MACHINE LEARNING DEPARTMENT

Introduction to Machine Learning

4. Perceptron and Kernels

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10-701x

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10-701: Machine Learning (f13)

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10-701 Classification Contest!

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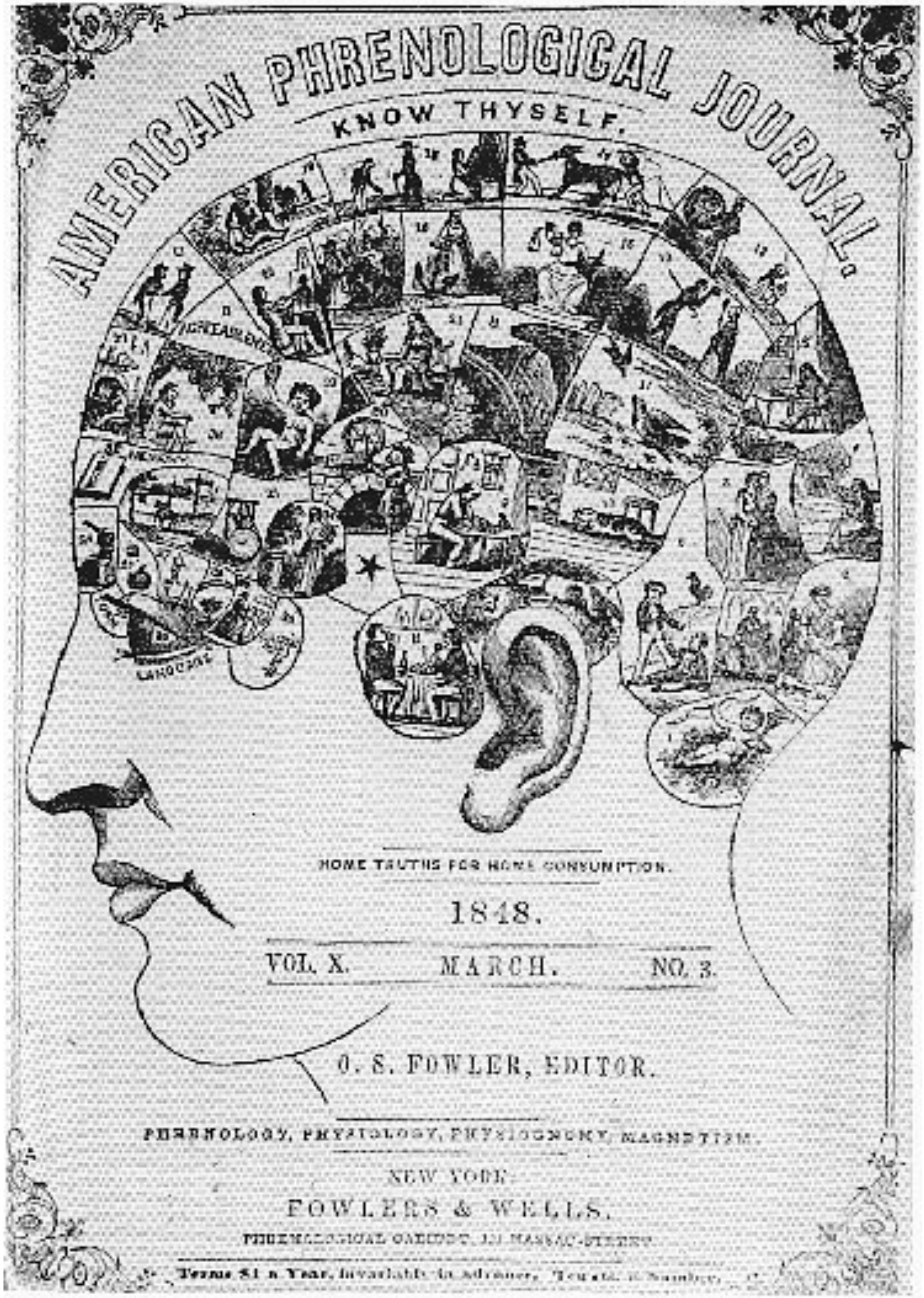
Outline

- Perceptron
  - Hebbian learning & biology
  - Algorithm
  - Convergence analysis
- Features and preprocessing
  - Nonlinear separation
  - Perceptron in feature space
- Kernels
  - Kernel trick
  - Properties
  - Examples

Perceptron

Frank Rosenblatt



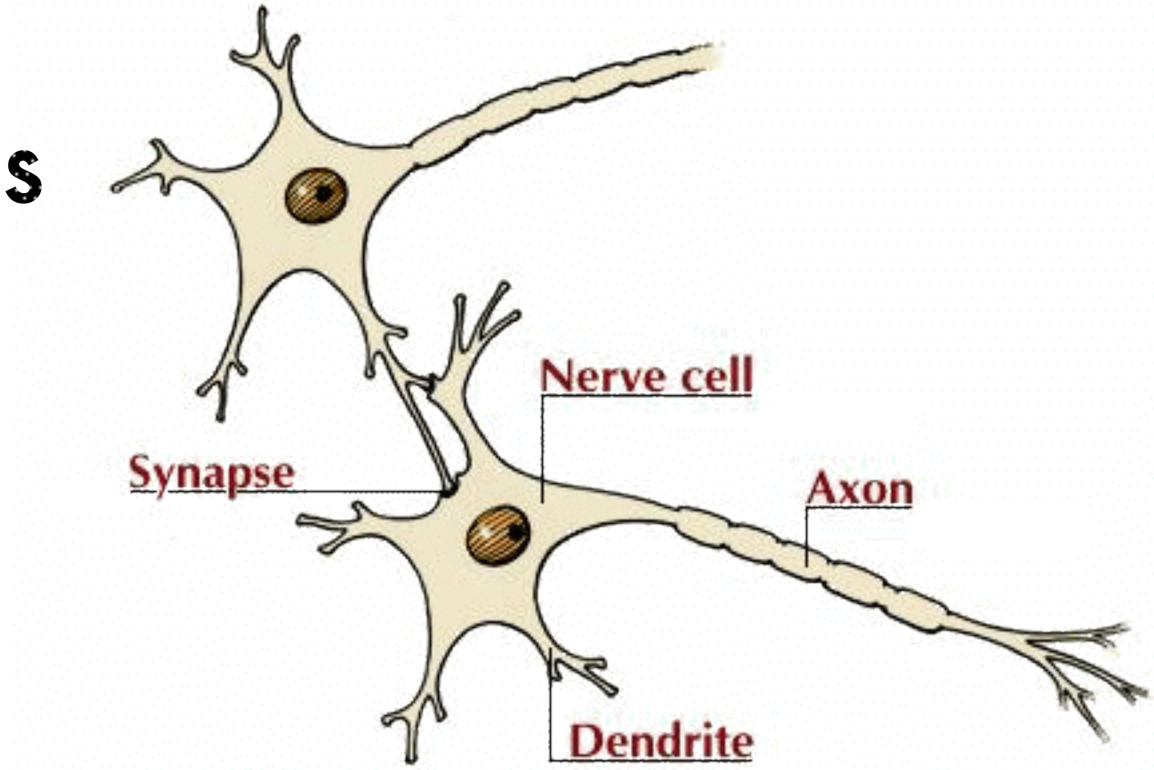
early theories of the brain

Biology and Learning

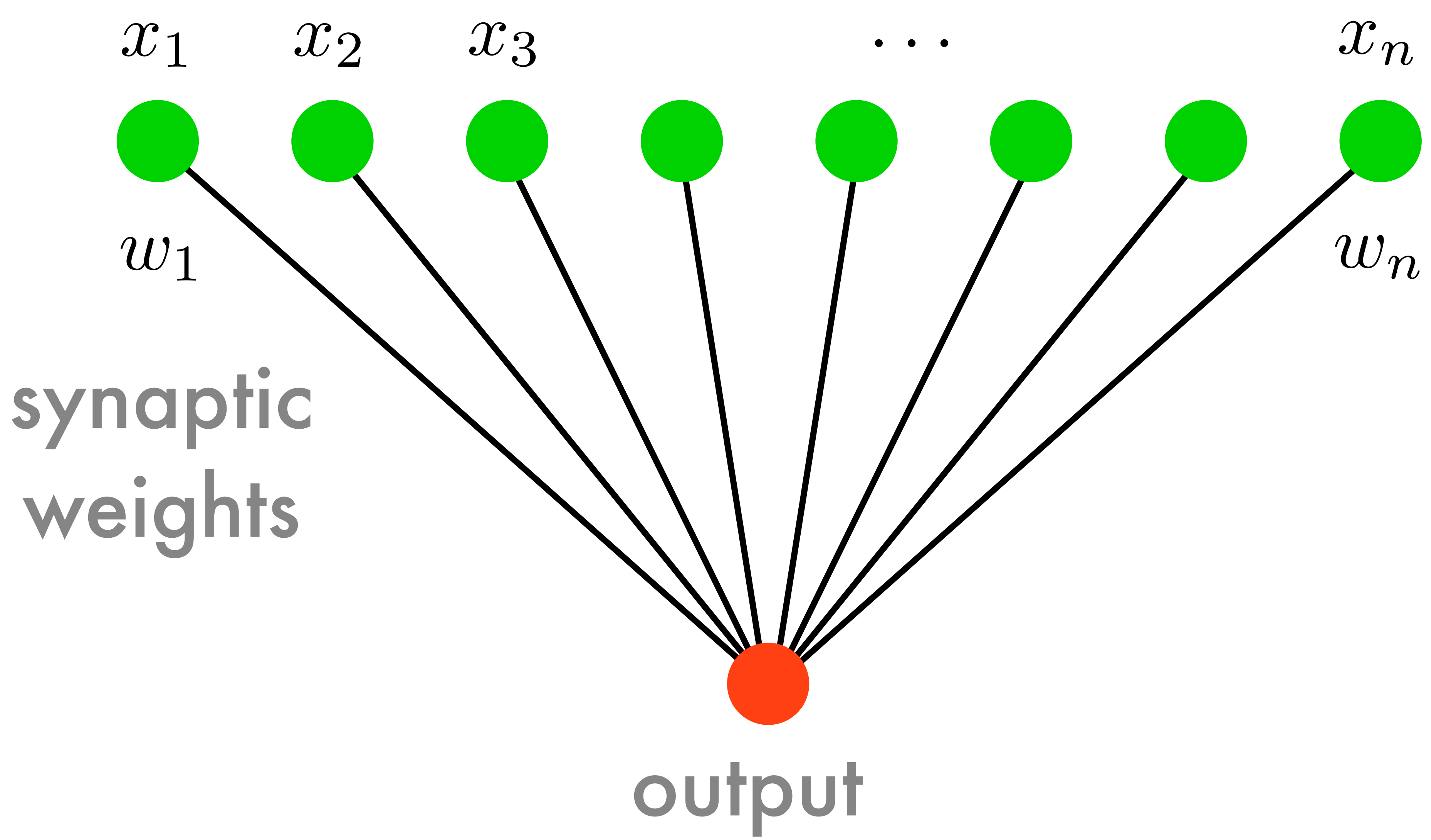
- Basic Idea
  - Good behavior should be rewarded, bad behavior punished (or not rewarded). This improves system fitness.
  - Killing a sabertooth tiger should be rewarded ...
  - Correlated events should be combined.
  - Pavlov's salivating dog.
- Training mechanisms
  - Behavioral modification of individuals (learning) Successful behavior is rewarded (e.g. food).
  - Hard-coded behavior in the genes (instinct) The wrongly coded animal does not reproduce.

Neurons

- Soma (CPU)
  Cell body - combines signals
- Dendrite (input bus)
  Combines the inputs from several other nerve cells
- Synapse (interface)
  Interface and parameter store between neurons
- Axon (cable)
  May be up to 1m long and will transport the activation signal to neurons at different locations



