Artificial Intelligence and Machine Learning

Barbara Caputo

Perceptron: Non-linearity and preprocessing

Nonlinear Features

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

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  - Map data into feature space $x \to \phi(x)$
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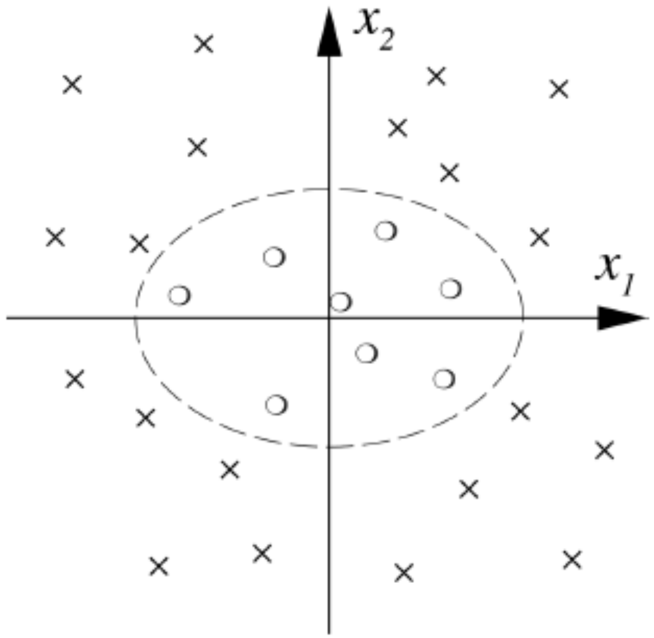
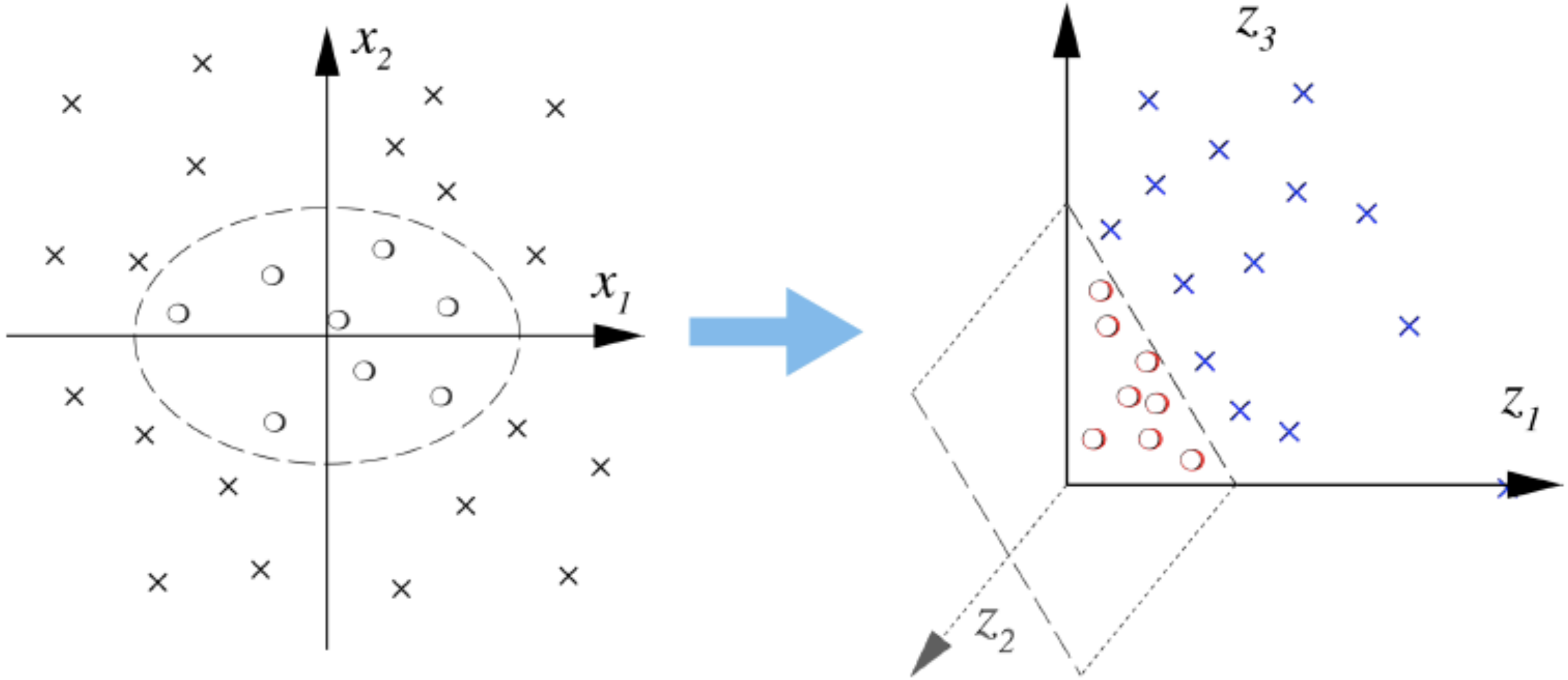
  - Query replace $\langle x, x' \rangle$ by $\langle \phi(x), \phi(x') \rangle$ for code
- Feature Perceptron
  - Solution in span of $\phi(x_i)$

