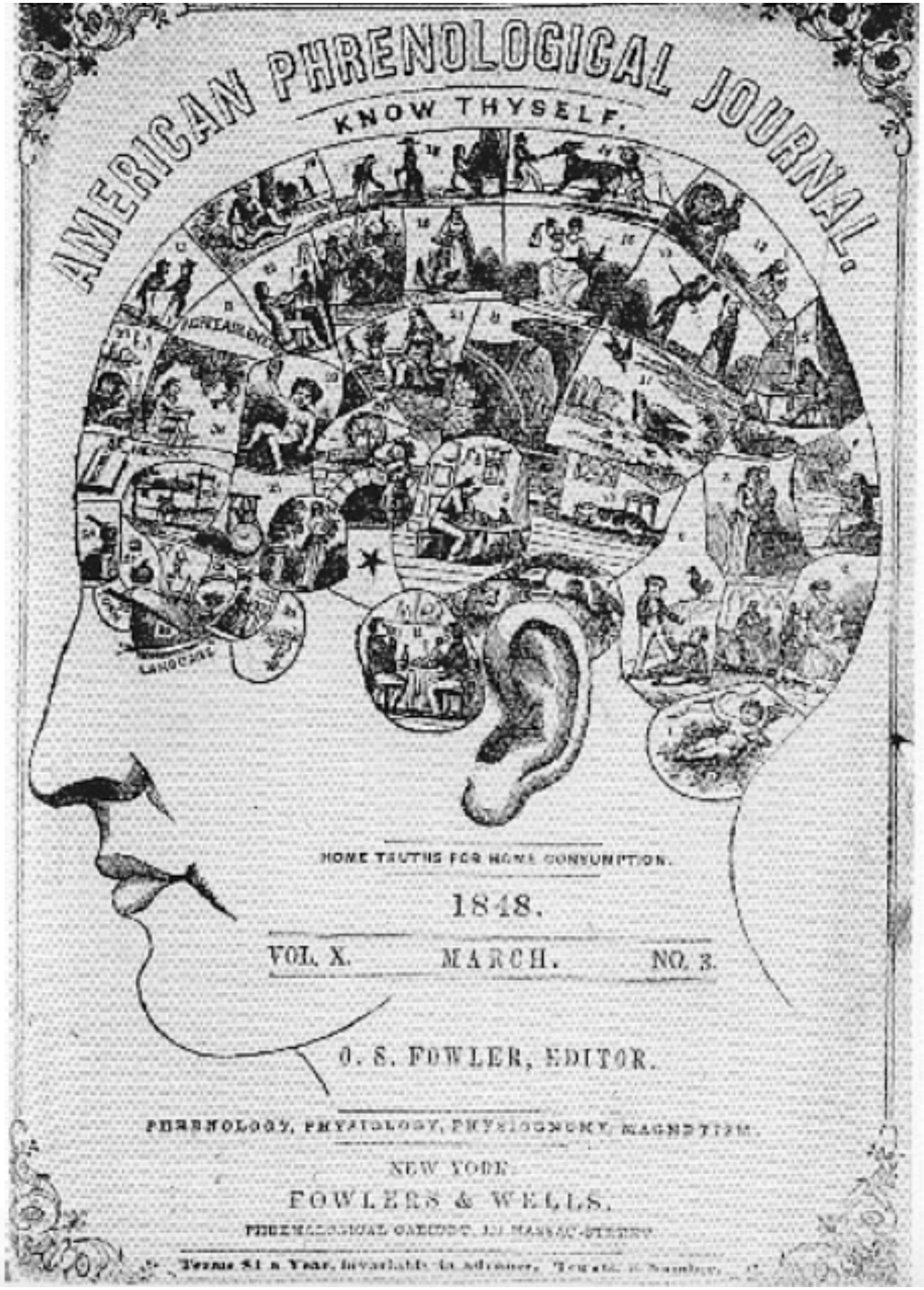
Artificial Intelligence and Machine Learning

Barbara Caputo

Outline

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

Perceptron



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.

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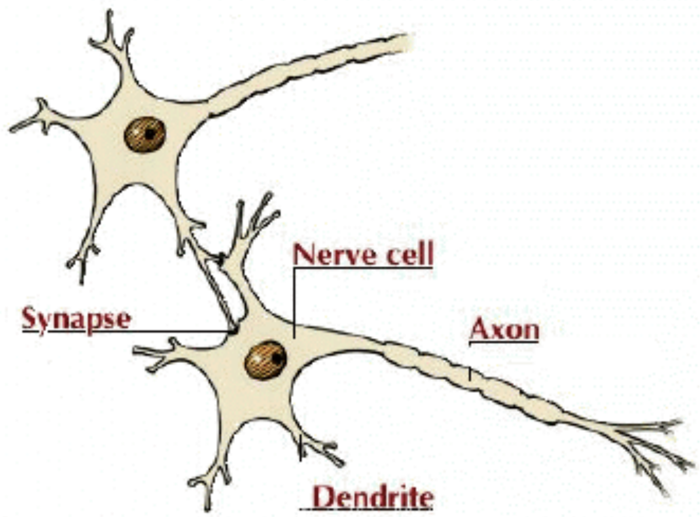
  - Pavlov's salivating dog.
- Training mechanisms
  - Behavioral modification of individuals (learning)
    Successful behavior is rewarded (e.g. food).
  - Hard-coded behavior in the genes (instinct)
    The wrongly coded animal does not reproduce.

Neurons

- Soma (CPU)
  Cell body - combines signals



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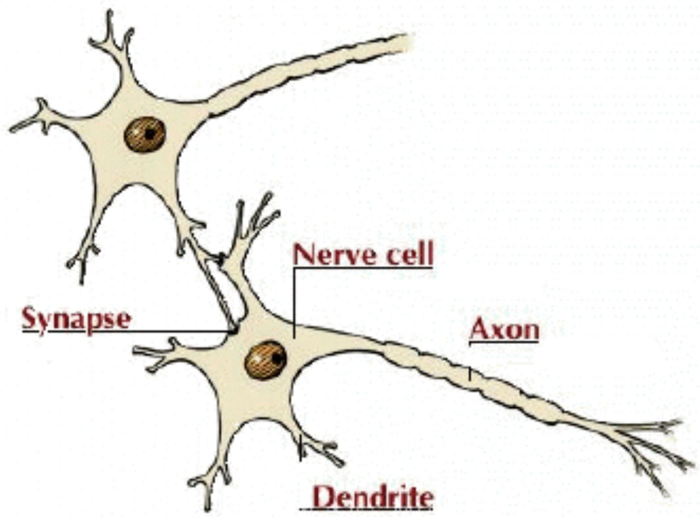
- Dendrite (input bus)
  Combines the inputs from several other nerve cells



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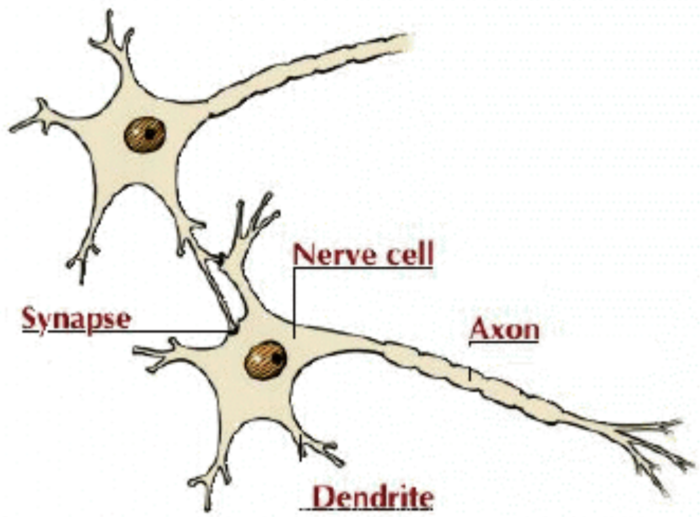
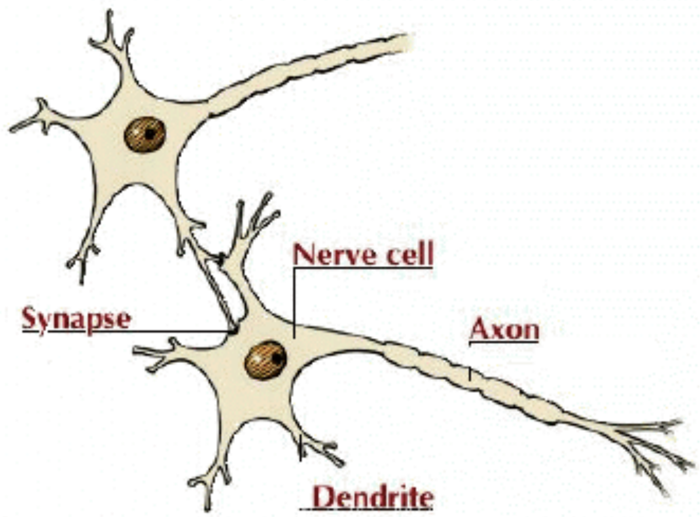
  Interface and parameter store between neurons



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



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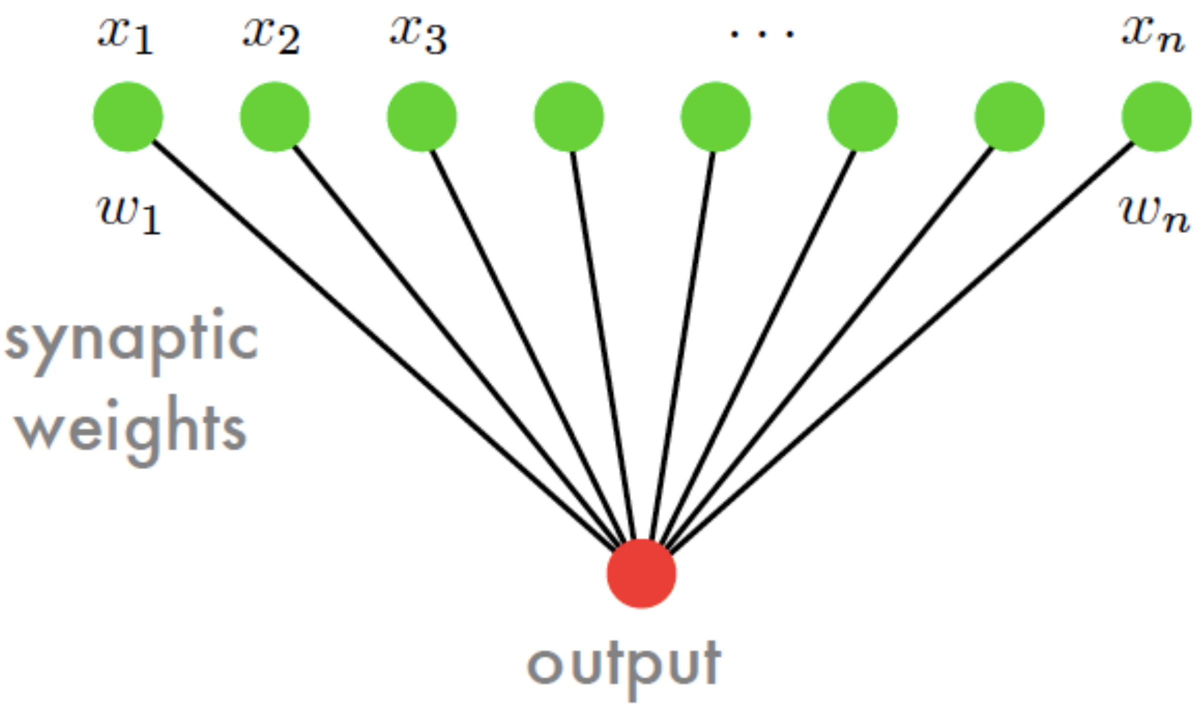