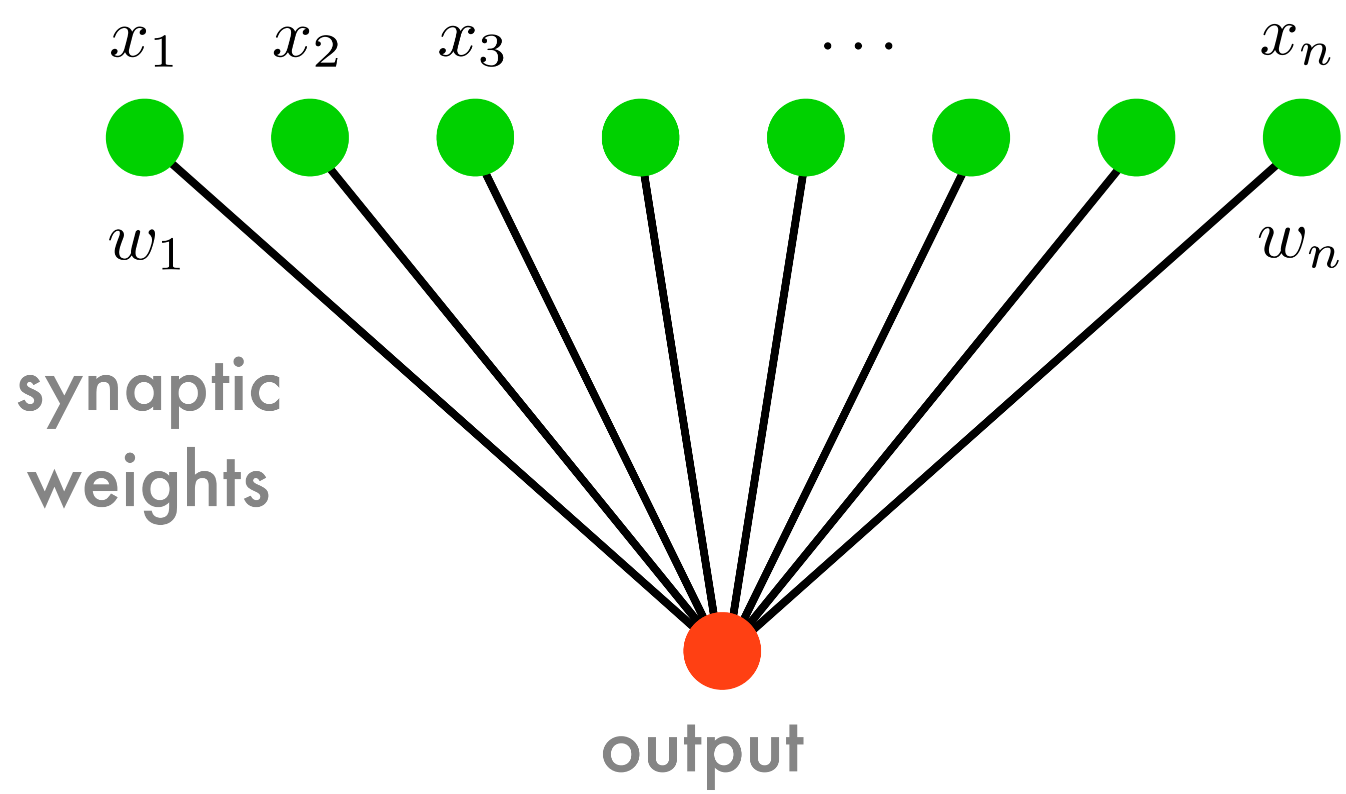
Neurons



$$f(x) = \sum_i w_i x_i = \langle w, x \rangle$$

Perceptron

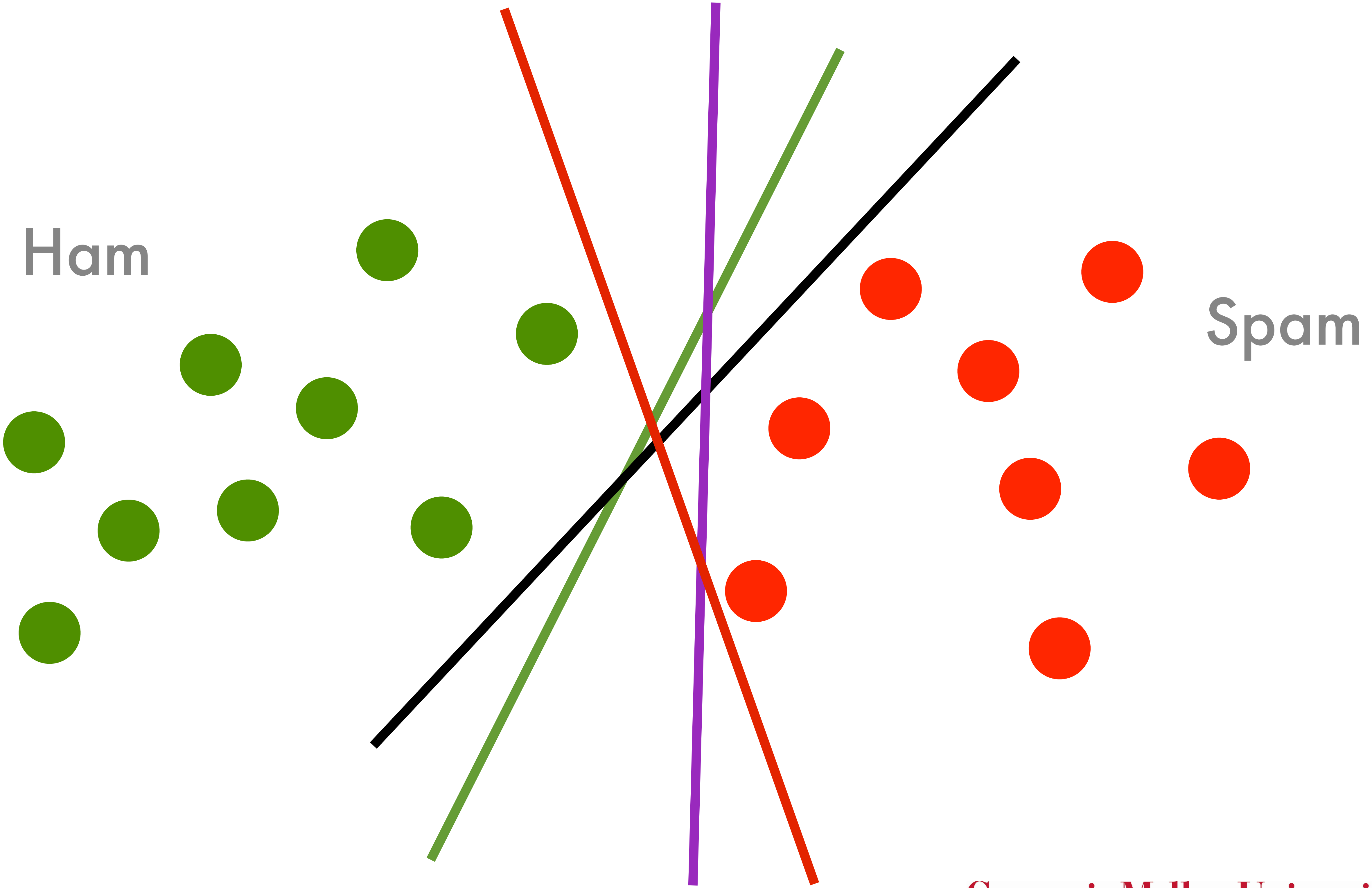
- Weighted linear combination
- Nonlinear decision function
- Linear offset (bias)



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

- Linear separating hyperplanes (spam/ham, novel/typical, click/no click)
- Learning
  Estimating the parameters w and b

Perceptron



The Perceptron

initialize $w = 0$ and $b = 0$
repeat
  if $y_i \left[\langle w, x_i \rangle + b\right] \leq 0$ **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 $f(x) = \sum_{i \in I} y_i \langle x_i, x \rangle + b$

Convergence Theorem

- If there exists some (w^*, b^*) with unit length and
$$y_i \left[\langle x_i, w^* \rangle + b^*\right] \geq \rho \text{ for all } i$$
then the perceptron converges to a linear separator after a number of steps bounded by
$$\left({b^*}^2 + 1\right)\left(r^2 + 1\right)\rho^{-2} \text{ where } \|x_i\| \leq r$$
- Dimensionality independent
- Order independent (i.e. also worst case)
- Scales with 'difficulty' of problem

Proof

Starting Point

We start from $w_1 = 0$ and $b_1 = 0$.

Step 1: Bound on the increase of alignment

Denote by w_i the value of w at step i (analogously b_i).

Alignment: $\langle (w_i, b_i), (w^*, b^*) \rangle$

For error in observation (x_i, y_i) we get

$$
\begin{aligned}
&\langle (w_{j+1}, b_{j+1}) \cdot (w^*, b^*) \rangle \\
&= \langle \left[(w_j, b_j) + y_i(x_i, 1) \right], (w^*, b^*) \rangle \\
&= \langle (w_j, b_j), (w^*, b^*) \rangle + y_i \langle (x_i, 1) \cdot (w^*, b^*) \rangle \\
&\geq \langle (w_j, b_j), (w^*, b^*) \rangle + \rho \\
&\geq j\rho.
\end{aligned}
$$

Alignment increases with number of errors.

Proof

Step 2: Cauchy-Schwartz for the Dot Product

$$\begin{aligned}\langle (w_{j+1}, b_{j+1}) \cdot (w^*, b^*) \rangle &\leq \|(w_{j+1}, b_{j+1})\| \, \|(w^*, b^*)\| \\ &= \sqrt{1 + (b^*)^2} \|(w_{j+1}, b_{j+1})\|\end{aligned}$$

Step 3: Upper Bound on $\|(w_j, b_j)\|$

If we make a mistake we have

$$\begin{aligned}\|(w_{j+1}, b_{j+1})\|^2 &= \|(w_j, b_j) + y_i(x_i, 1)\|^2 \\ &= \|(w_j, b_j)\|^2 + 2y_i \langle (x_i, 1), (w_j, b_j) \rangle + \|(x_i, 1)\|^2 \\ &\leq \|(w_j, b_j)\|^2 + \|(x_i, 1)\|^2 \\ &\leq j(R^2 + 1).\end{aligned}$$

Step 4: Combination of first three steps

$$j\rho \leq \sqrt{1 + (b^*)^2} \|(w_{j+1}, b_{j+1})\| \leq \sqrt{j(R^2 + 1)((b^*)^2 + 1)}$$

Solving for j proves the theorem.

Consequences

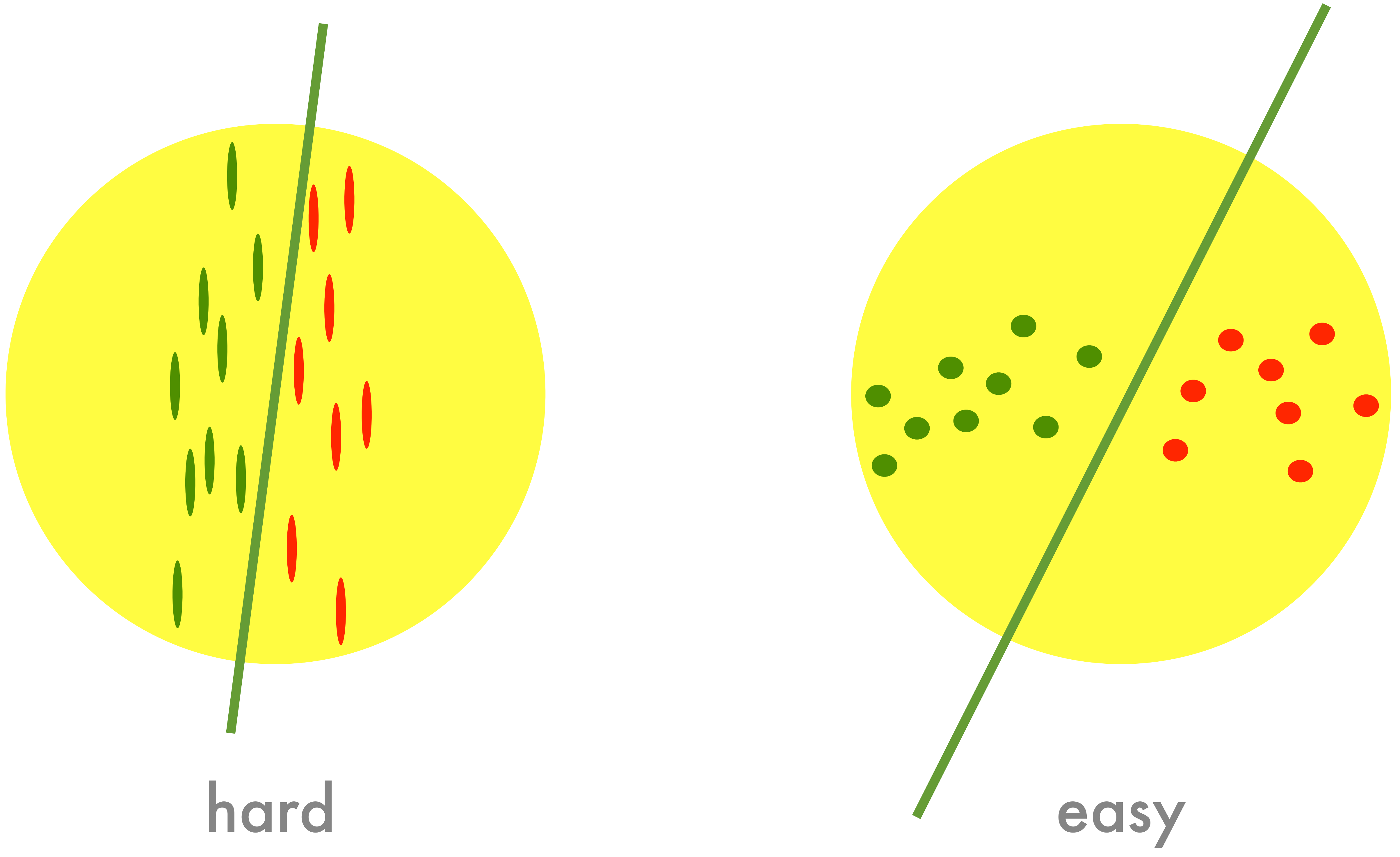
- Only need to store errors.
  This gives a compression bound for perceptron.
- Stochastic gradient descent on hinge loss

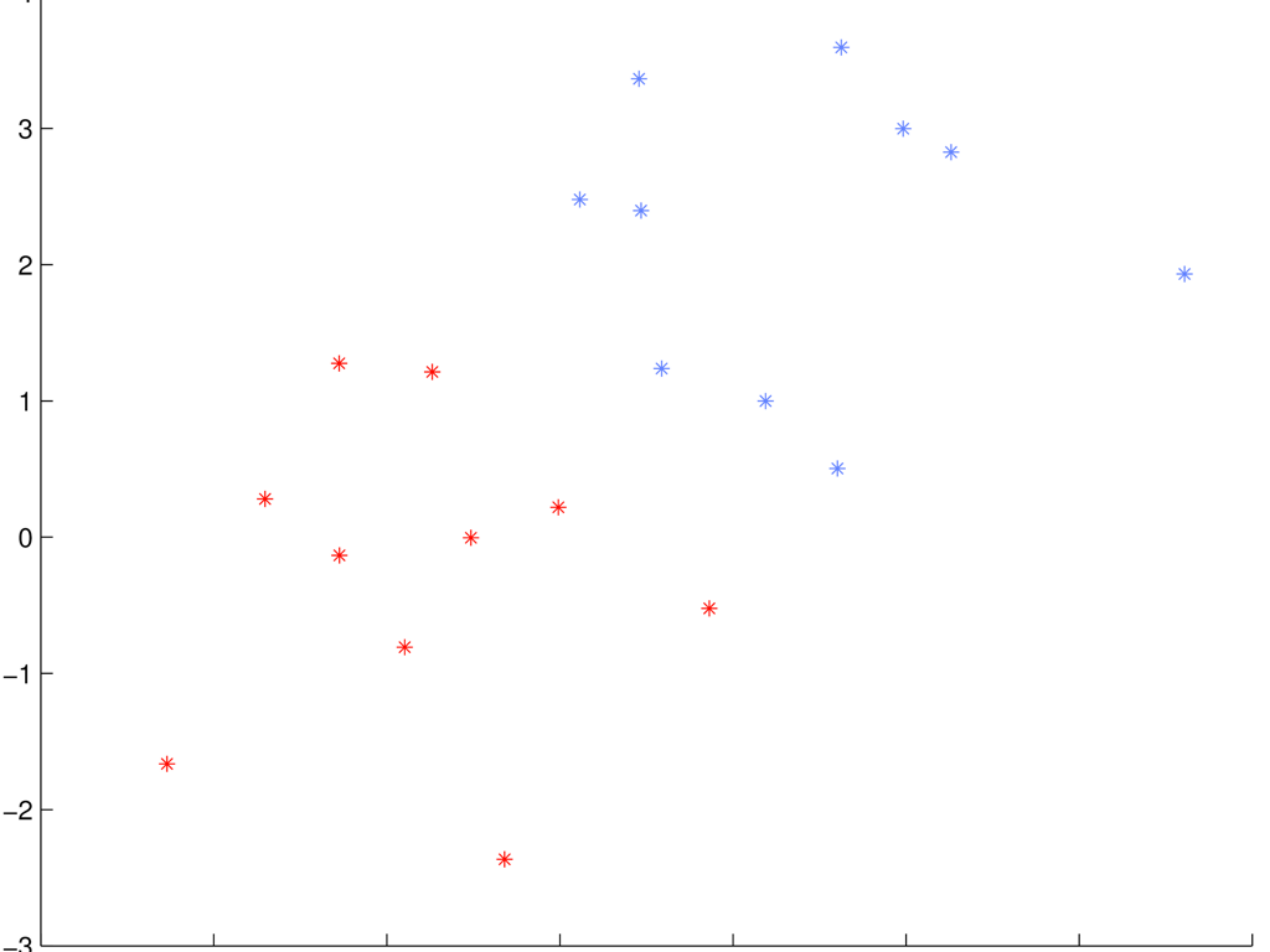
$$l(x_i, y_i, w, b) = \max\left(0, 1 - y_i\left[\langle w, x_i\rangle + b\right]\right)$$