Quadratic Features

Quadratic Features



Quadratic Features



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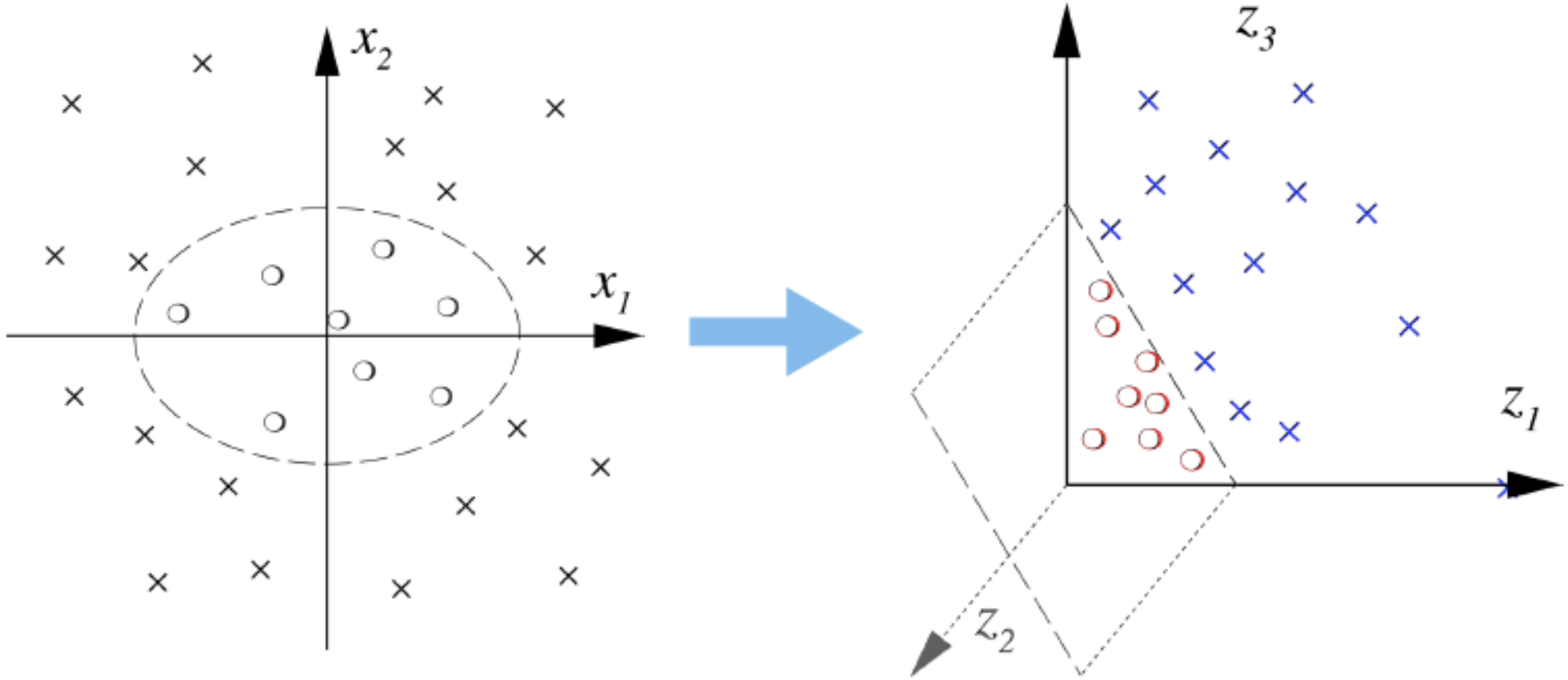