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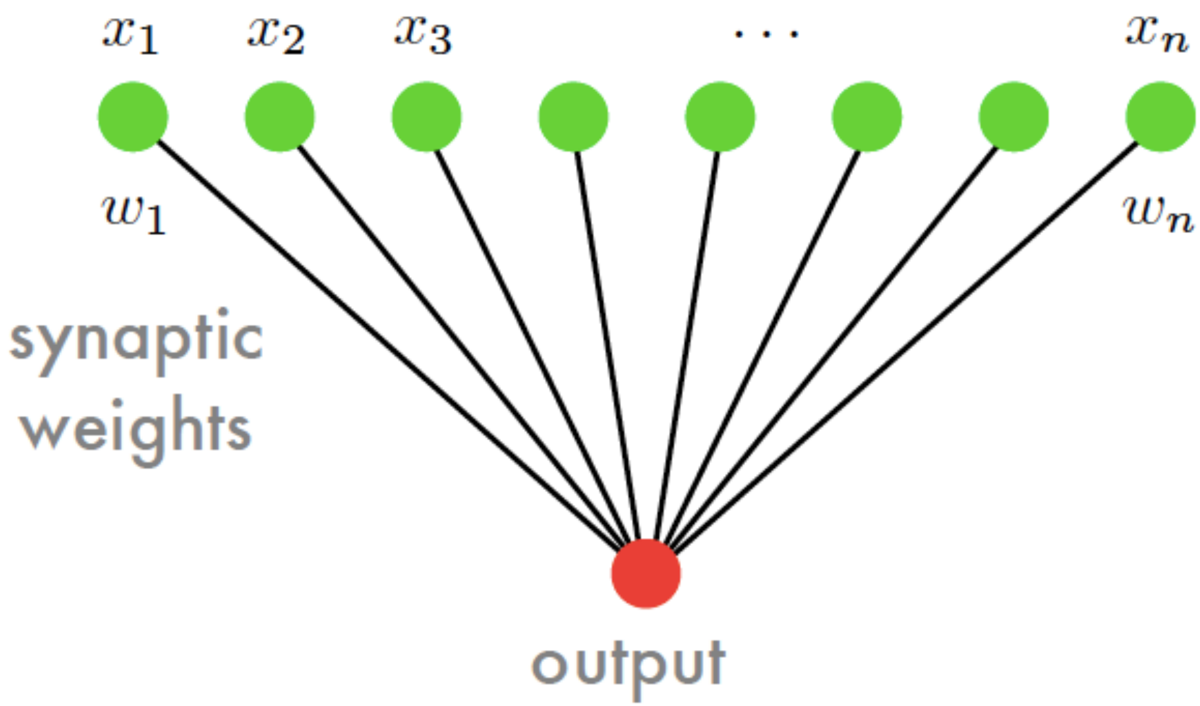
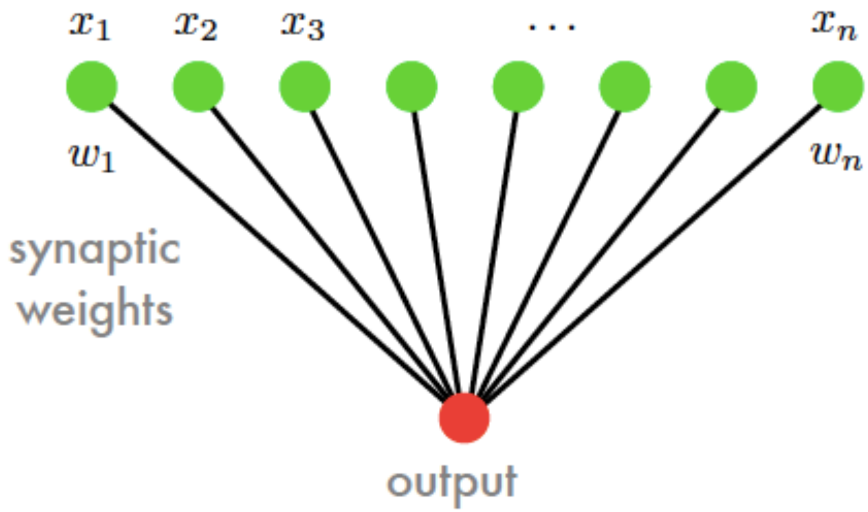


$$f(x) = \sum_i w_i x_i = \langle w, x \rangle$$

Perceptron

- Weighted linear combination



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

Perceptron

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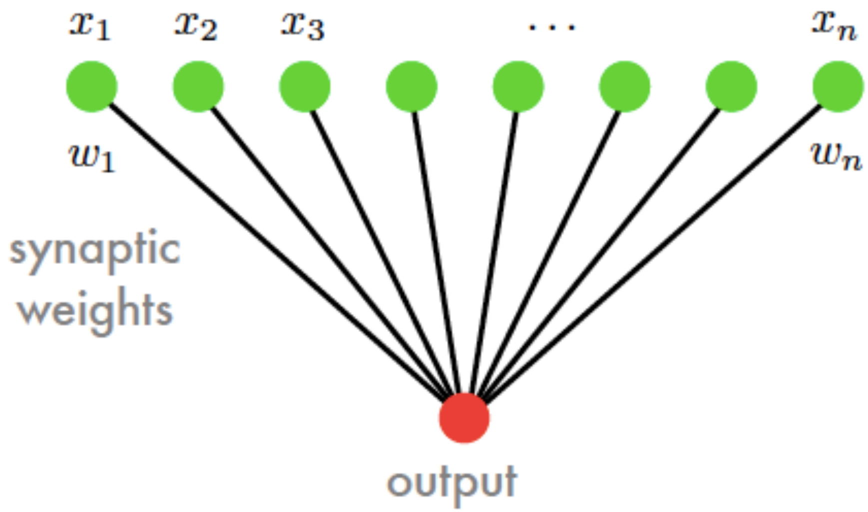
- Nonlinear decision function



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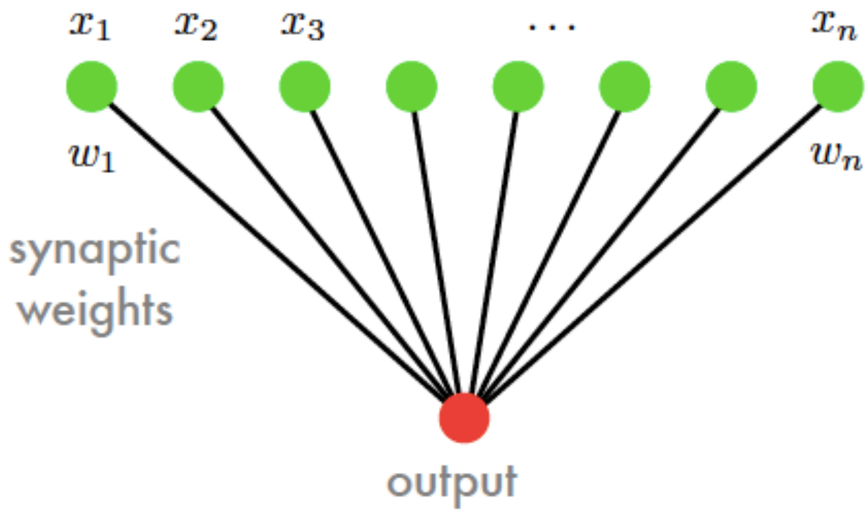

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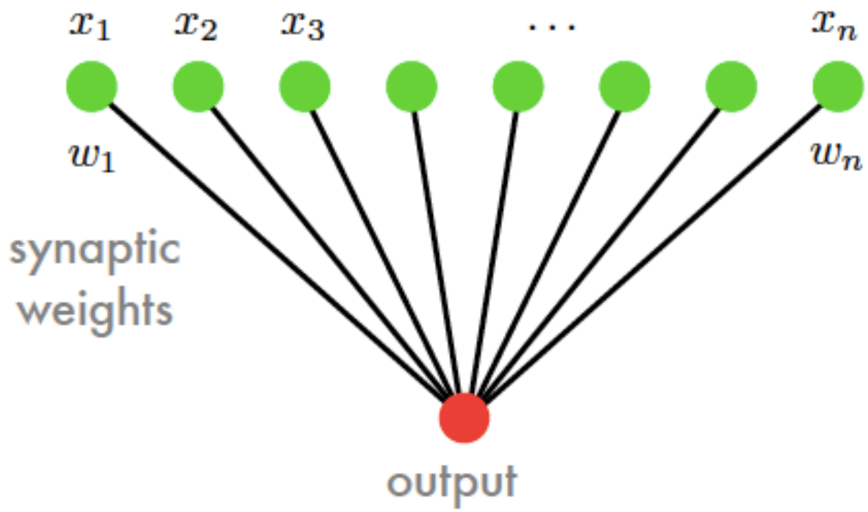

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- Linear separating hyperplanes (spam/ham, novel/typical, click/no click)
- Learning
  Estimating the parameters w and b