- Fails with noisy data

do NOT train your avatar with perceptrons

Hardness
margin vs. size





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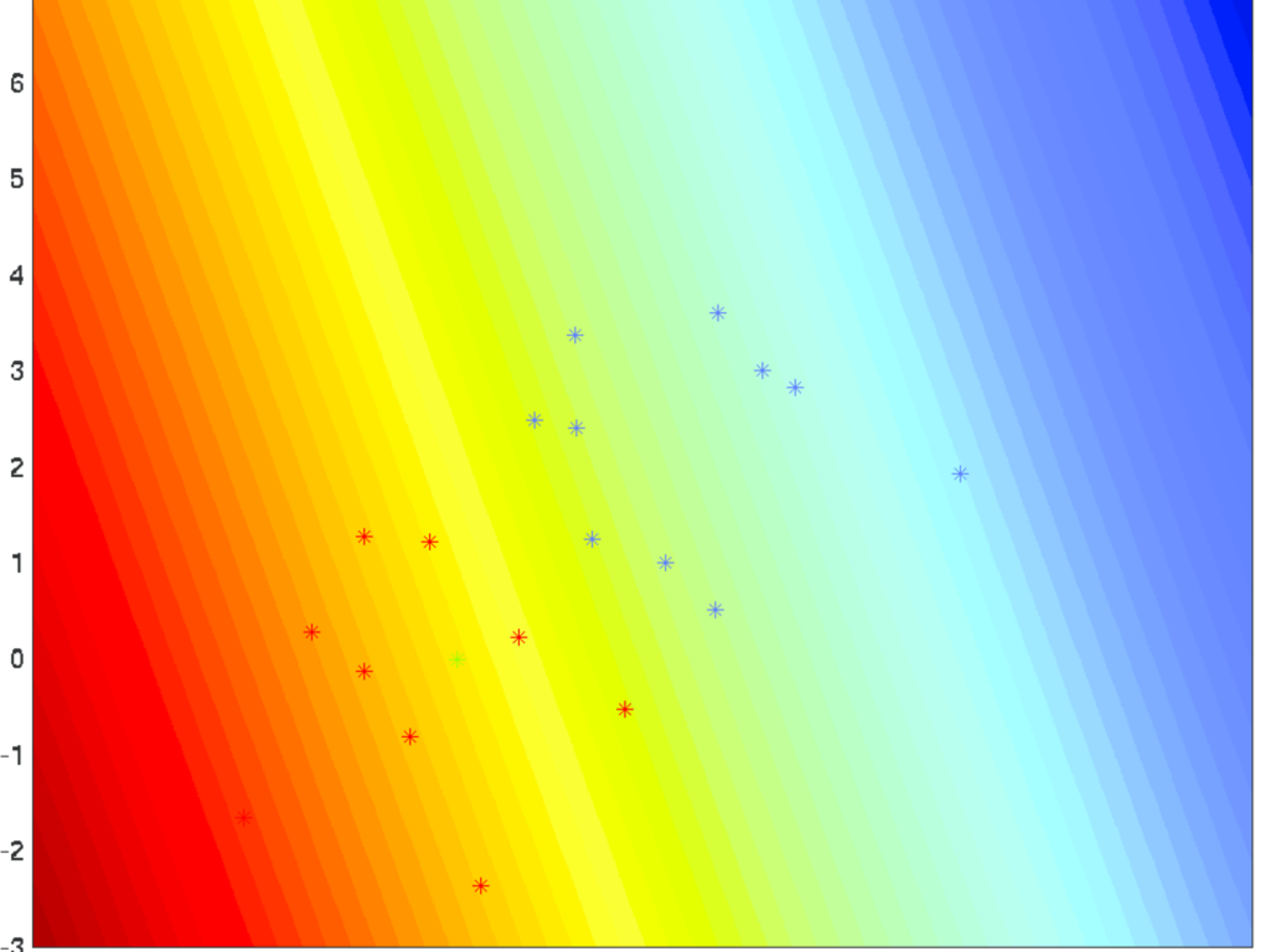
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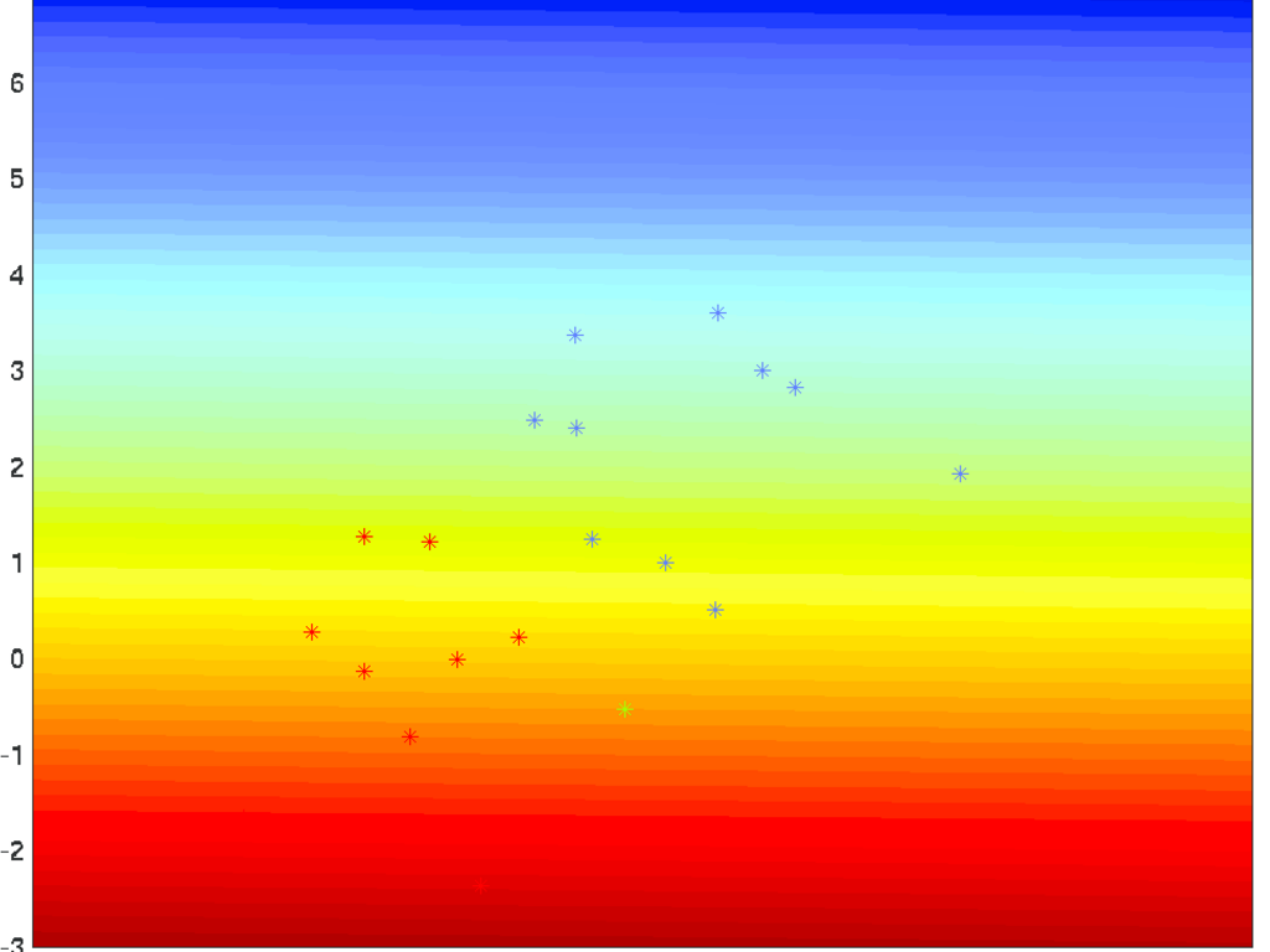
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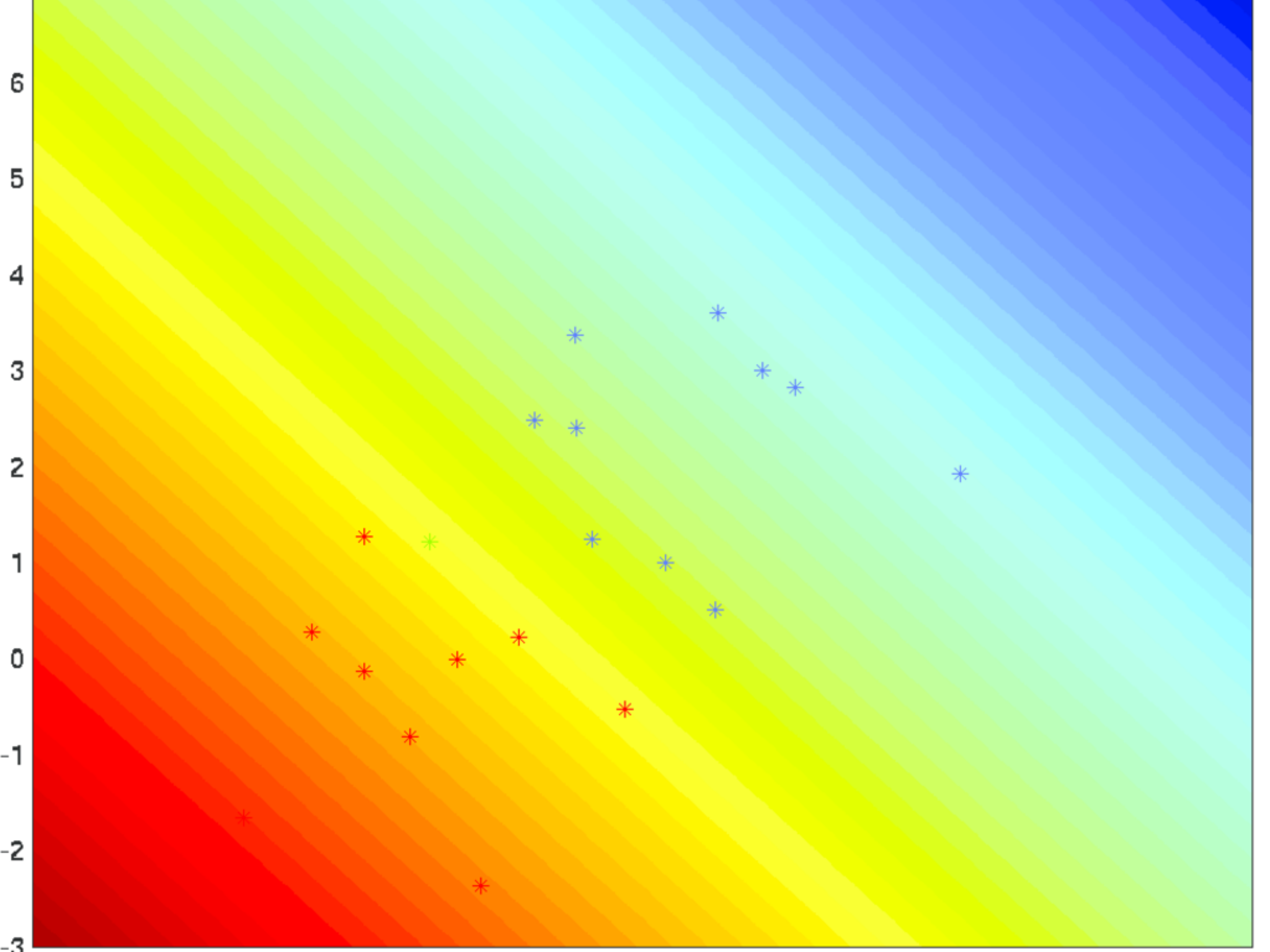
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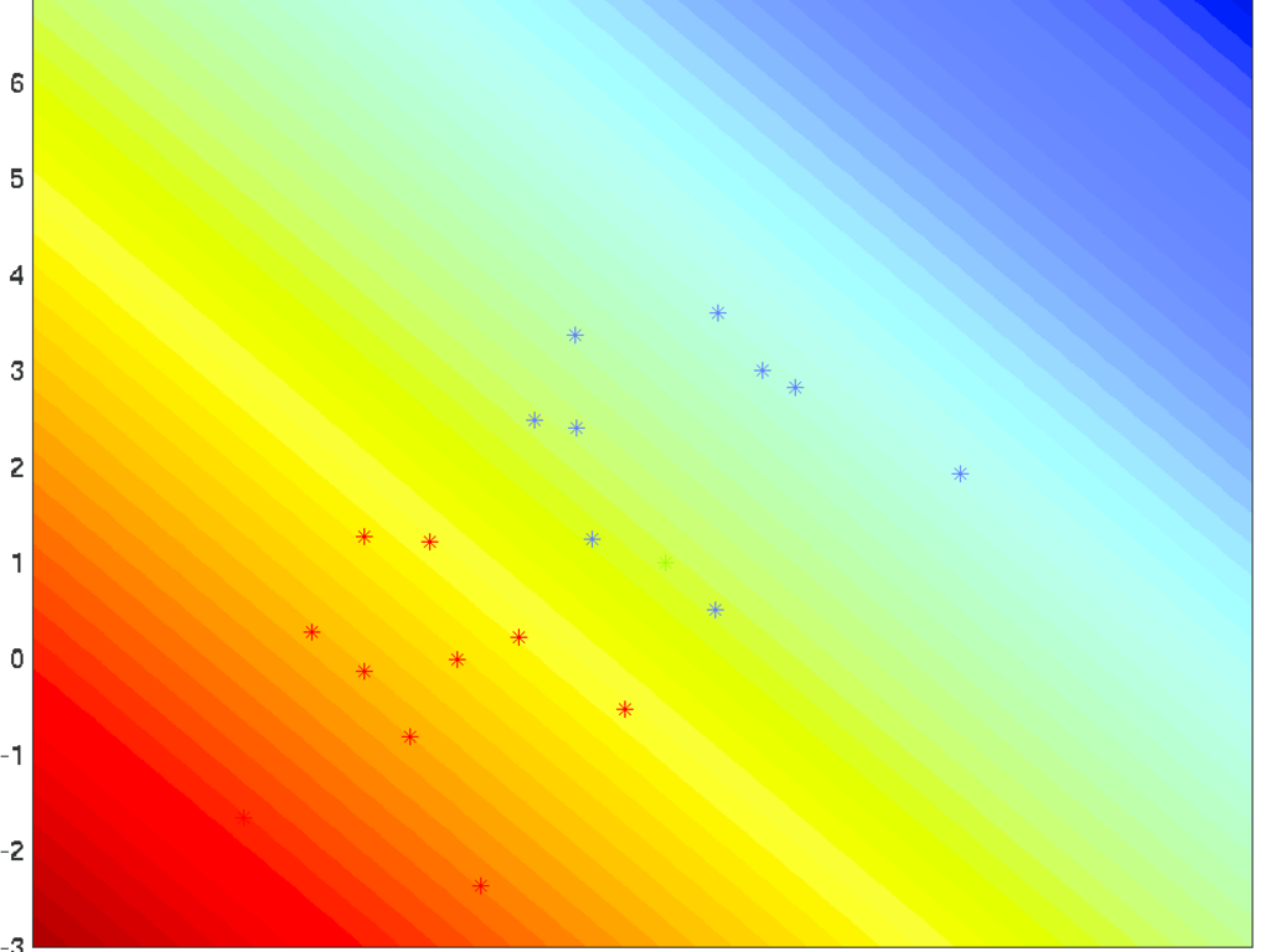