- Separating surfaces are
  Circles, hyperbolae, parabolae

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

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permitted nor denied by best guess record for domain of alex
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        Tue, 03 Jan 2012 14:17:48 -0800 (PST)
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To: alex@smola.org
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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

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    if $y_i(w \cdot \Phi(x_i) + b) \leq 0$ then

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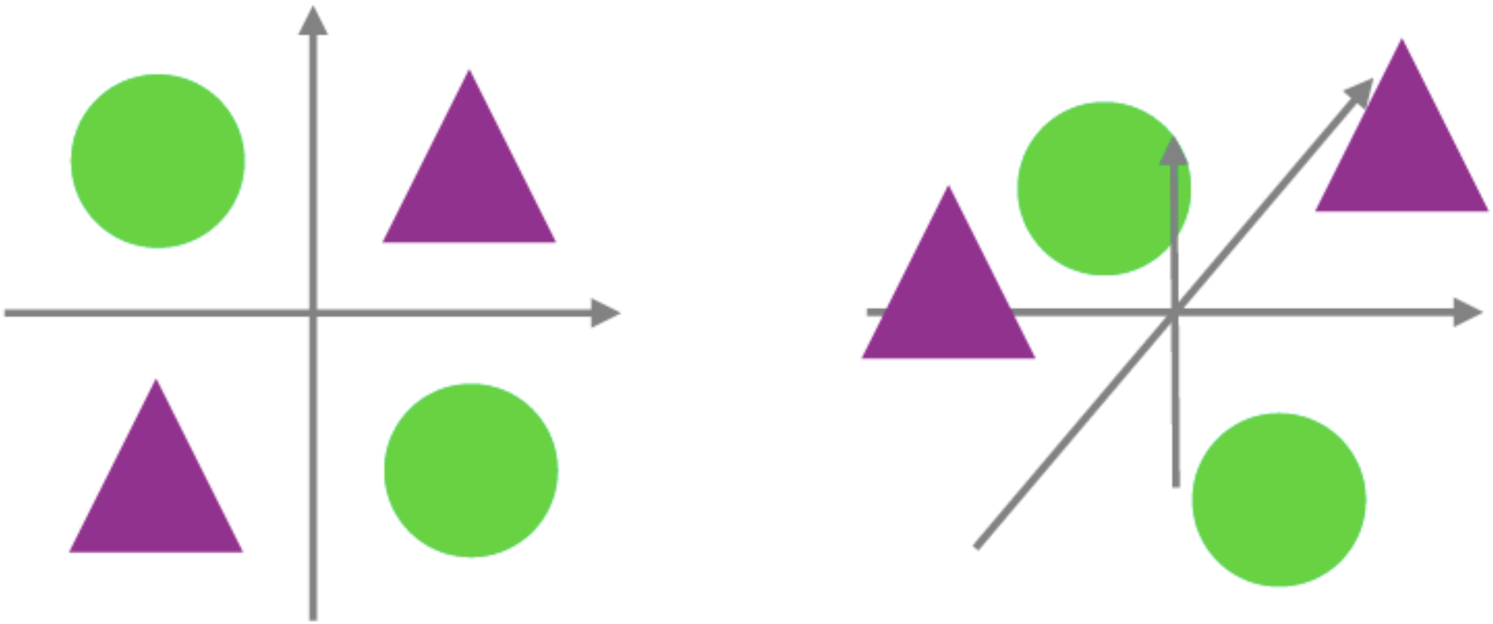
- Weight vector is linear combination $w = \sum_{i \in I} y_i \phi(x_i)$
- Classifier is linear combination of inner products $f(x) = \sum_{i \in I} y_i \langle \phi(x_i), \phi(x) \rangle + b$