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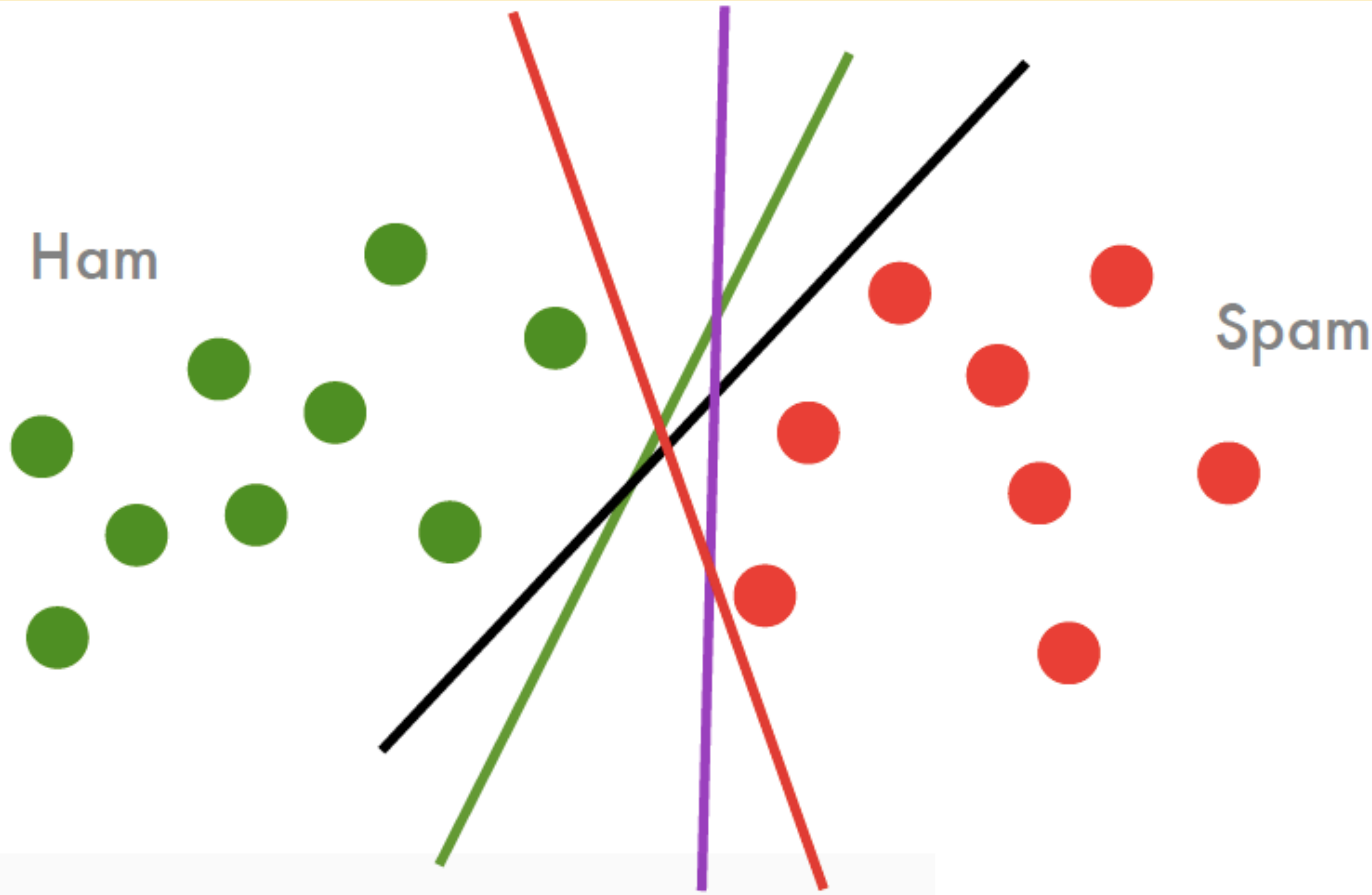

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- Weight vector is linear combination $w = \sum_{i \in I} y_i x_i$
- Classifier is linear combination of inner products $f(x) = \sum_{i \in I} y_i \langle x_i, x \rangle + b$

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- 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).

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

For error in observation (x_i, y_i) we get

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

Alignment increases with number of errors.

Proof