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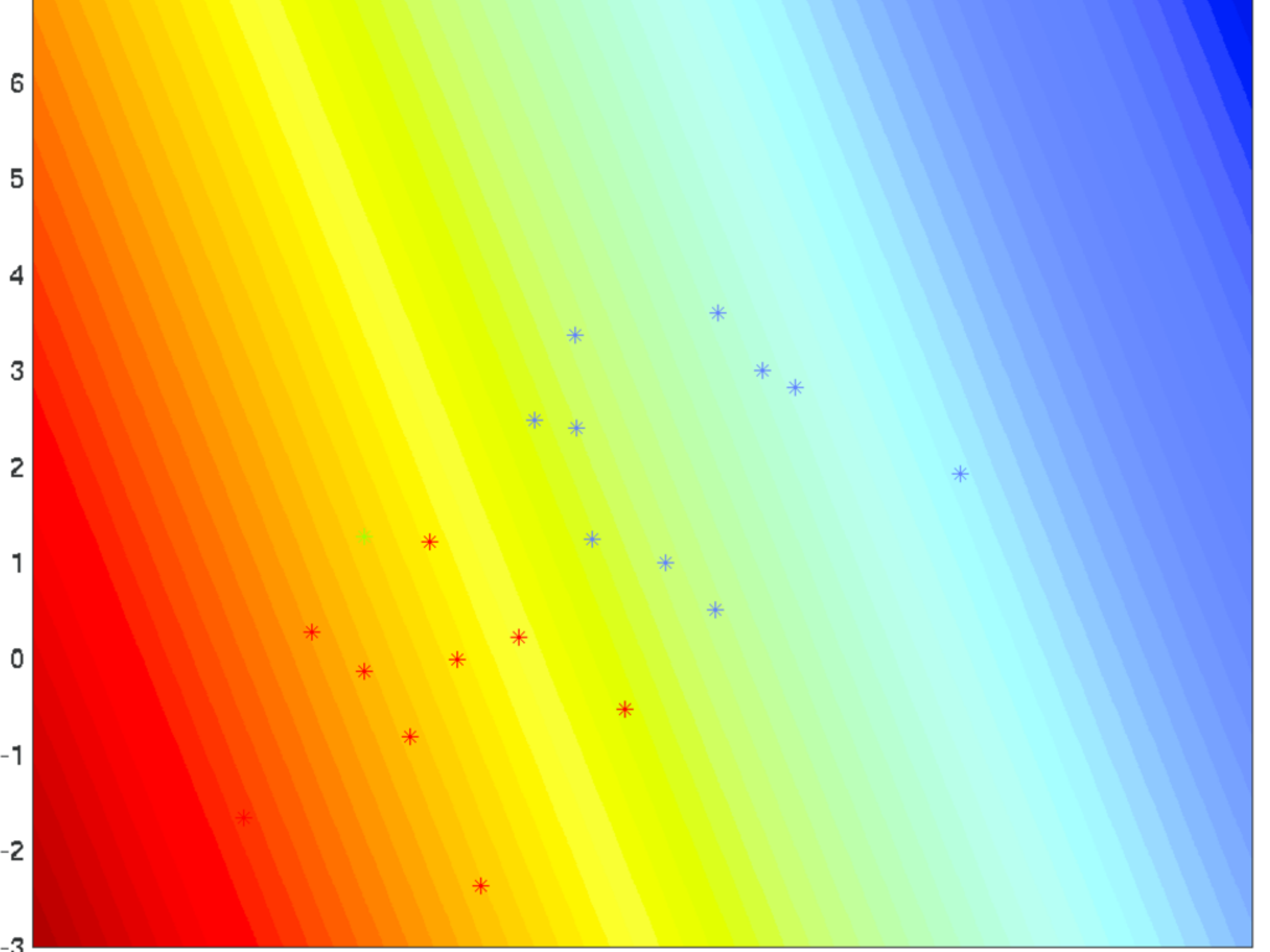

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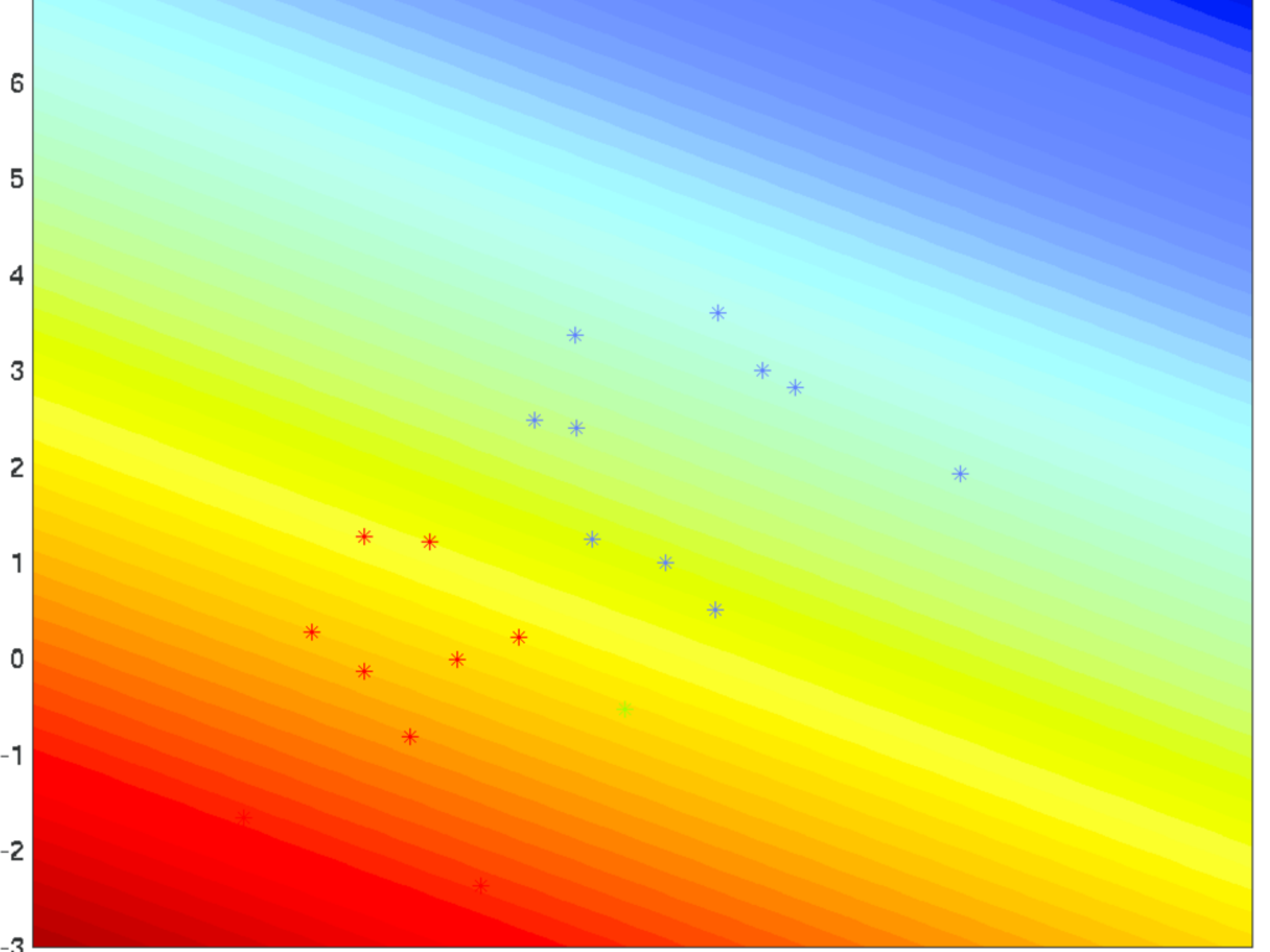