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

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 in $\mathbb{R}^2$

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

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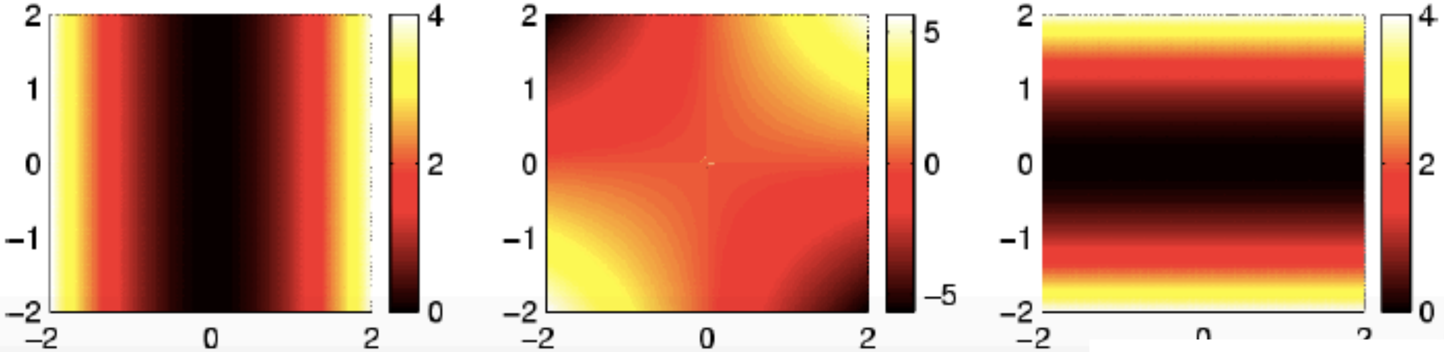
Insight

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

5 minutes break

Polynomial Kernels

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

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

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

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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

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

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

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

where x_i are the training patterns.

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

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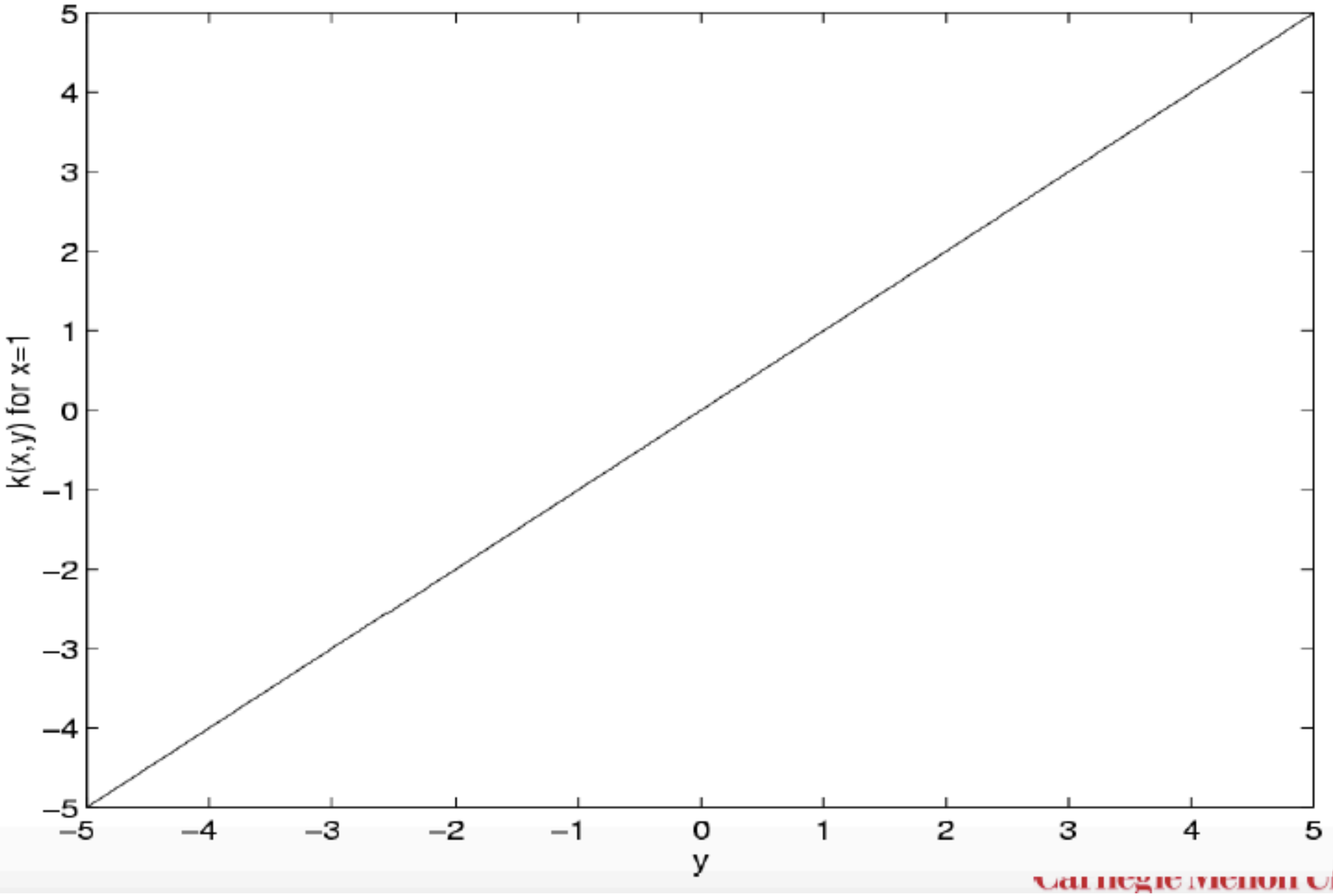
Cond. Expectation	$\mathbf{E}_c[p(x\|c)p(x'\|c)]$