Step 2: Cauchy-Schwartz for the Dot Product

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

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

If we make a mistake we have

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

Step 4: Combination of first three steps

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

Solving for j proves the theorem.

5 minutes break

Consequences

- Only need to store errors.
  This gives a compression bound for perceptron.

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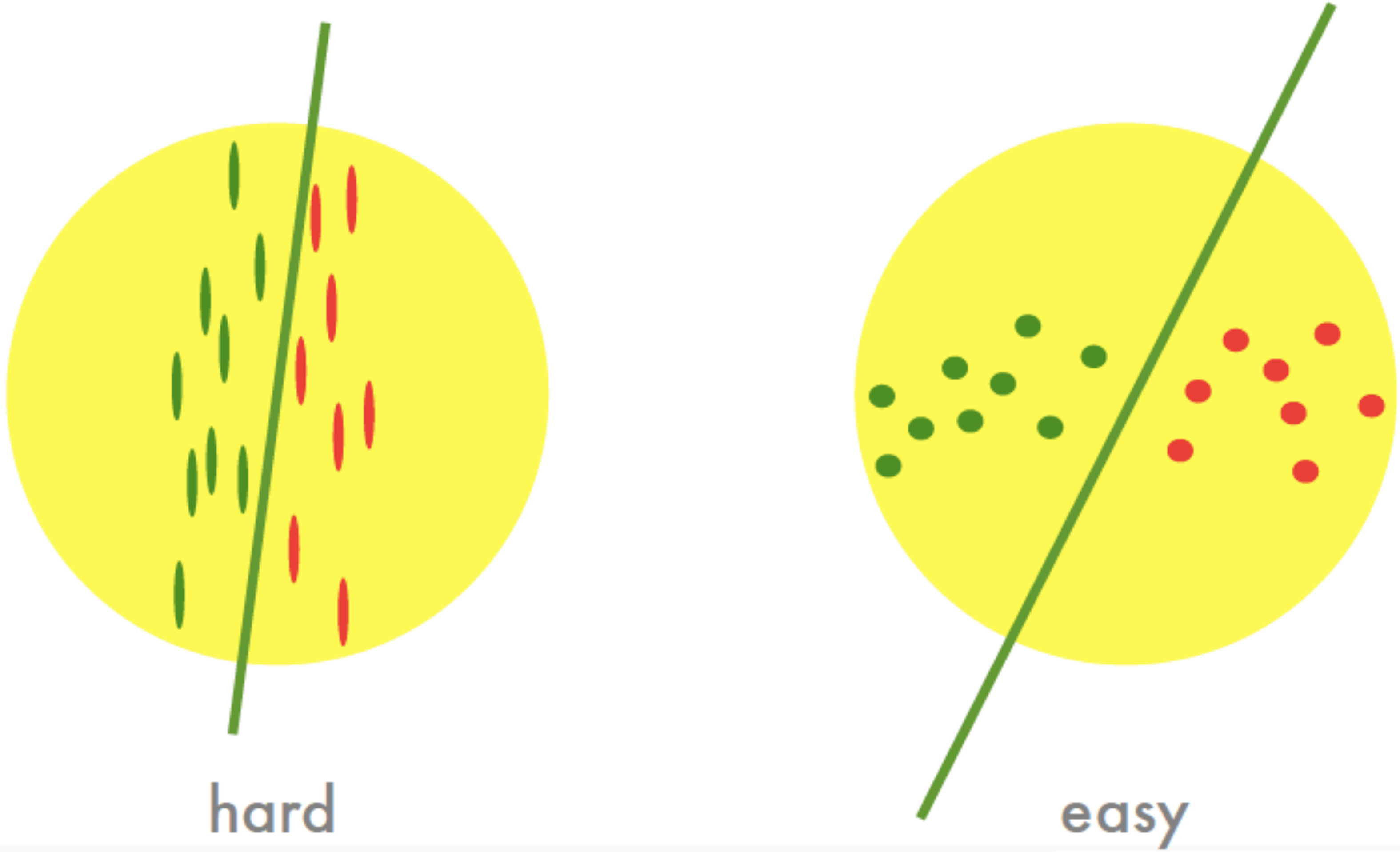
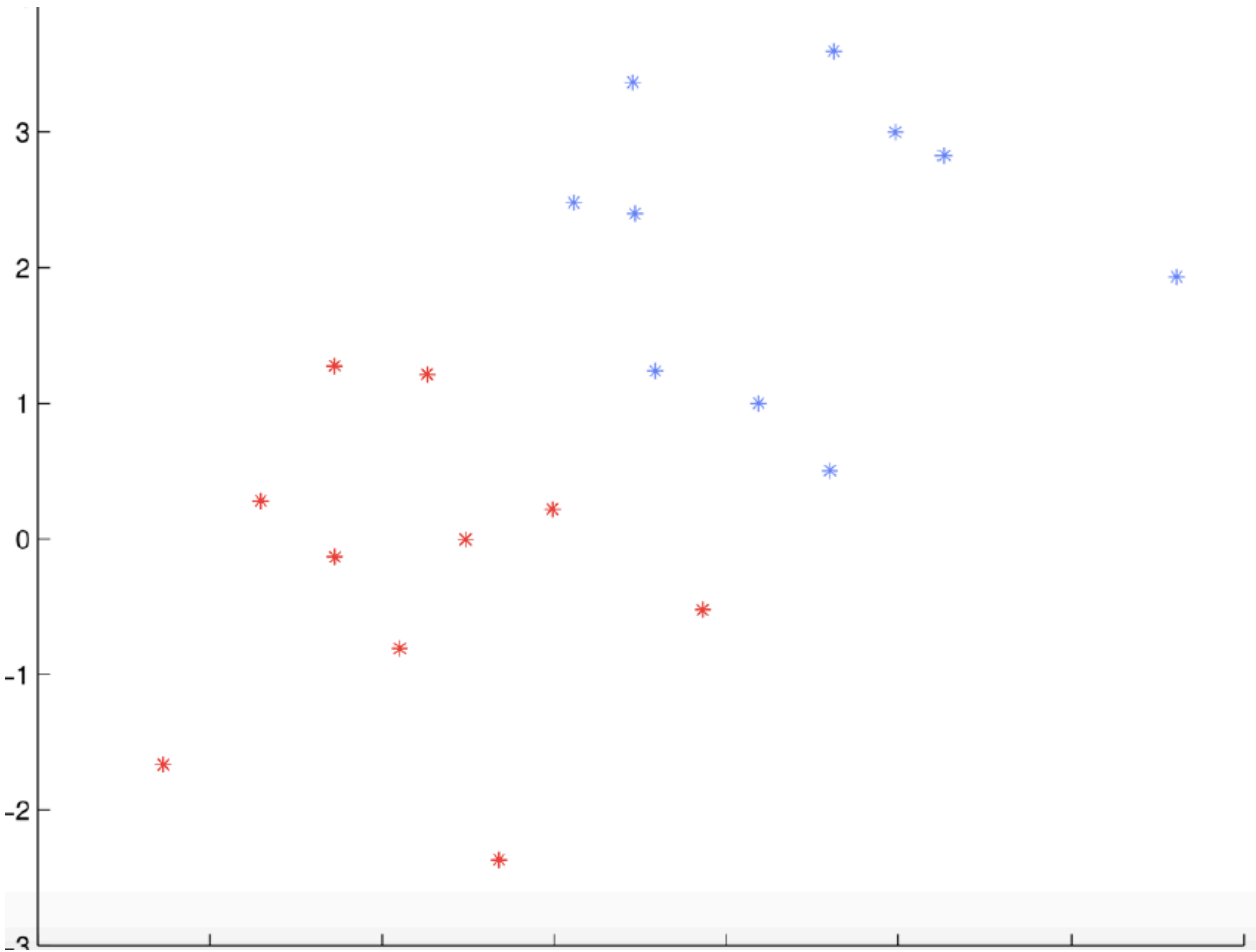
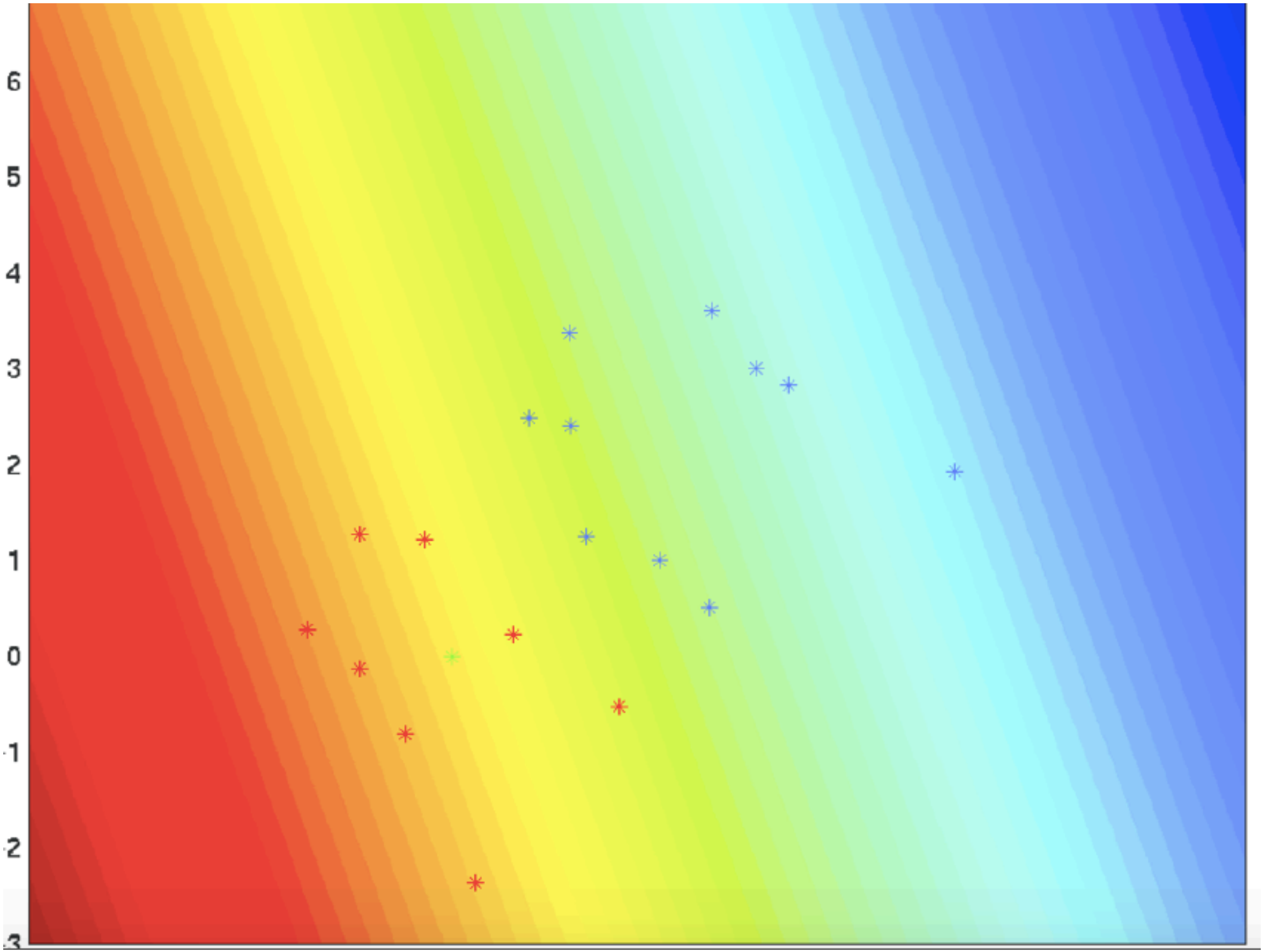
- Fails with noisy data