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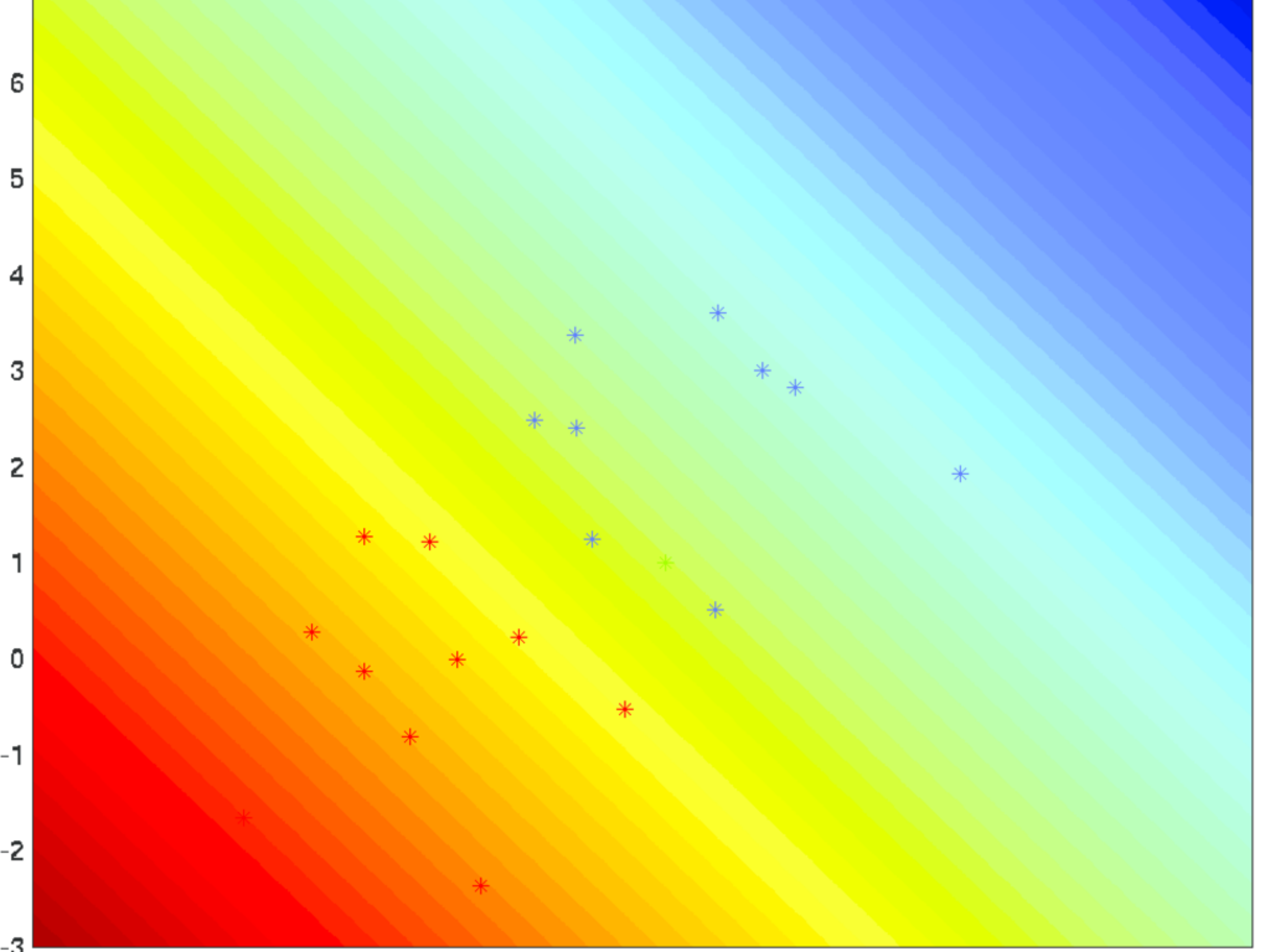
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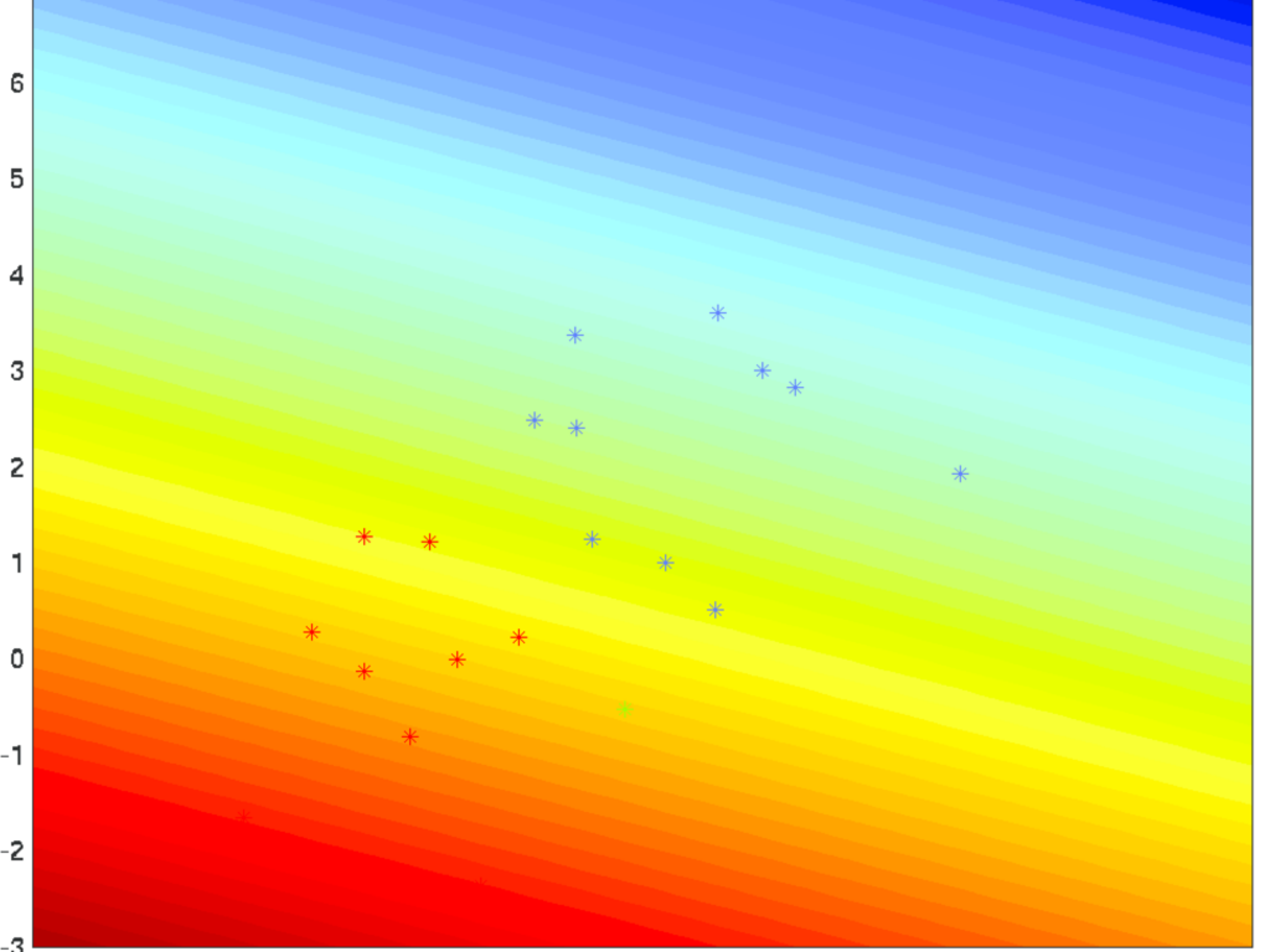
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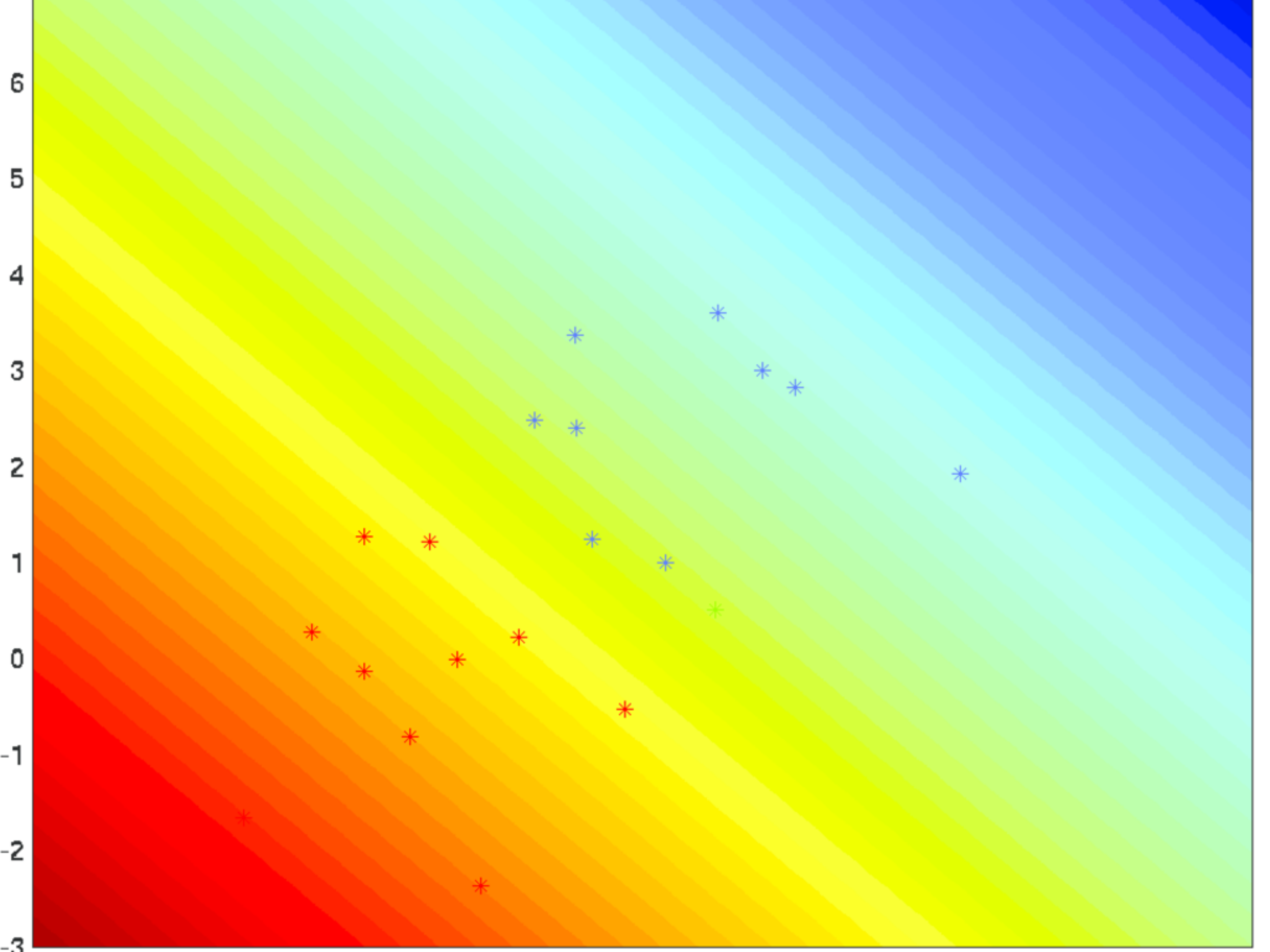
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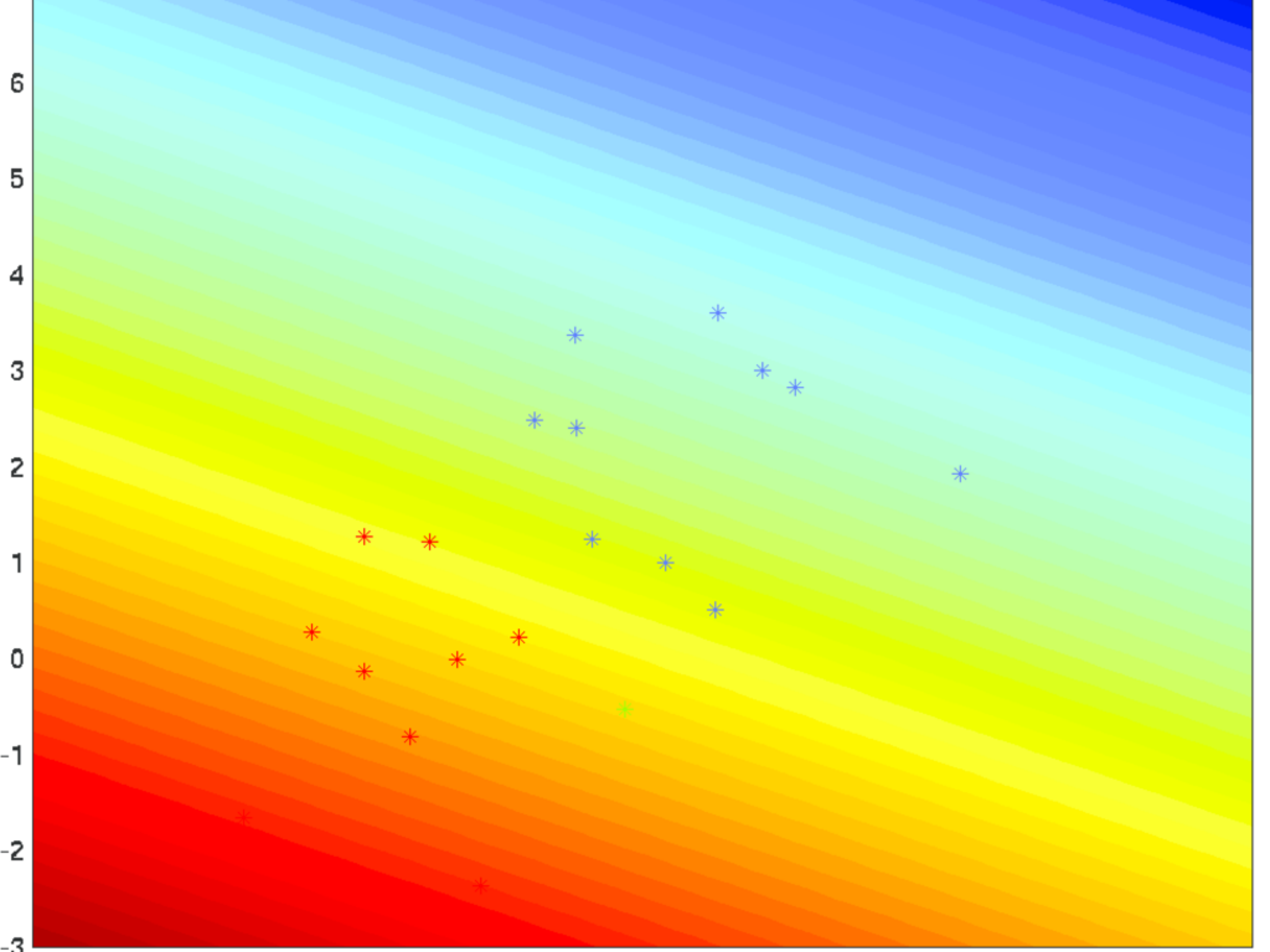
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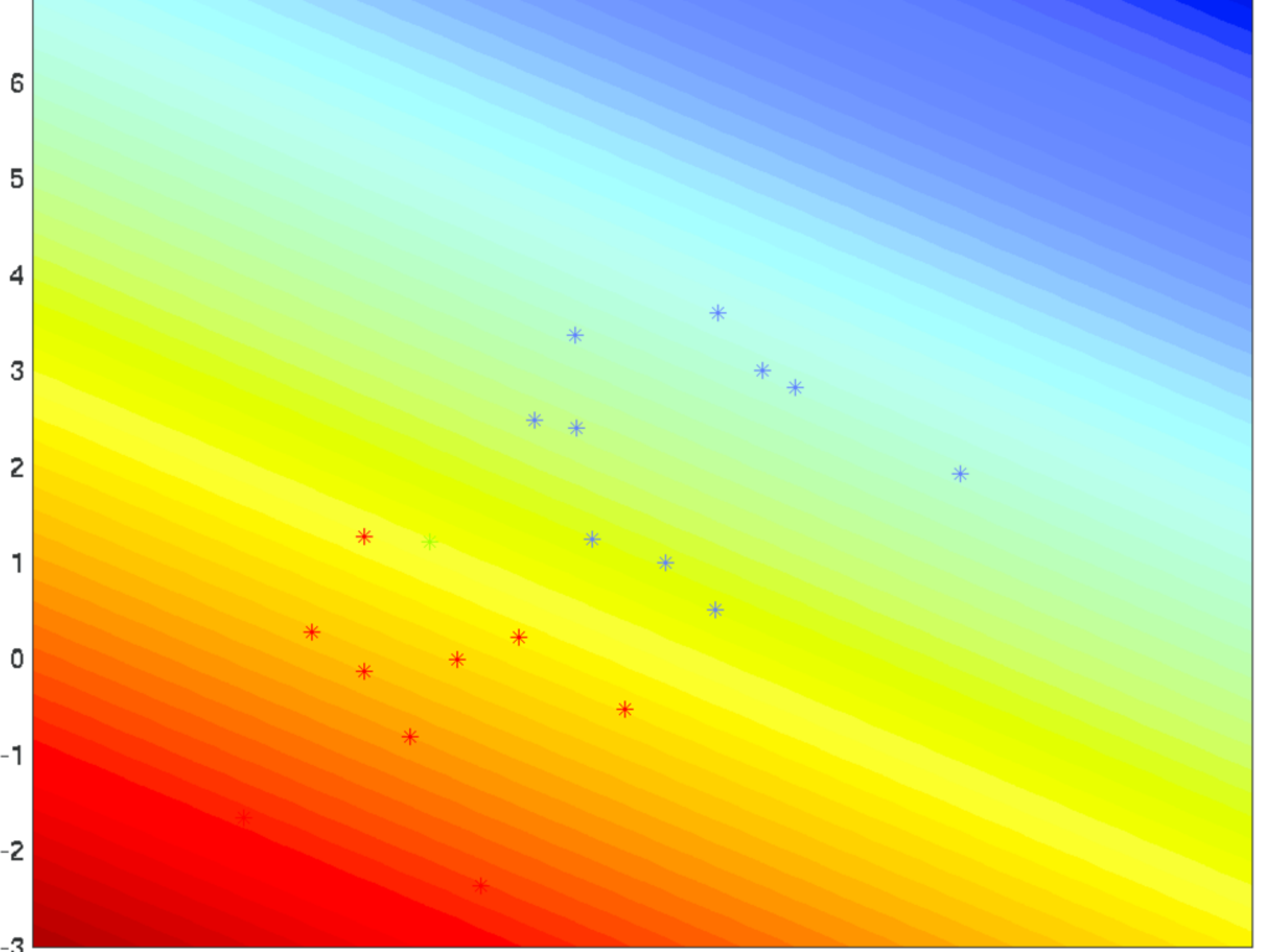
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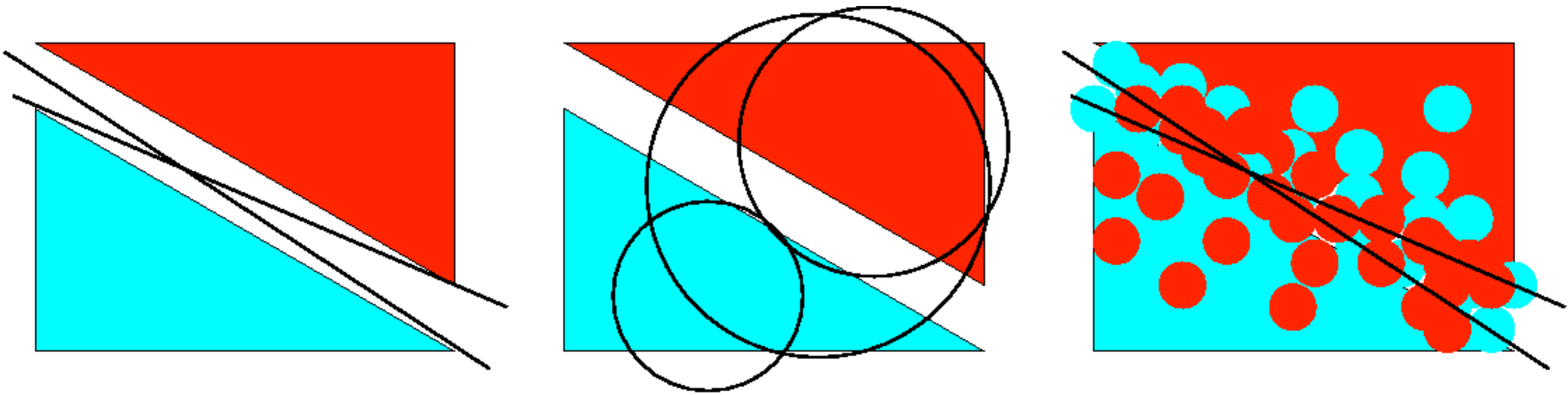
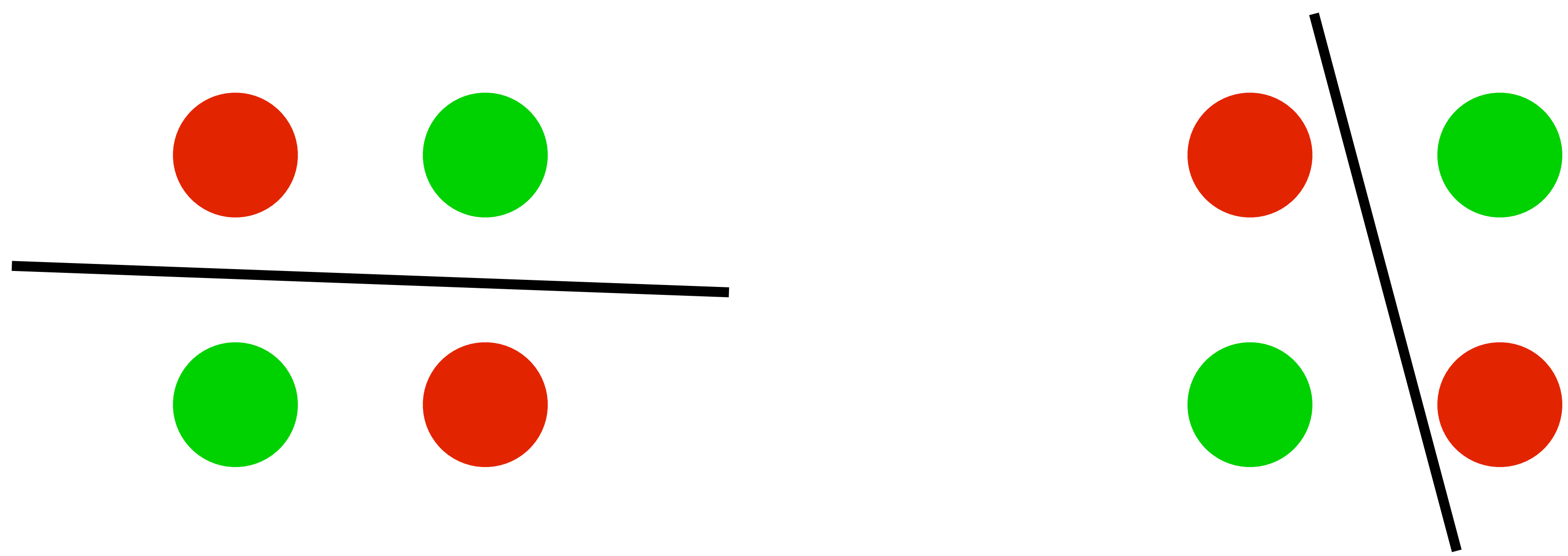
Concepts & version space