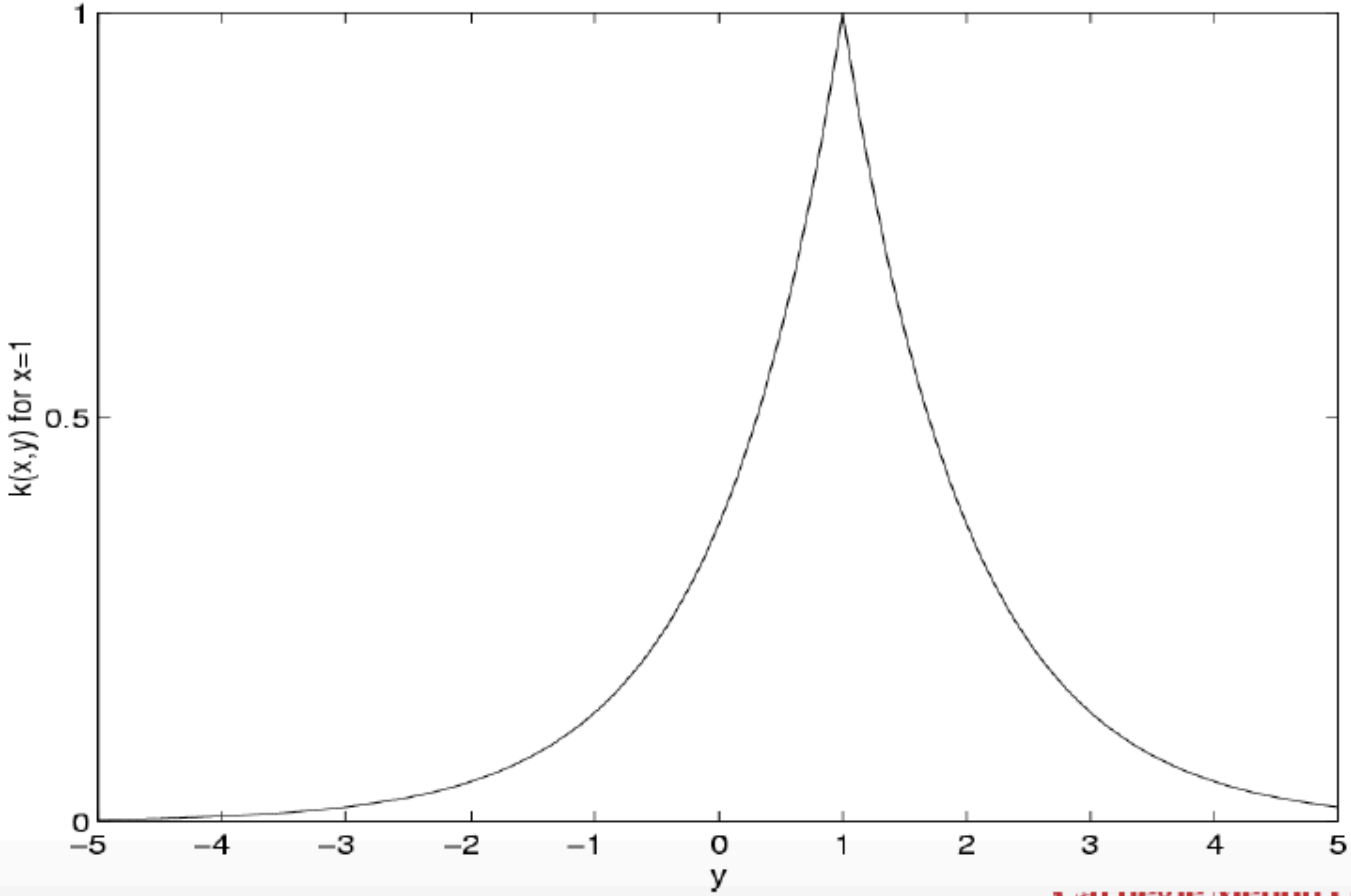
Simple trick for checking Mercer's condition