do NOT train your avatar with perceptrons

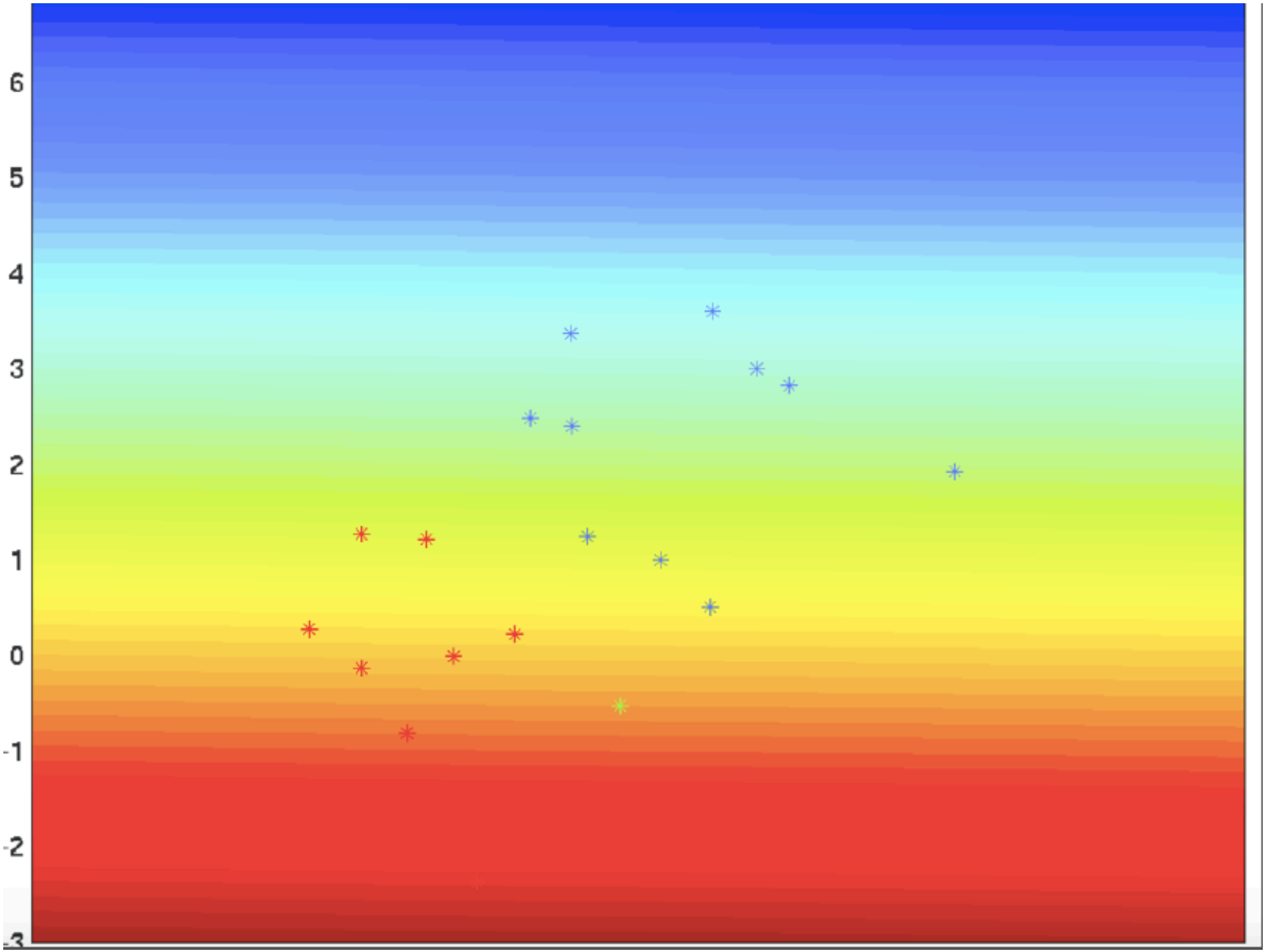
Hardness
margin vs. size




3
2
1
0
-1
-2
-3



6
5
4
3
2
1
0
-1
-2
-3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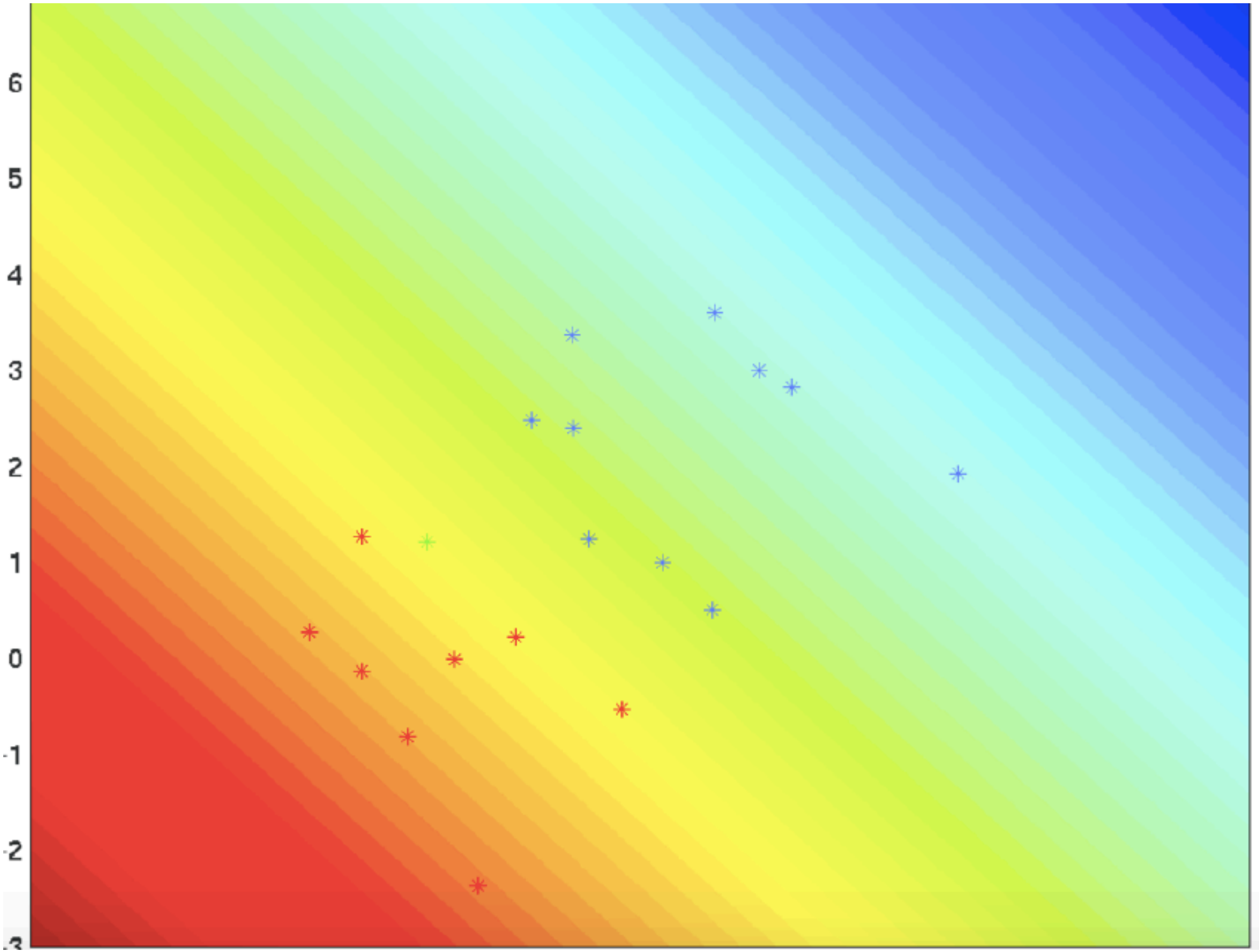
-3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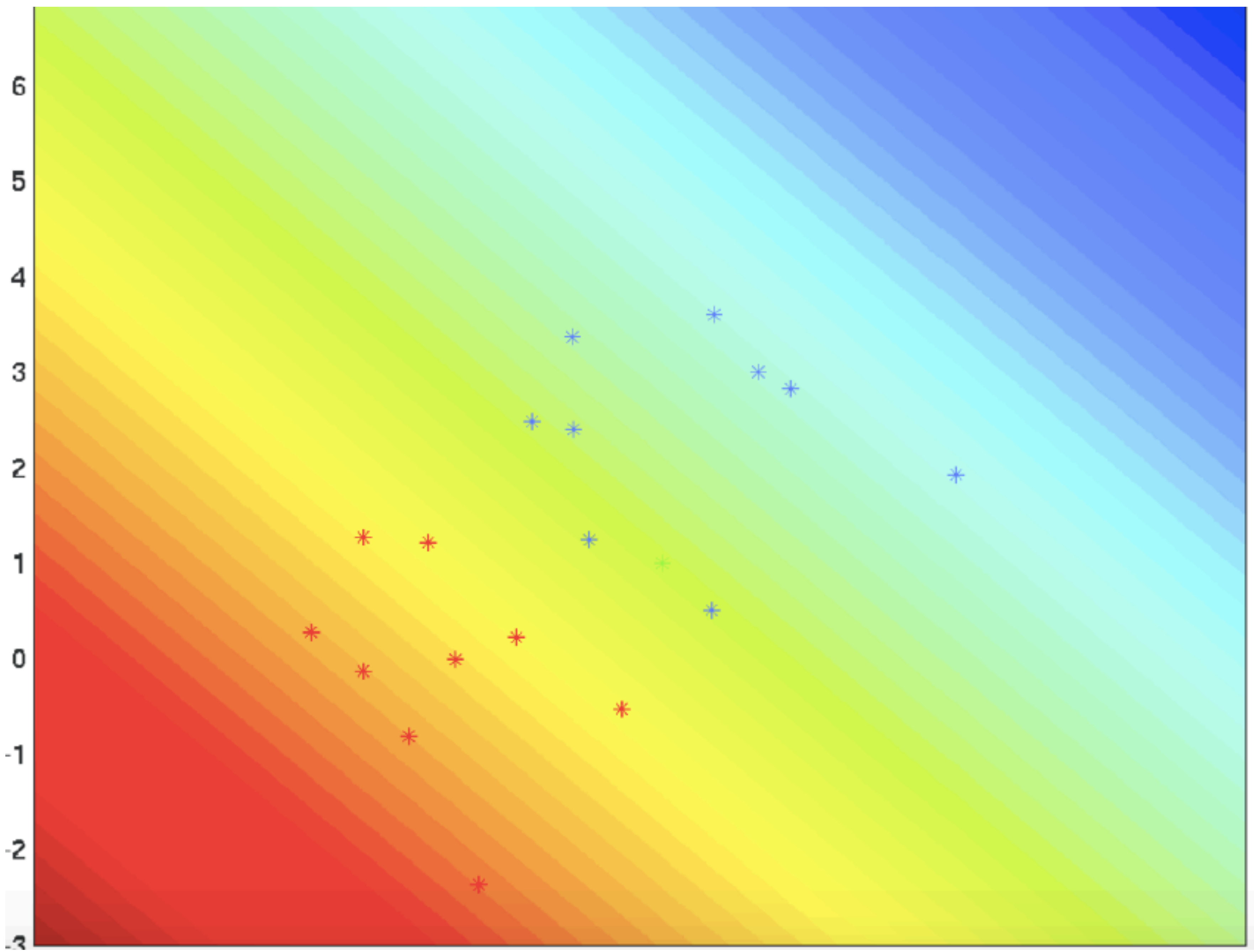
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Concepts & version space

- Realizable concepts
  - Some function exists that can separate data and is included in the concept space
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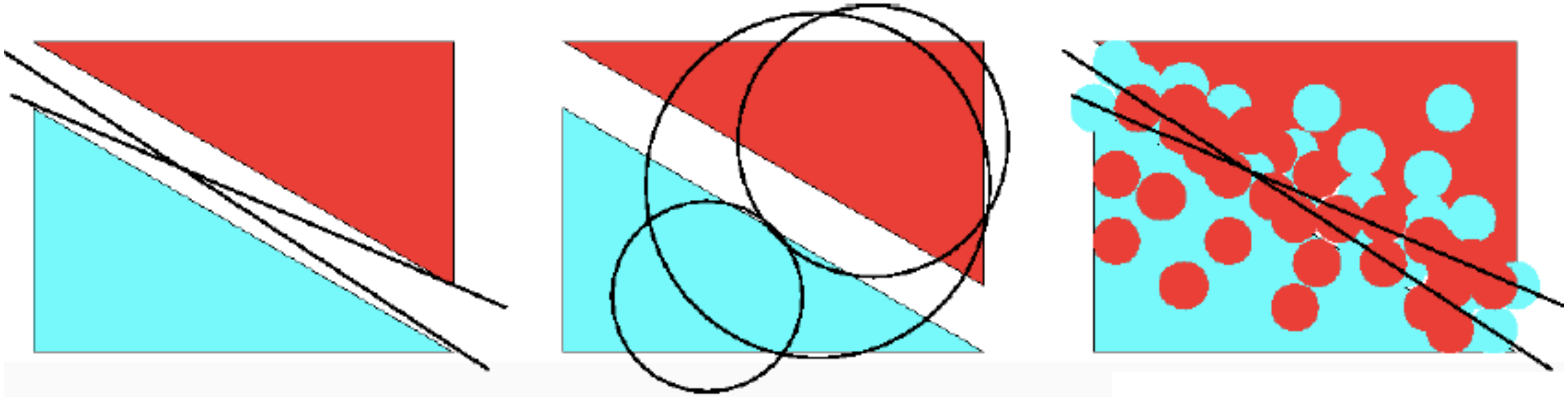

Minimum error separation

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- XOR - not linearly separable
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- 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).

Non-linearity and preprocessing

Nonlinear Features

- Perceptron

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  - Map data into feature space $x \to \phi(x)$
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  - 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

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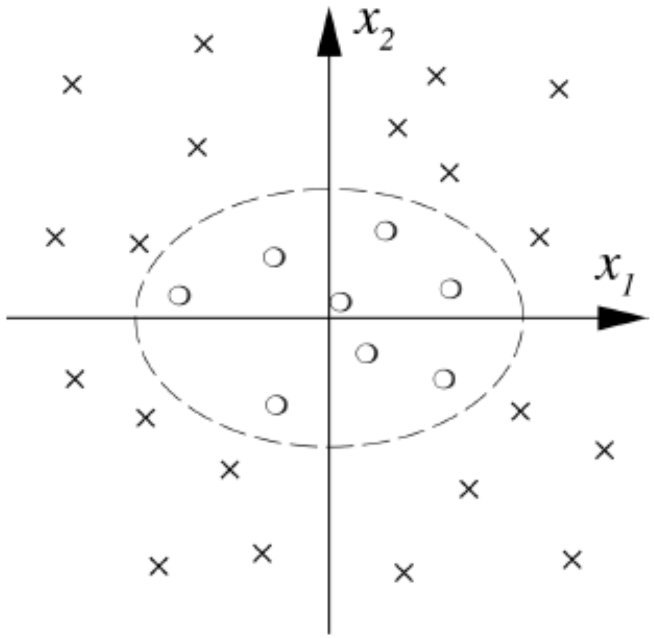