- Realizable concepts
  - Some function exists that can separate data and is included in the concept space
  - For perceptron - data is linearly separable
- Unrealizable concept
  - Data not separable
  - We don't have a suitable function class (often hard to distinguish)

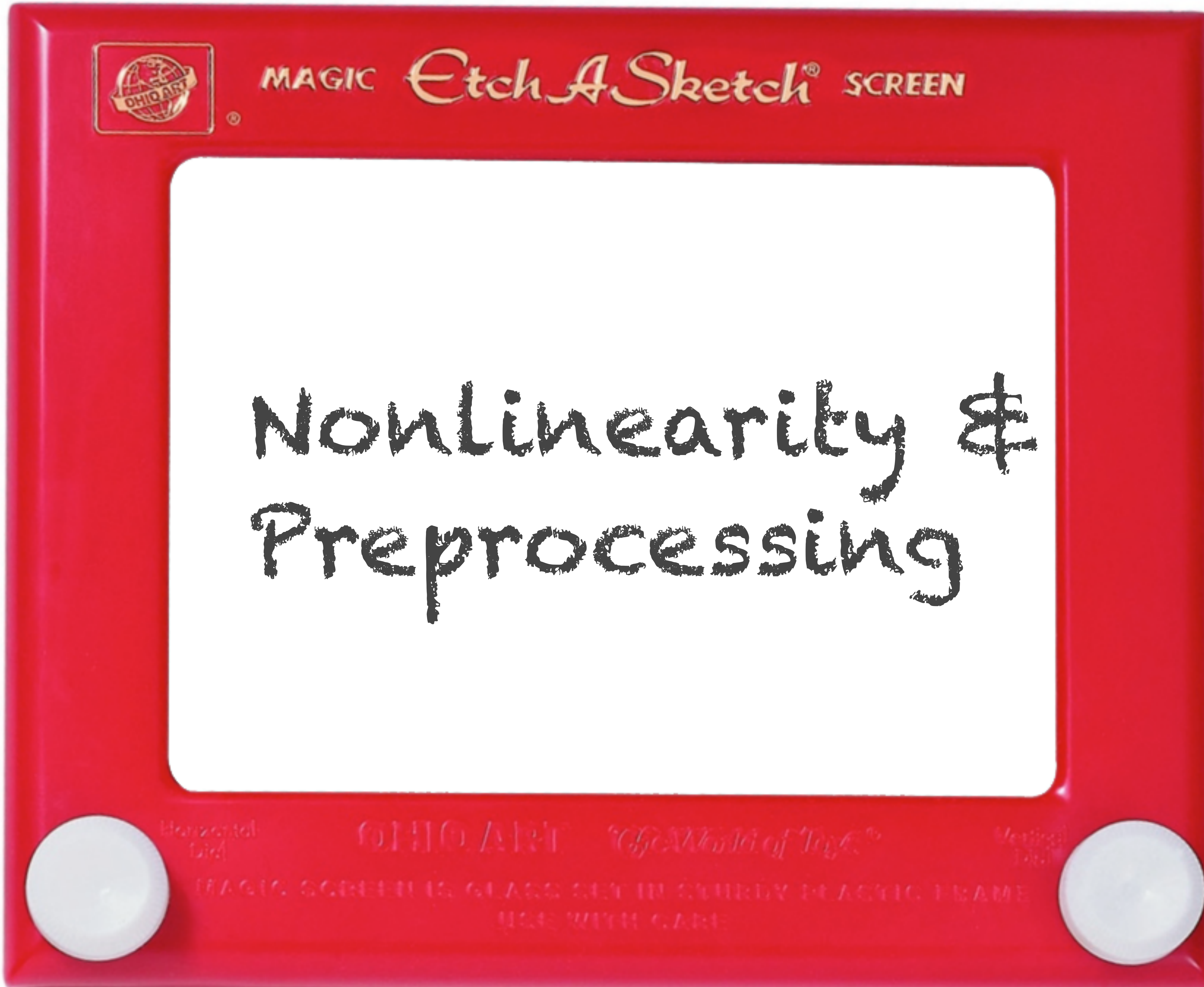


Minimum error separation



- XOR - not linearly separable
- Nonlinear separation is trivial
- Caveat (Minsky & Papert)
  Finding the minimum error linear separator
  is NP hard (this killed Neural Networks in the 70s).

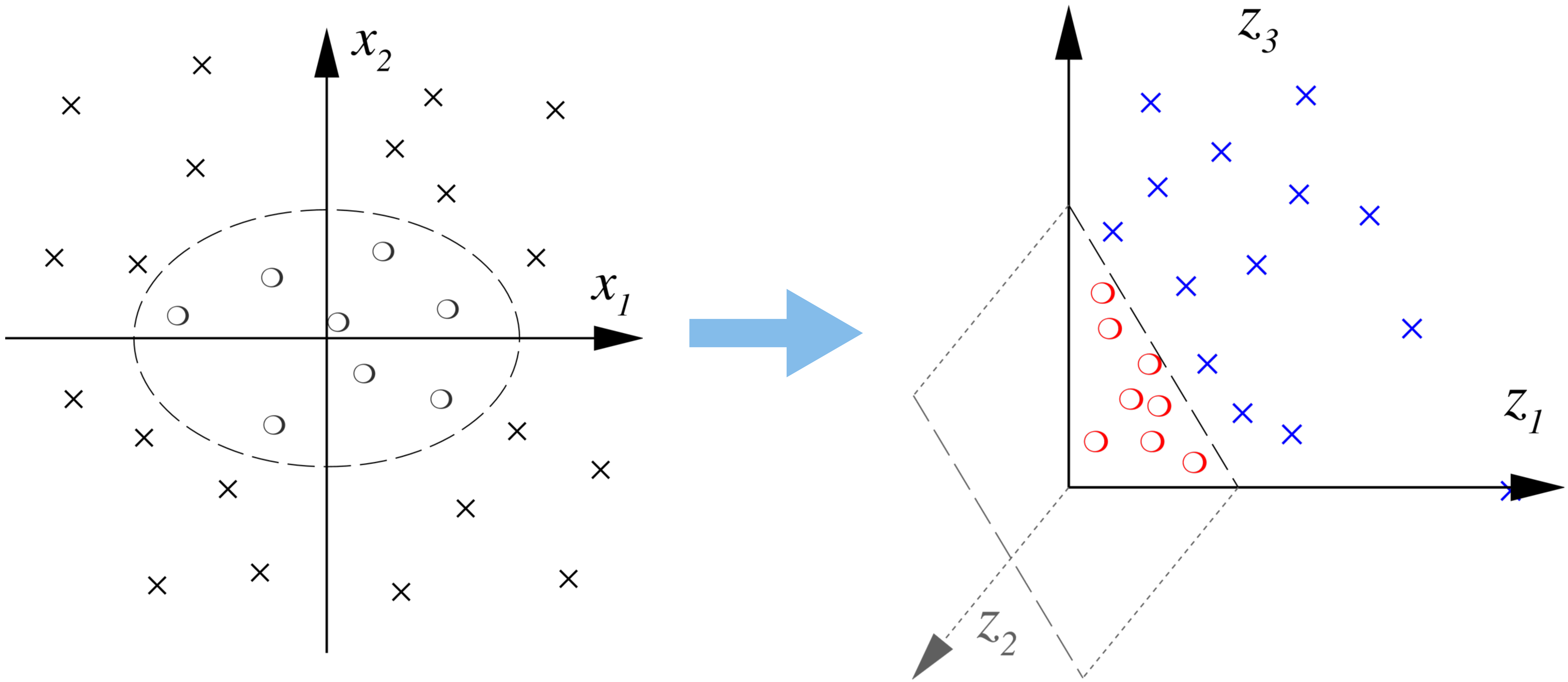
Nonlinearity & Preprocessing



Nonlinear 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 $\phi(x_i)$

Quadratic Features



- Separating surfaces are
Circles, hyperbolae, parabolae

Constructing Features (very naive OCR system)

	1	2	3	4	5	6	7	8	9	0
Loops	0	0	0	1	0	1	0	2	1	1
3 Joints	0	0	0	0	0	1	0	0	1	0
4 Joints	0	0	0	1	0	0	0	1	0	0
Angles	0	1	1	1	1	0	1	0	0	0
Ink	1	2	2	2	2	2	1	3	2	2

Feature Engineering for Spam Filtering

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```

- bag of words
- pairs of words
- date & time
- recipient path
- IP number
- sender
- encoding
- links
- ... secret sauce ...