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

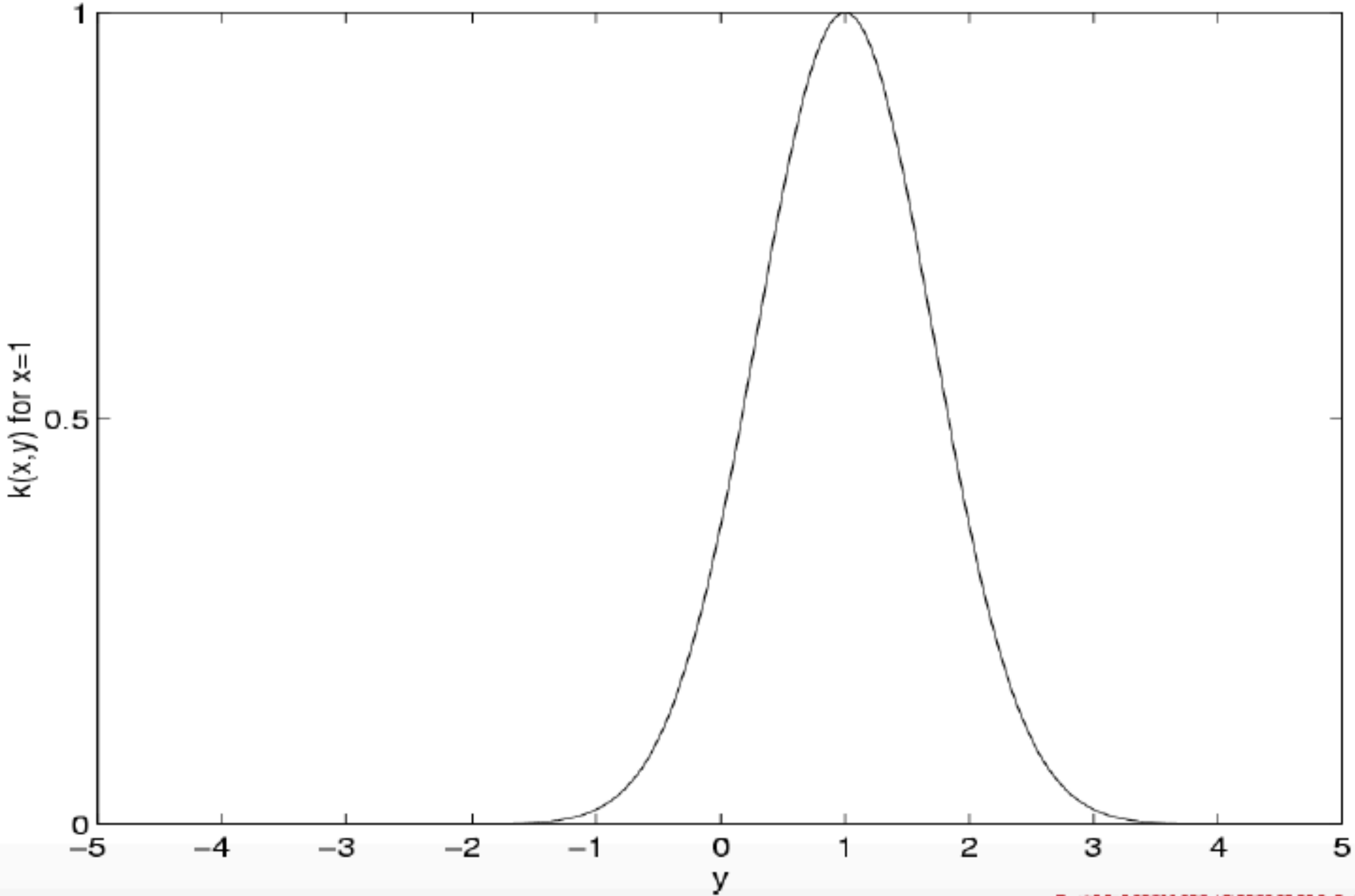