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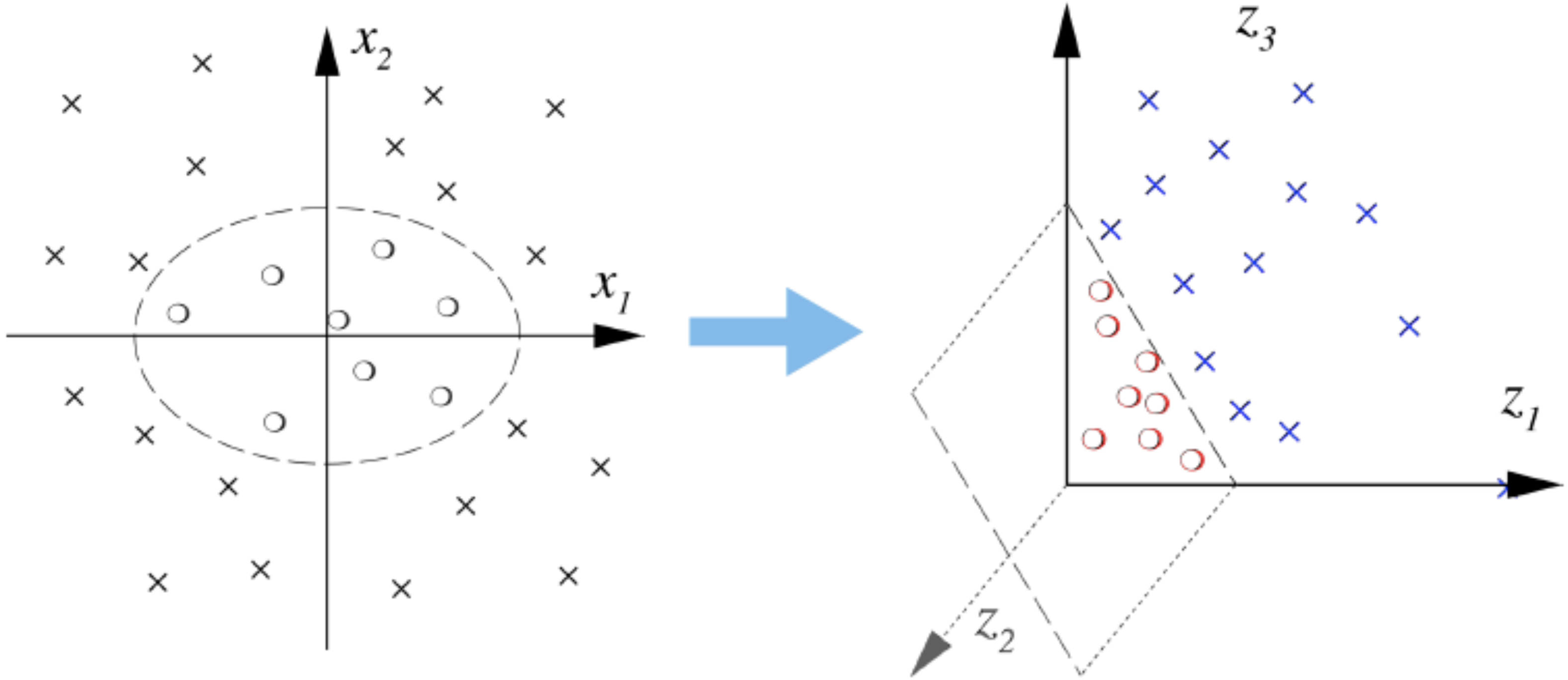

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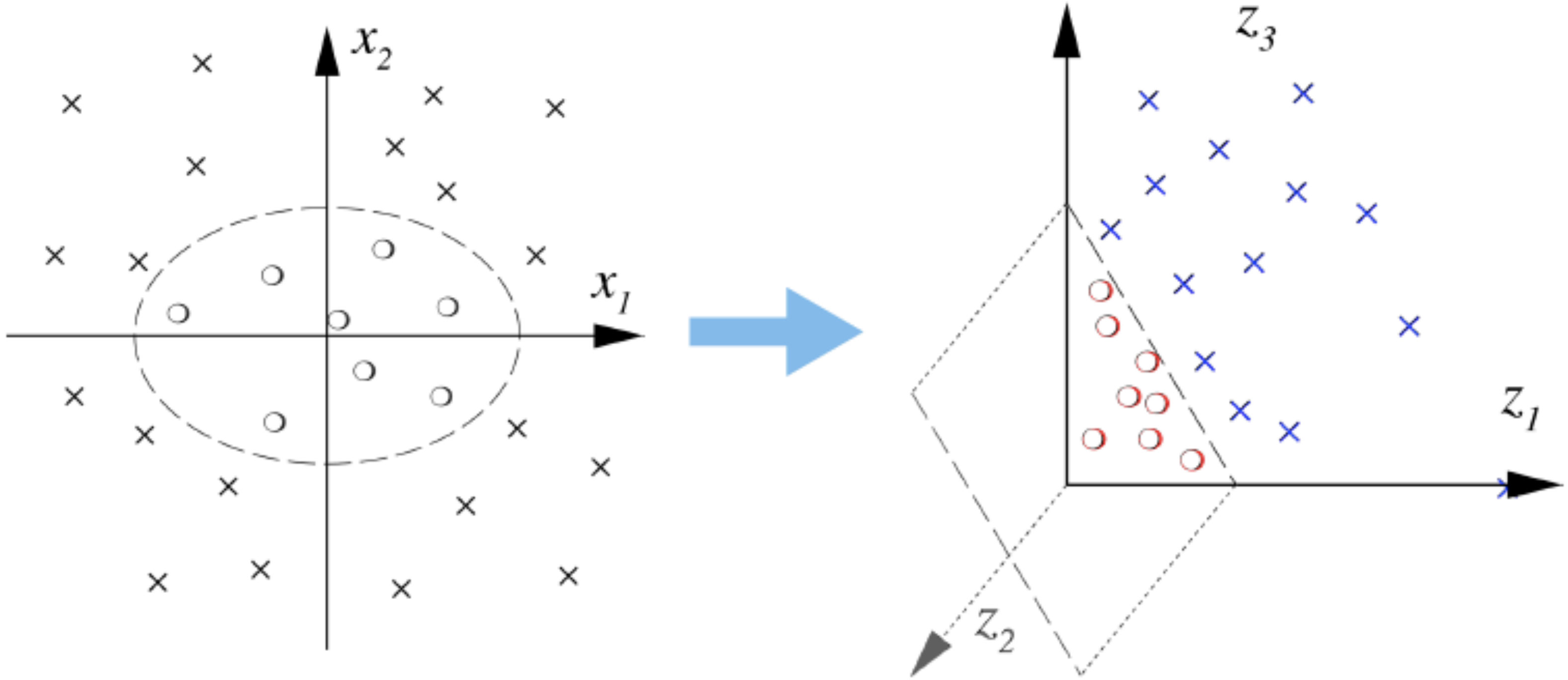

- Separating surfaces are
  Circles, hyperbolae, parabolae

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

```
Delivered-To: alex.smola@gmail.com
Received: by 10.216.47.73 with SMTP id s51cs361171web;
        Tue, 3 Jan 2012 14:17:53 -0800 (PST)
Received: by 10.213.17.145 with SMTP id s17mr2519891eba.147.1325629071725;
        Tue, 03 Jan 2012 14:17:51 -0800 (PST)
Return-Path: <alex+caf_=alex.smola=gmail.com@smola.org>
Received: from mail-ey0-f175.google.com (mail-ey0-f175.google.com [209.85.215.175])
        by mx.google.com with ESMTPS id n4si29264232eef.57.2012.01.03.14.17.51
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permitted nor denied by best guess record for domain of alex
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        h=mime-version:sender:date:x-google-sender-auth:message-id:subject
         :from:to:content-type;
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From: Tim Althoff <althoff@eecs.berkeley.edu>
To: alex@smola.org
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Content-Type: text/plain; charset=ISO-8859-1
```

- 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

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- Classifier is linear combination of inner products $f(x) = \sum_{i \in I} y_i \langle \phi(x_i), \phi(x) \rangle + b$

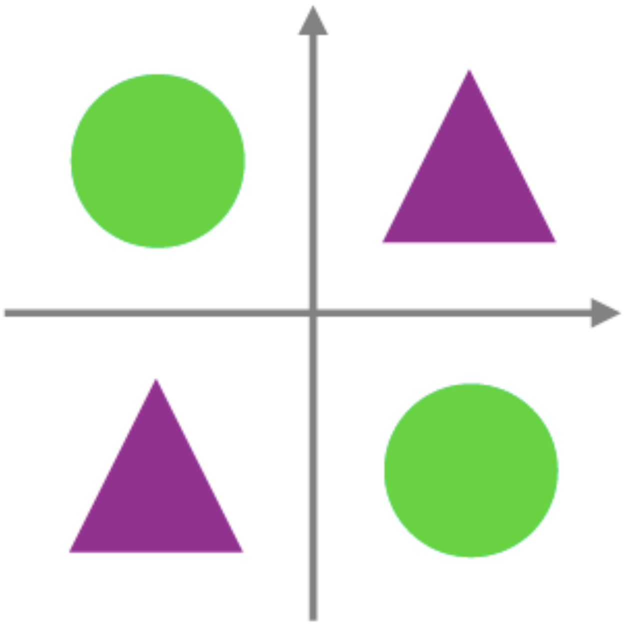
Problems

- 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

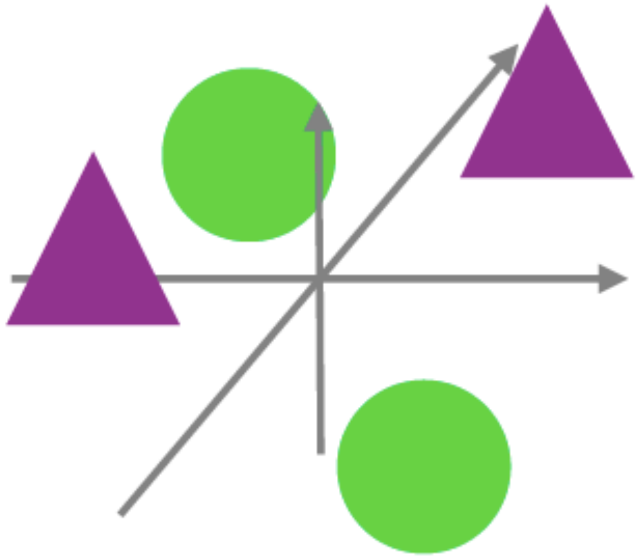
5 minutes break

Kernels

Solving XOR



(x_1, x_2)



(x_1, x_2, x_1x_2)

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

Quadratic Features

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

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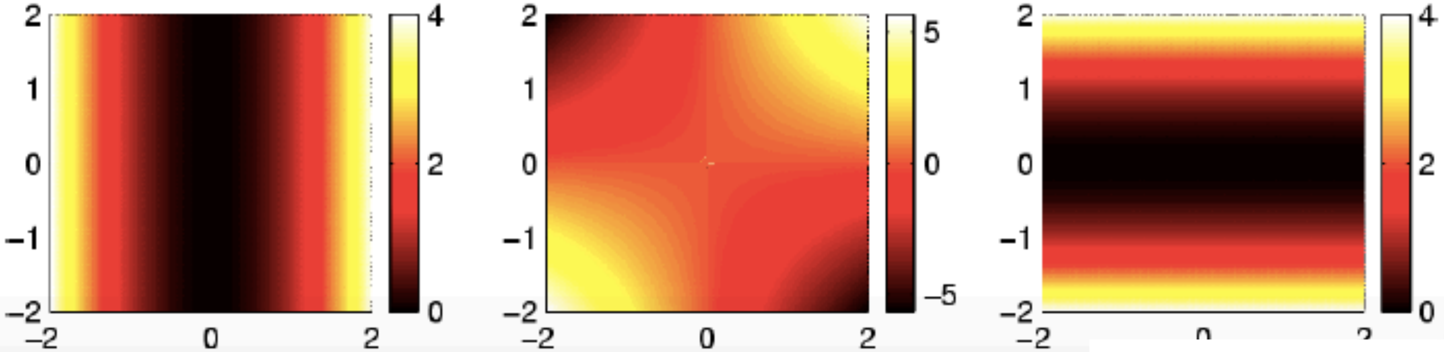
Insight

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



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.