More feature engineering

- Two Interlocking Spirals
  Transform the data into a radial and angular part
  $$(x_1, x_2) = (r \sin\phi, r \cos\phi)$$
- Handwritten Japanese Character Recognition
  - Break down the images into strokes and recognize it
  - Lookup based on stroke order
- Medical Diagnosis
  - Physician's comments
  - Blood status / ECG / height / weight / temperature ...
  - Medical knowledge
- Preprocessing
  - Zero mean, unit variance to fix scale issue (e.g. weight vs. income)
  - Probability integral transform (inverse CDF) as alternative

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

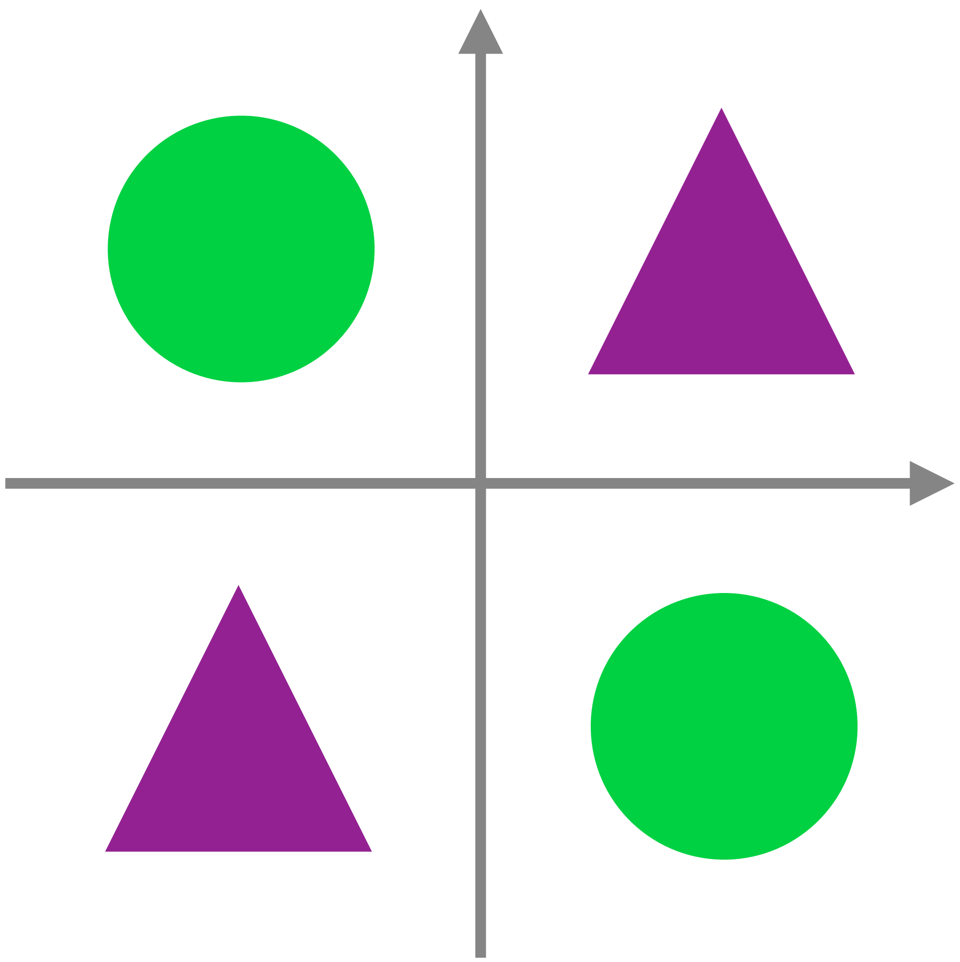
Problems

- Problems
  - Need domain expert (e.g. Chinese OCR)
  - Often expensive to compute
  - Difficult to transfer engineering knowledge
- Shotgun Solution
  - Compute many features
  - Hope that this contains good ones
  - Do this efficiently

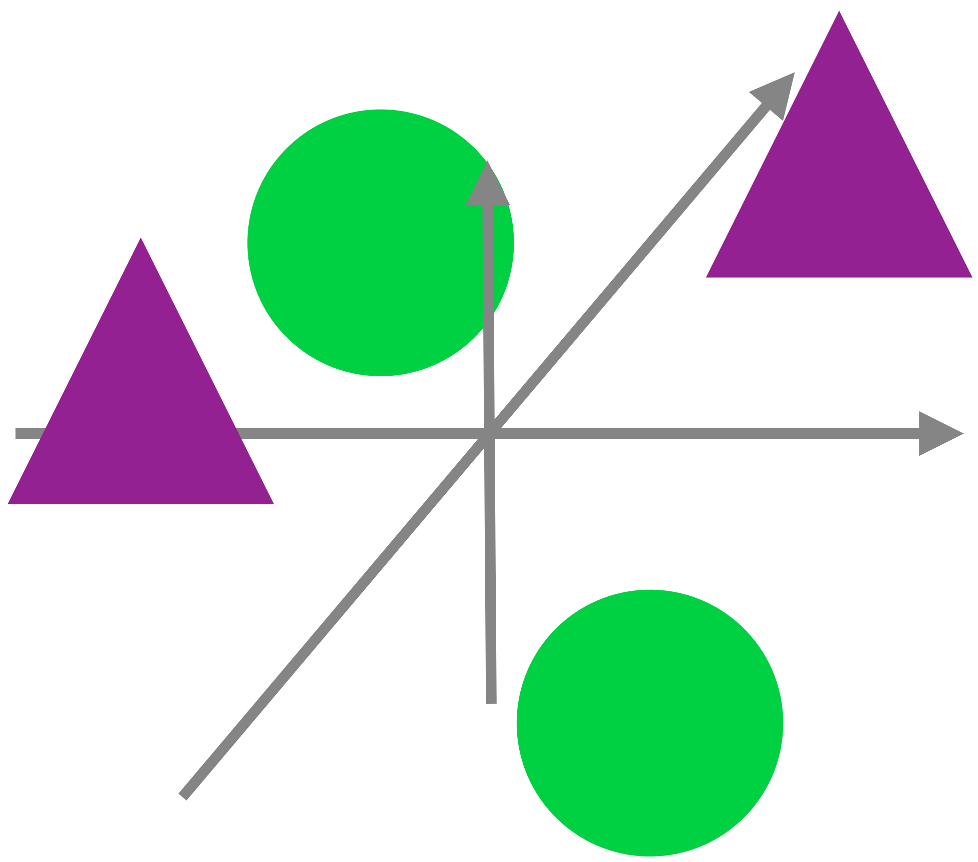
Kernels

Grace Wahba

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

Quadratic Features

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

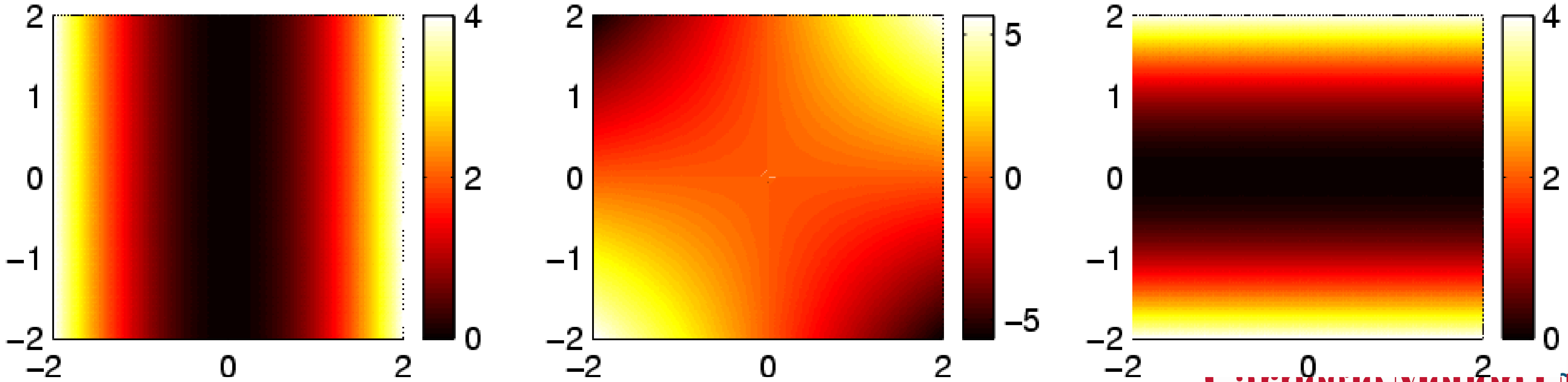
$$\Phi(x) := \left(x_1^2, \sqrt{2}x_1x_2, x_2^2\right)$$

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 d via $\langle x, x' \rangle^d$.



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 $\Phi(x)$ ...

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

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

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 $\Phi_i(x)$.

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?

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

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

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.

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

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

A Counterexample

A Candidate for a Kernel

$$k(x, x') = \begin{cases} 1 & \text{if } \|x - x'\| \leq 1 \\ 0 & \text{otherwise} \end{cases}$$

This is symmetric and gives us some information about the proximity of points, yet it is not a proper kernel …

Kernel Matrix

We use three points, $x_1 = 1, x_2 = 2, x_3 = 3$ and compute the resulting “kernelmatrix” K. This yields

$$K = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{bmatrix}$$ and eigenvalues $(\sqrt{2}-1)^{-1}, 1$ and $(1-\sqrt{2})$.

as eigensystem. Hence k is not a kernel.

