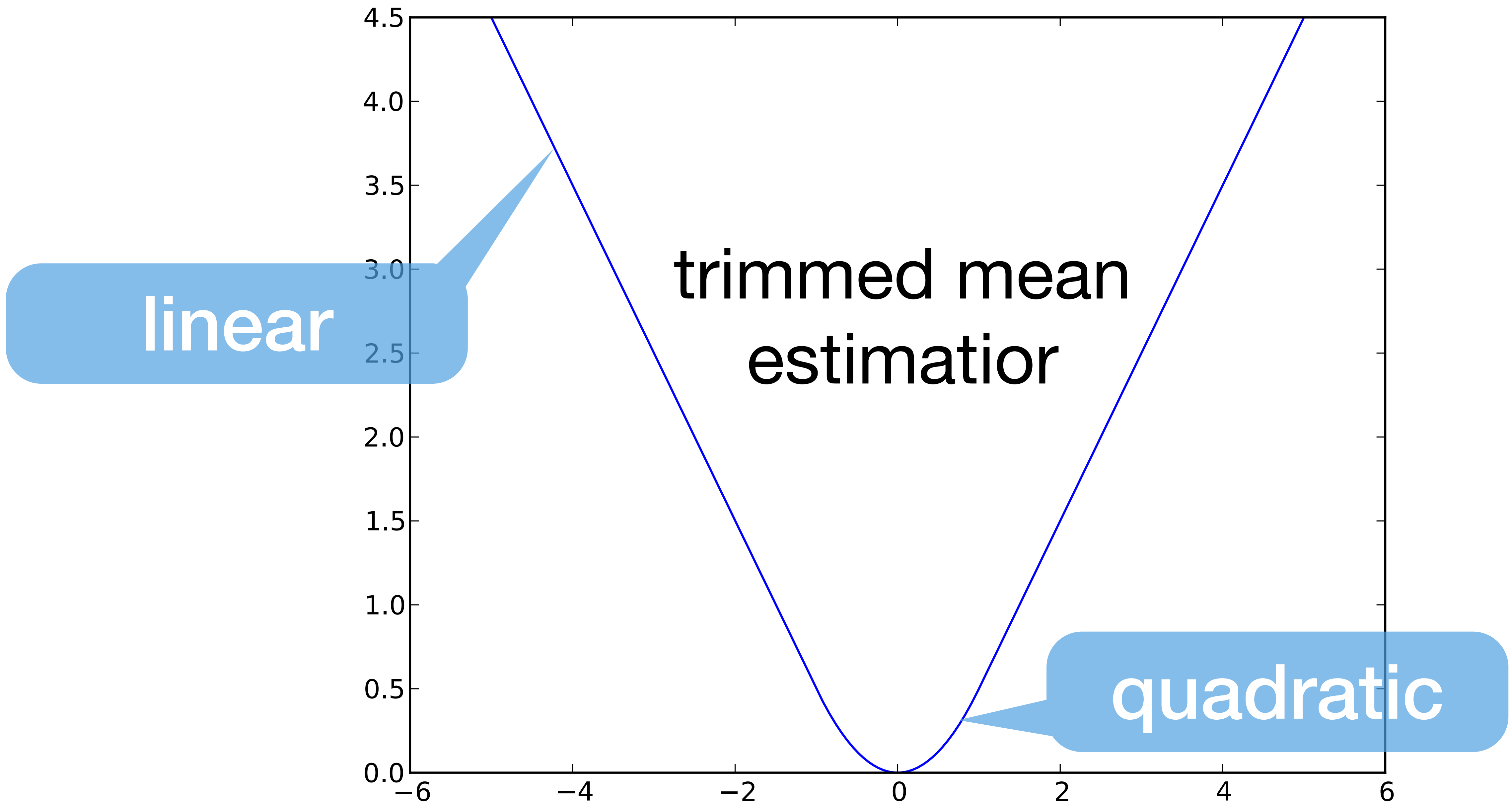
Huber's robust loss

$$l(y, f(x)) = \begin{cases} \frac{1}{2}(y - f(x))^2 & \text{if } |y - f(x)| < 1 \\ |y - f(x)| - \frac{1}{2} & \text{otherwise} \end{cases}$$



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Summary

- Advantages:
  - Kernels allow very flexible hypotheses
  - Poly-time exact optimization methods rather than approximate methods
  - Soft-margin extension permits mis-classified examples
  - Variable-sized hypothesis space
  - Excellent results (1.1% error rate on handwritten digits vs. LeNet's 0.9%)

- Disadvantages:
  - Must choose kernel parameters
  - Very large problems computationally intractable
  - Batch algorithm

slide by Sanja Fidler

Software

- `SVM`^{light}: one of the most widely used SVM packages. Fast optimization, can handle very large datasets, C++ code.
- `LIBSVM`
- Both of these handle multi-class, weighted SVM for unbalanced data, etc.
- There are several new approaches to solving the SVM objective that can be much faster:
  - Stochastic subgradient method (discussed in a few lectures)
  - Distributed computation (also to be discussed)
- See `http://mloss.org`, “machine learning open source software”

slide by Alex Smola

Next Lecture:

Decision Trees