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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

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initialize $f = 0$
repeat
    Pick (x_i, y_i) from data
    if $y_i f(x_i) \leq 0$ then
        $f(\cdot) \leftarrow f(\cdot) + y_i k(x_i, \cdot) + y_i$
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- 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

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- 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.

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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

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

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

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Dot Product in Feature Space

Is there always a Φ such that k really is a dot product?

Mercer's Theorem

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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

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

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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

Properties

Distance in Feature Space

Distance between points in feature space via

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

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Kernel Matrix

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

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

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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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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:

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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

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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 . . .

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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	$\exp\left(-\lambda \lVert x - x' \rVert\right)$
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	$\mathbf{E}_c[p(x\|c)p(x'\|c)]$

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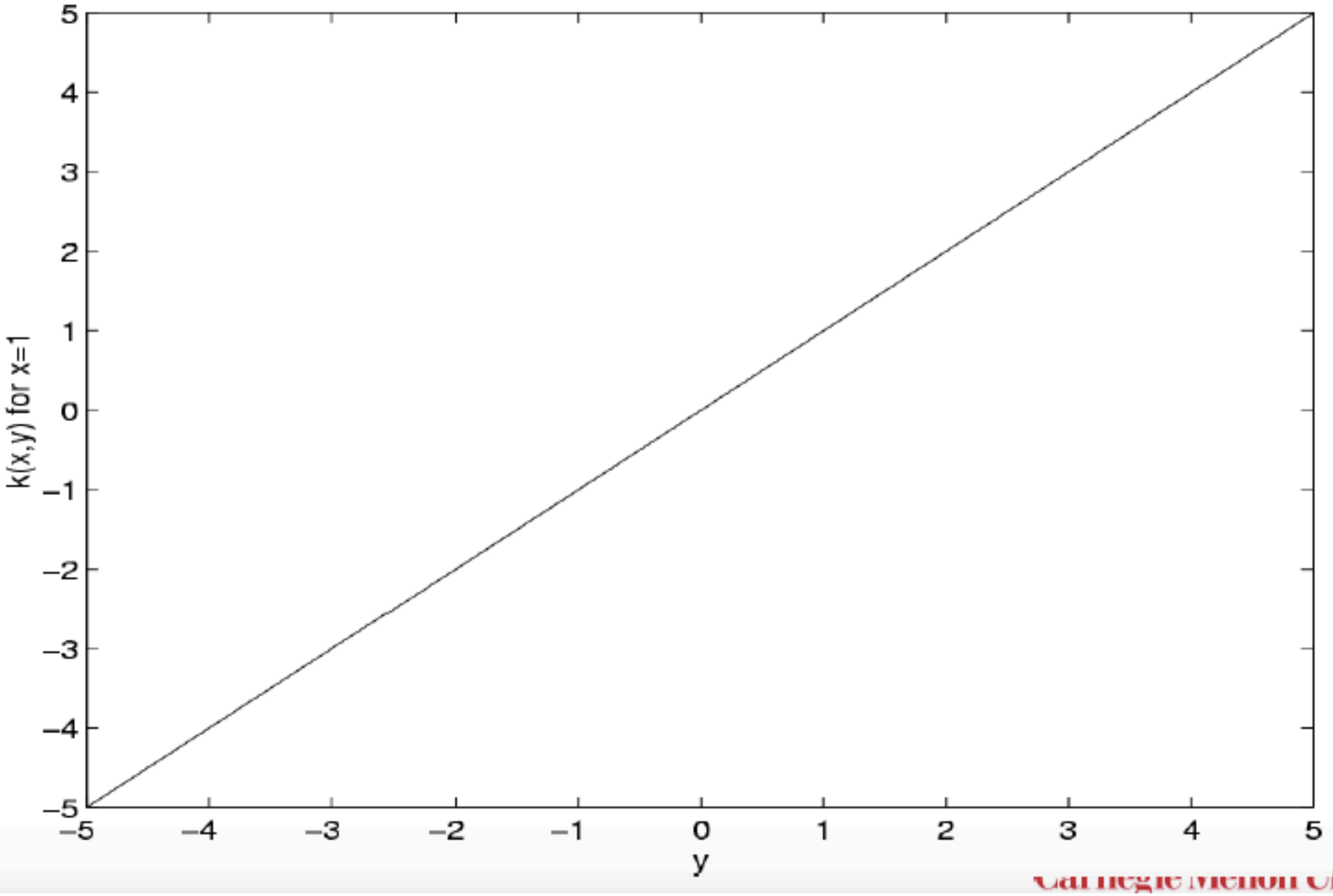
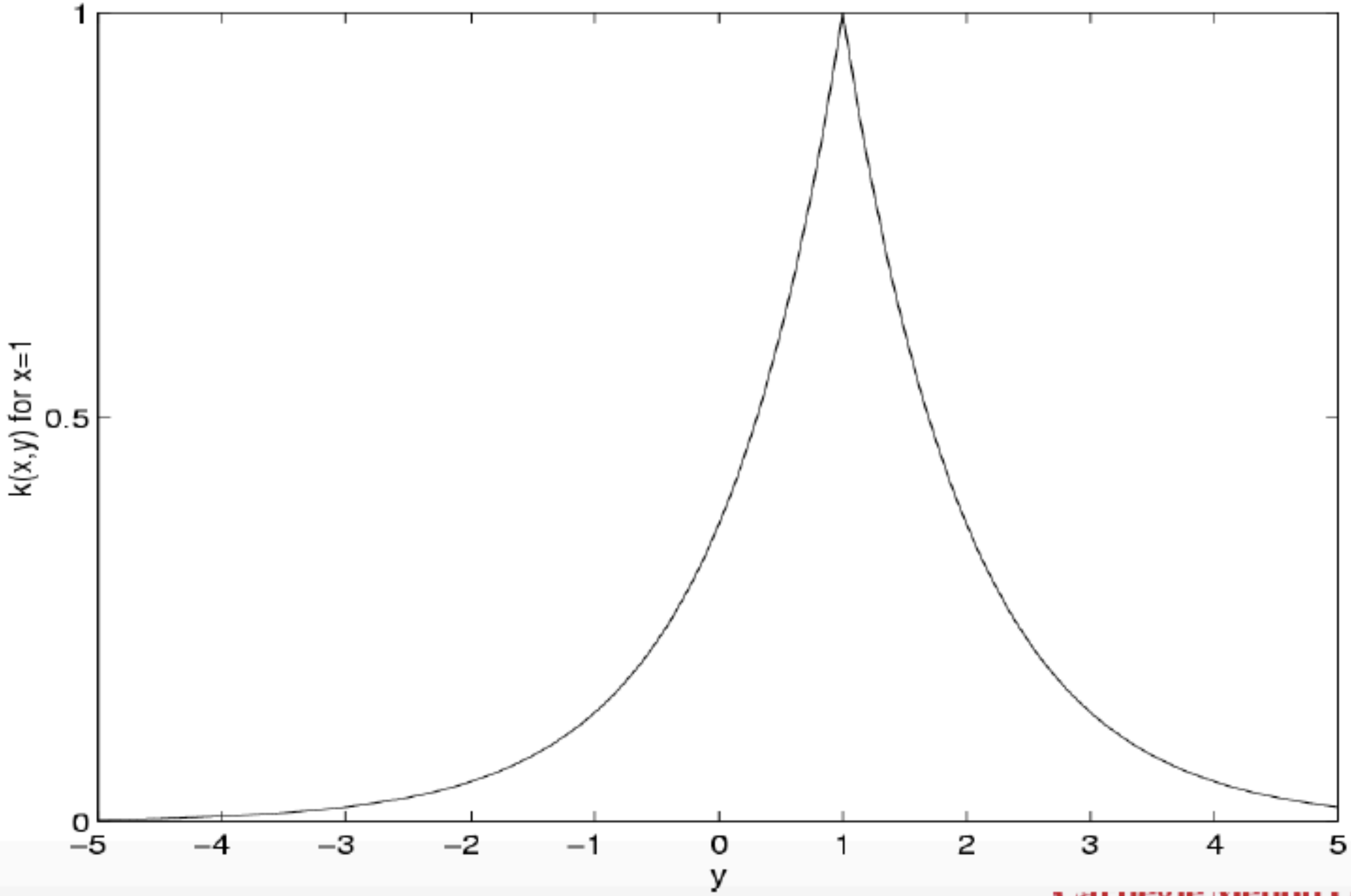
Simple trick for checking Mercer's condition