Examples

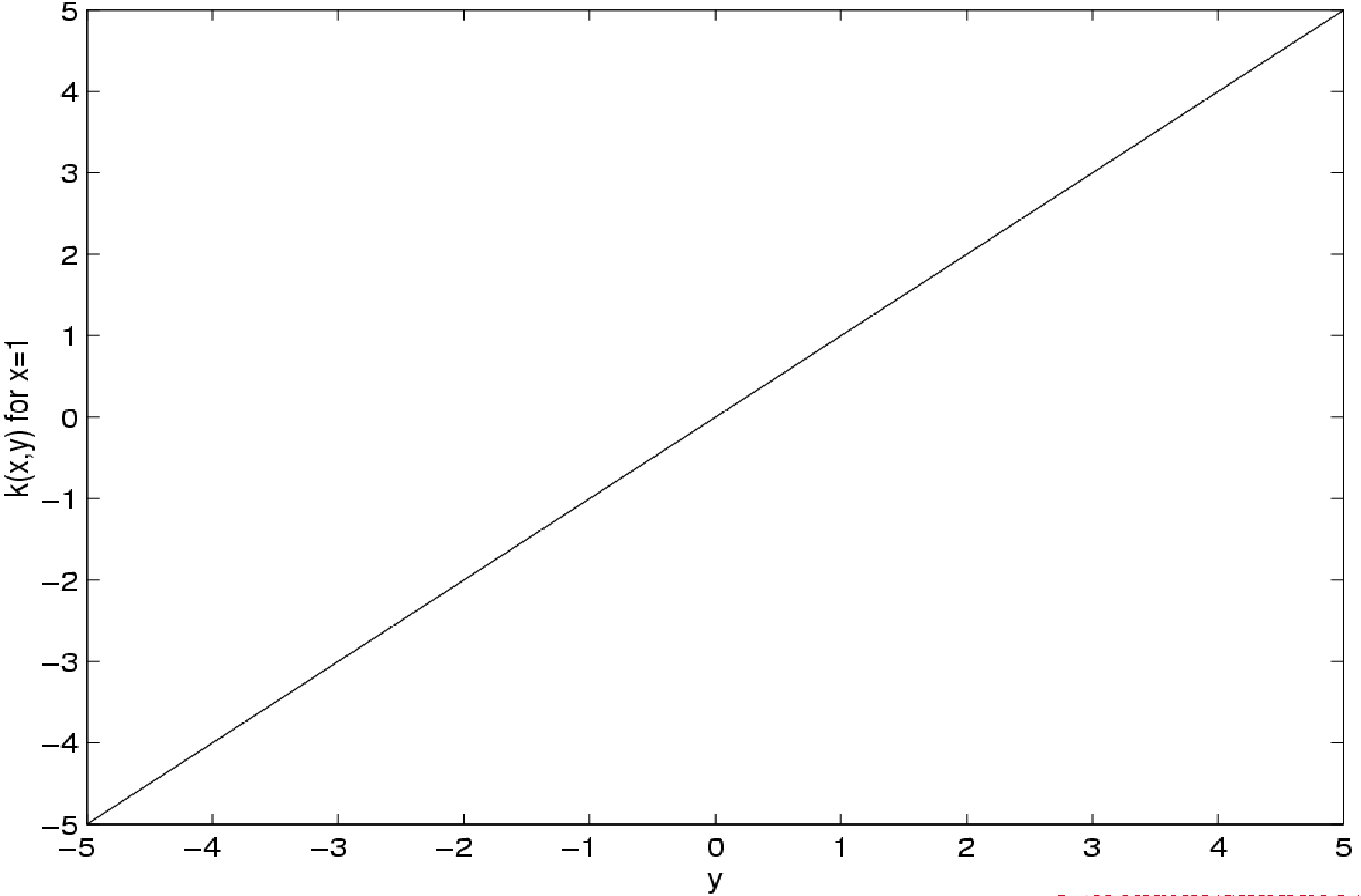
Examples of kernels $k(x, x')$

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

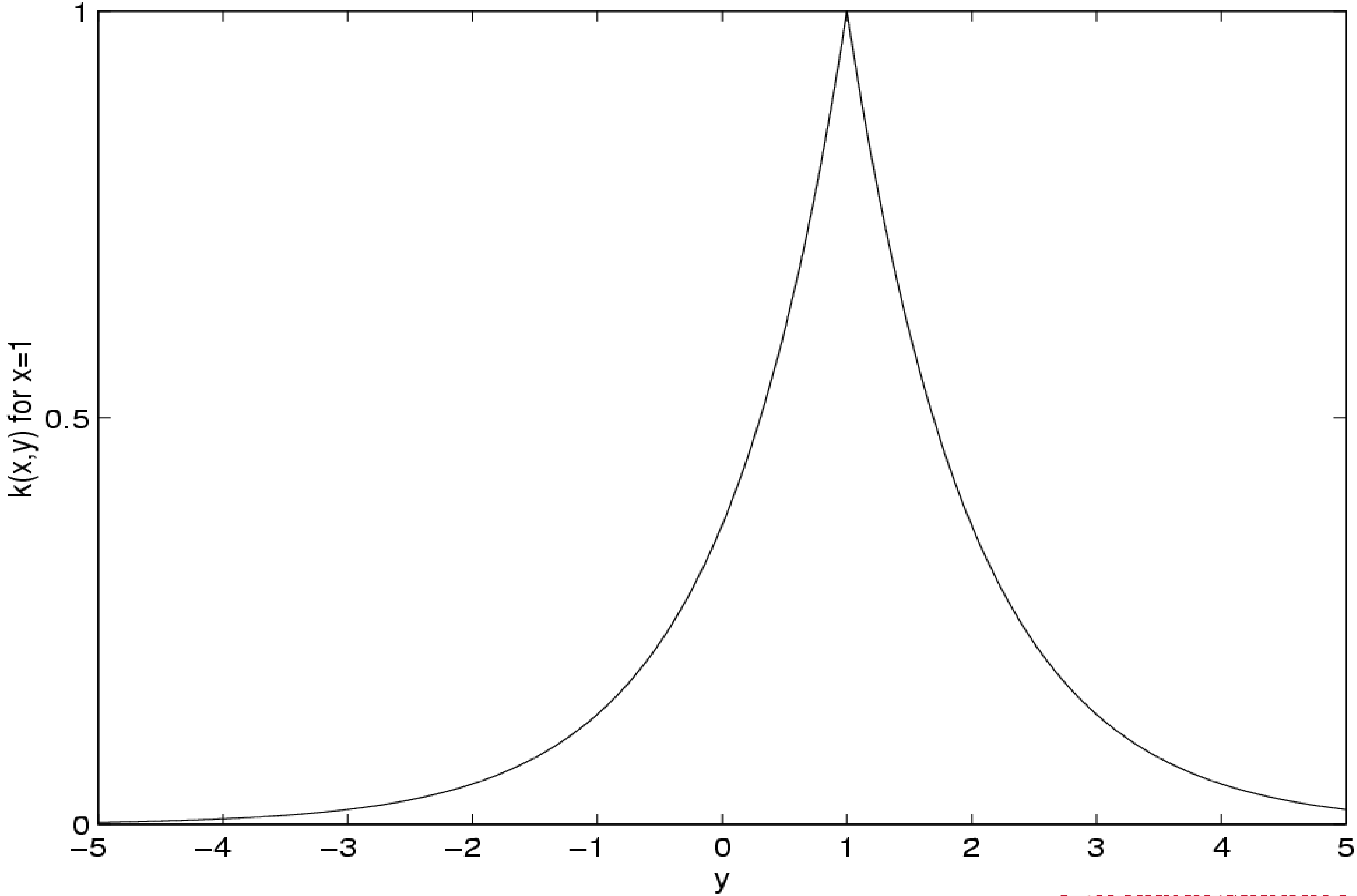
Simple trick for checking Mercer's condition

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

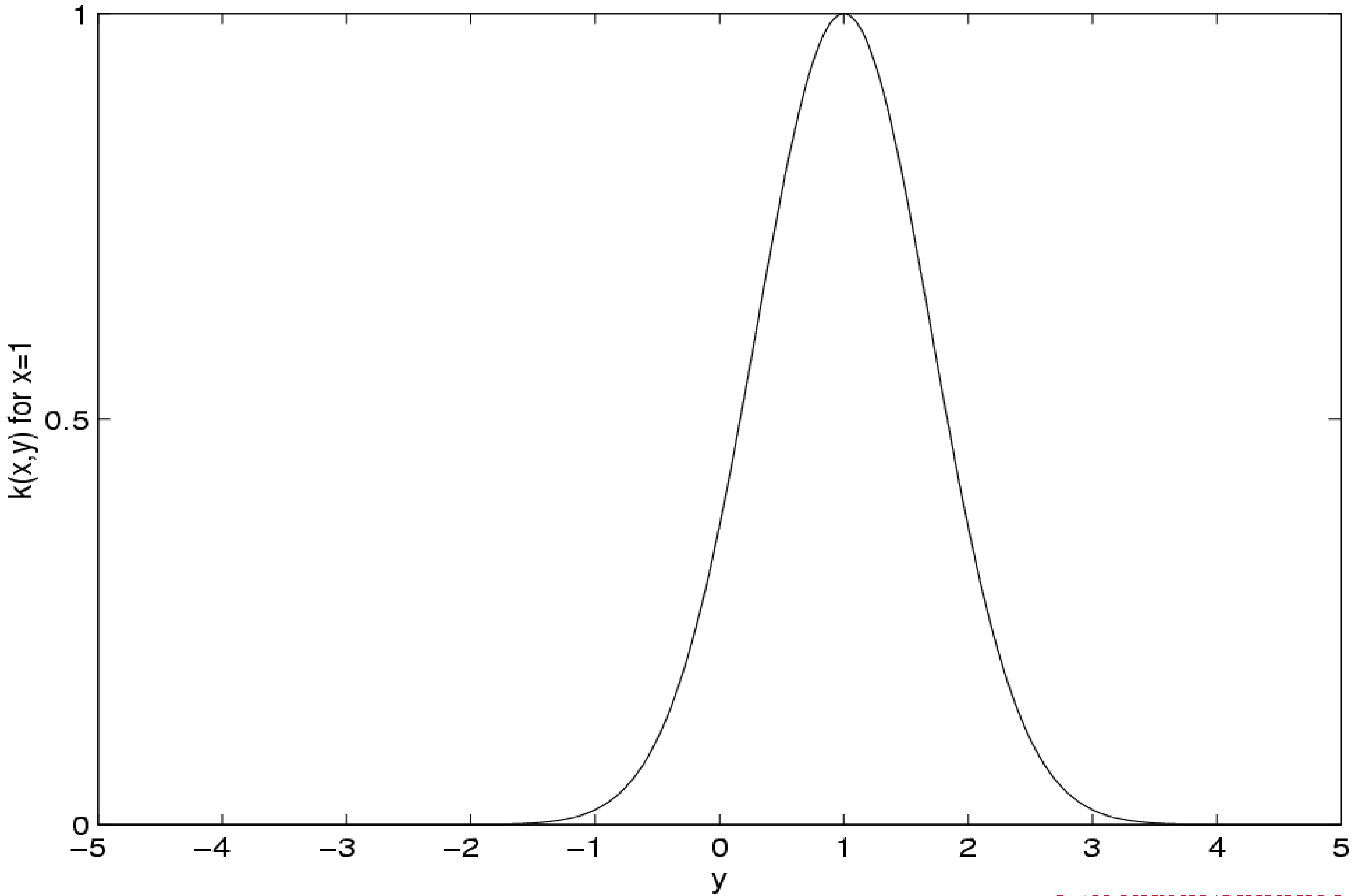
Linear Kernel



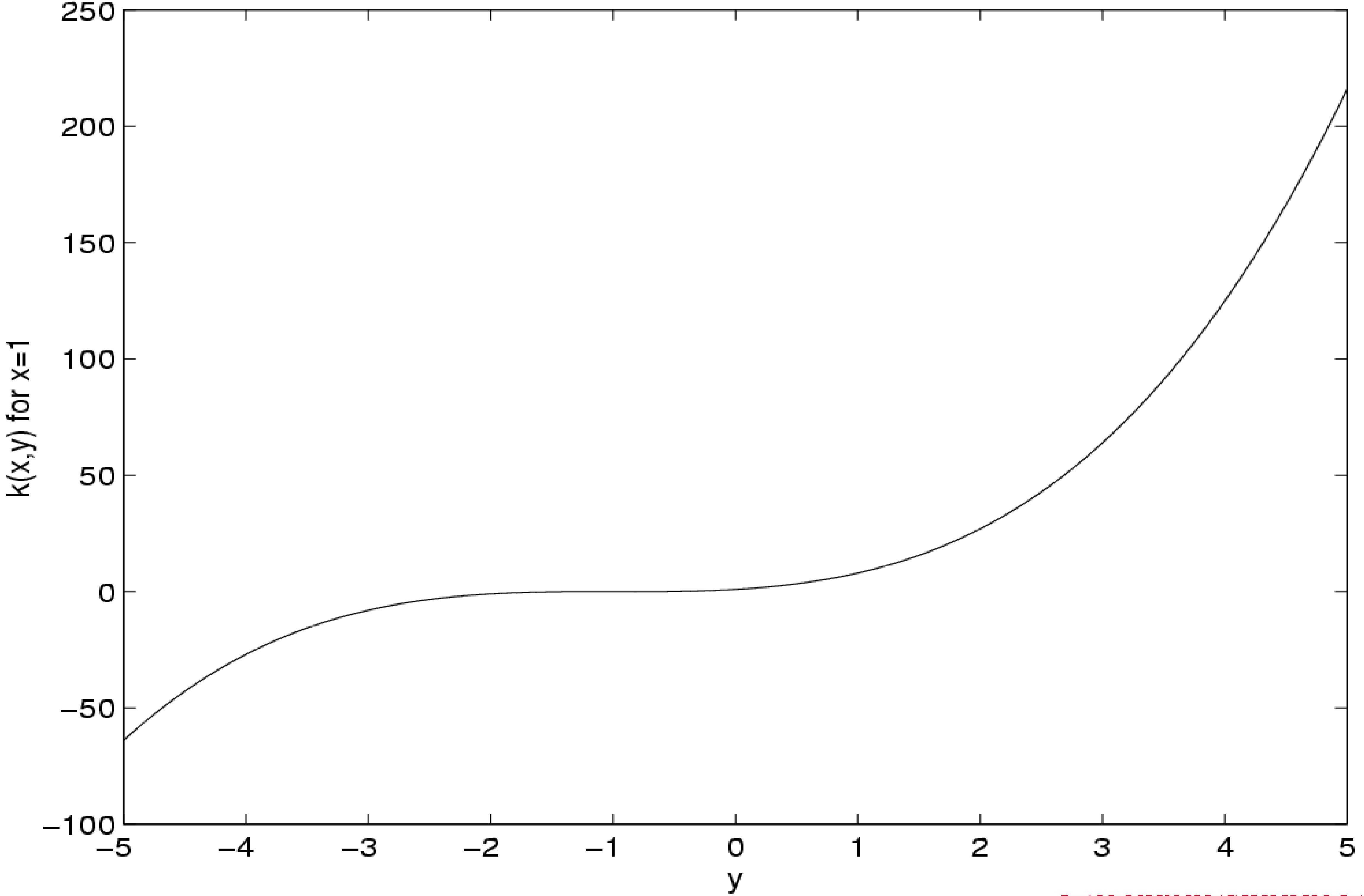
Laplacian Kernel



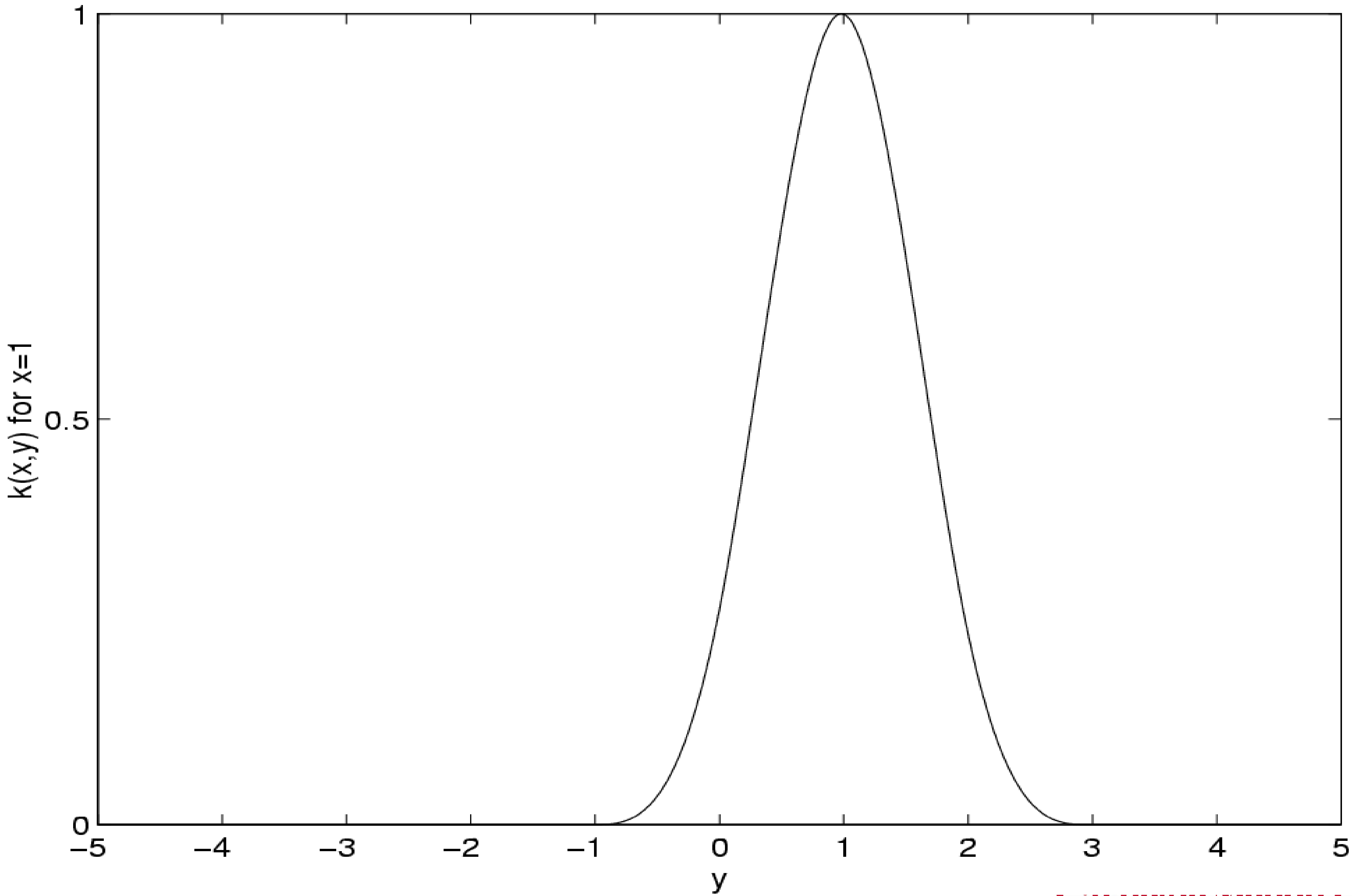
Gaussian Kernel



Polynomial of order 3



B_3 Spline Kernel



Summary

- Perceptron
  - Hebbian learning & biology
  - Algorithm
  - Convergence analysis
- Features and preprocessing
  - Nonlinear separation
  - Perceptron in feature space
- Kernels
  - Kernel trick
  - Properties
  - Examples