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

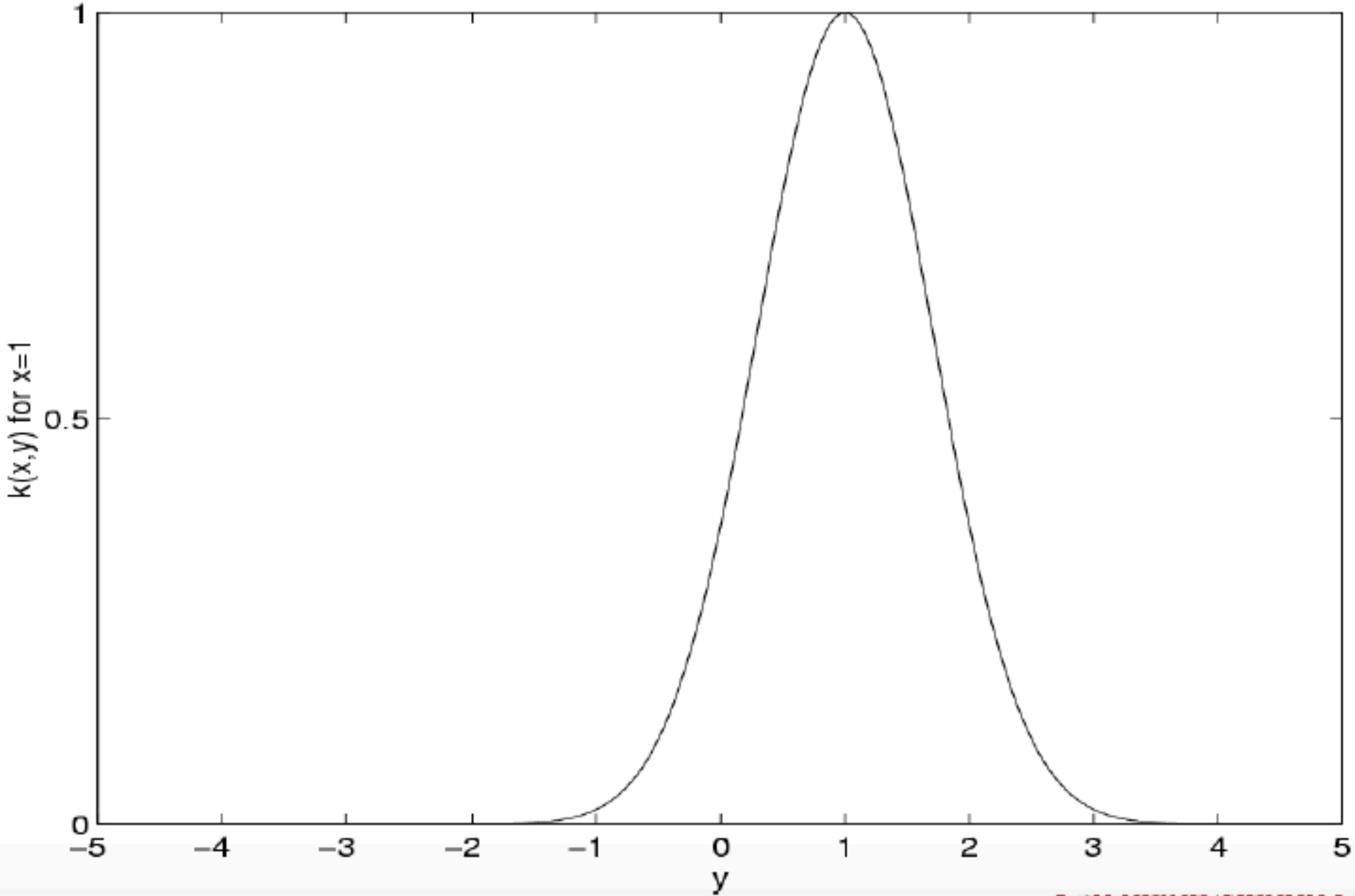
Linear Kernel



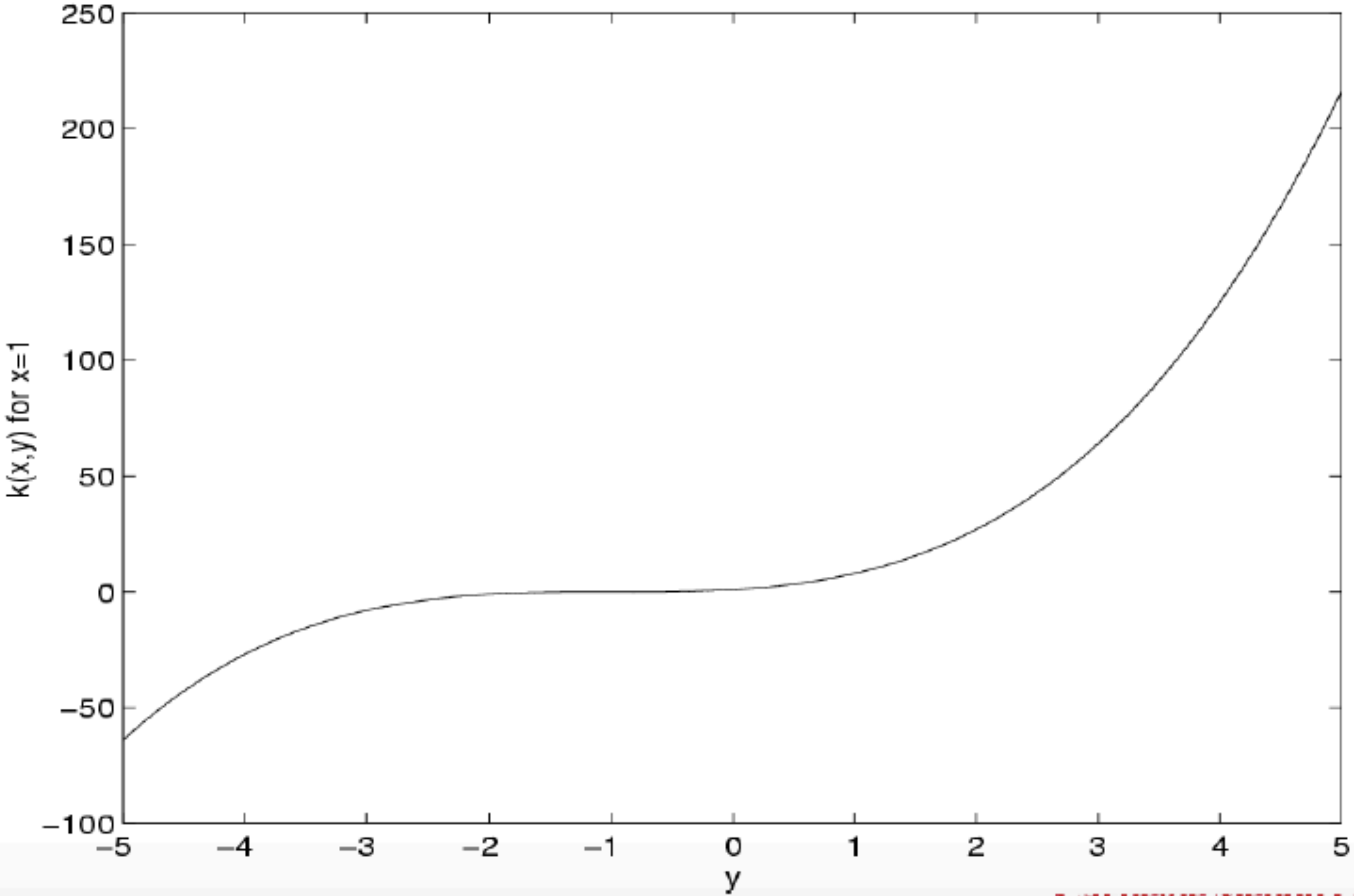
Laplacian Kernel



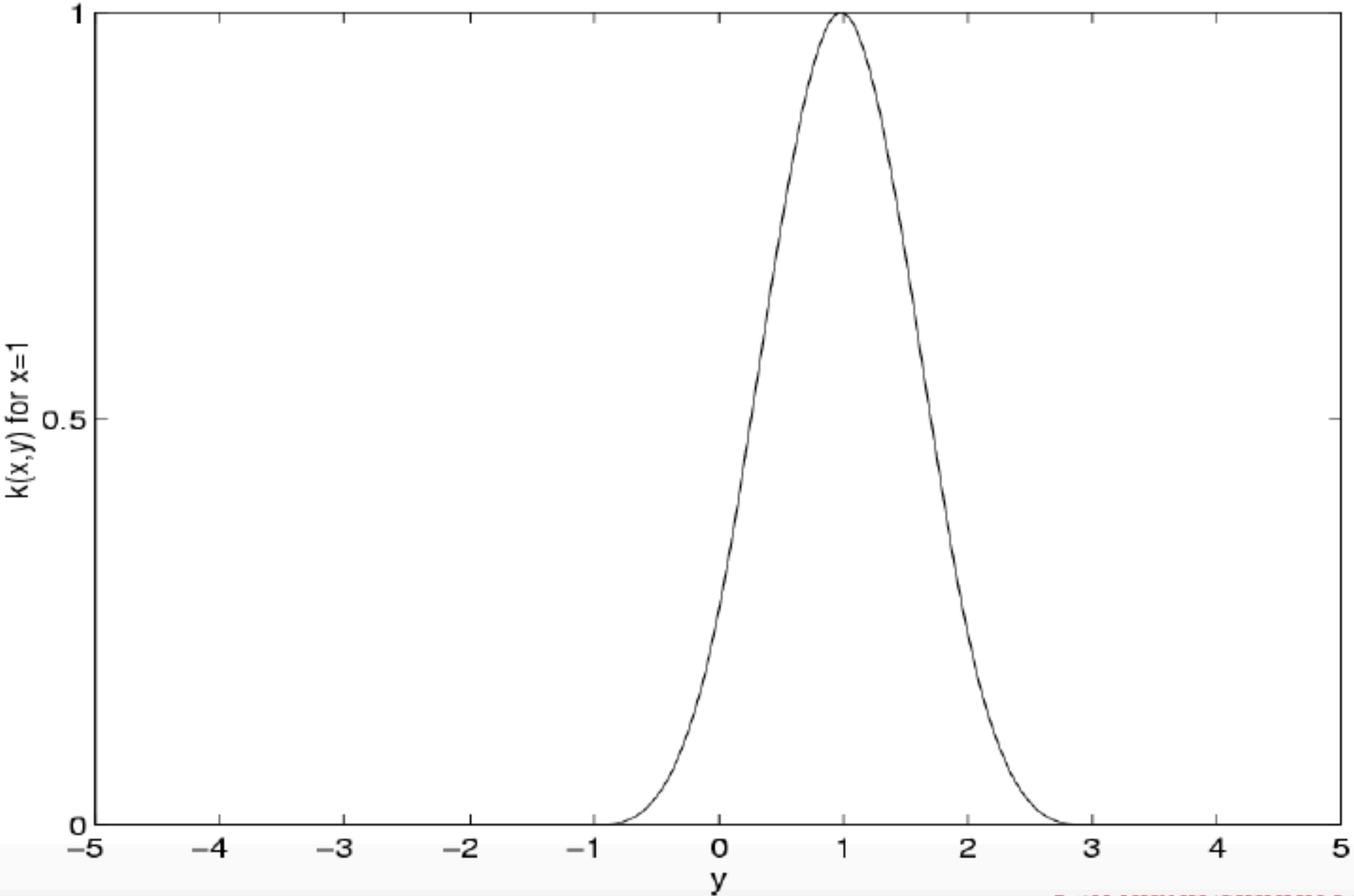
Gaussian Kernel



Polynomial of order 3



B_3 Spline Kernel



That’s all!