Linear Kernel



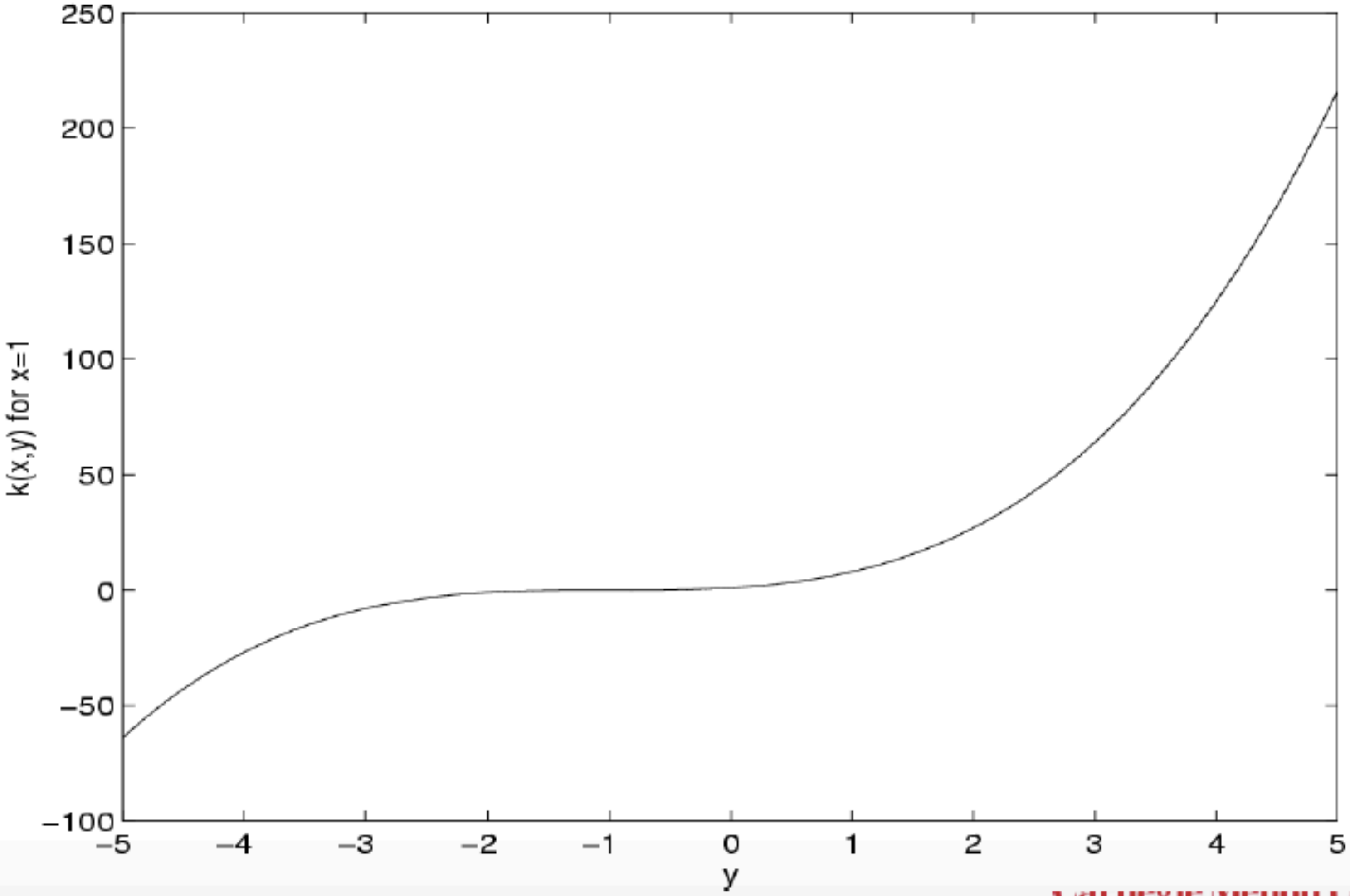
Laplacian Kernel



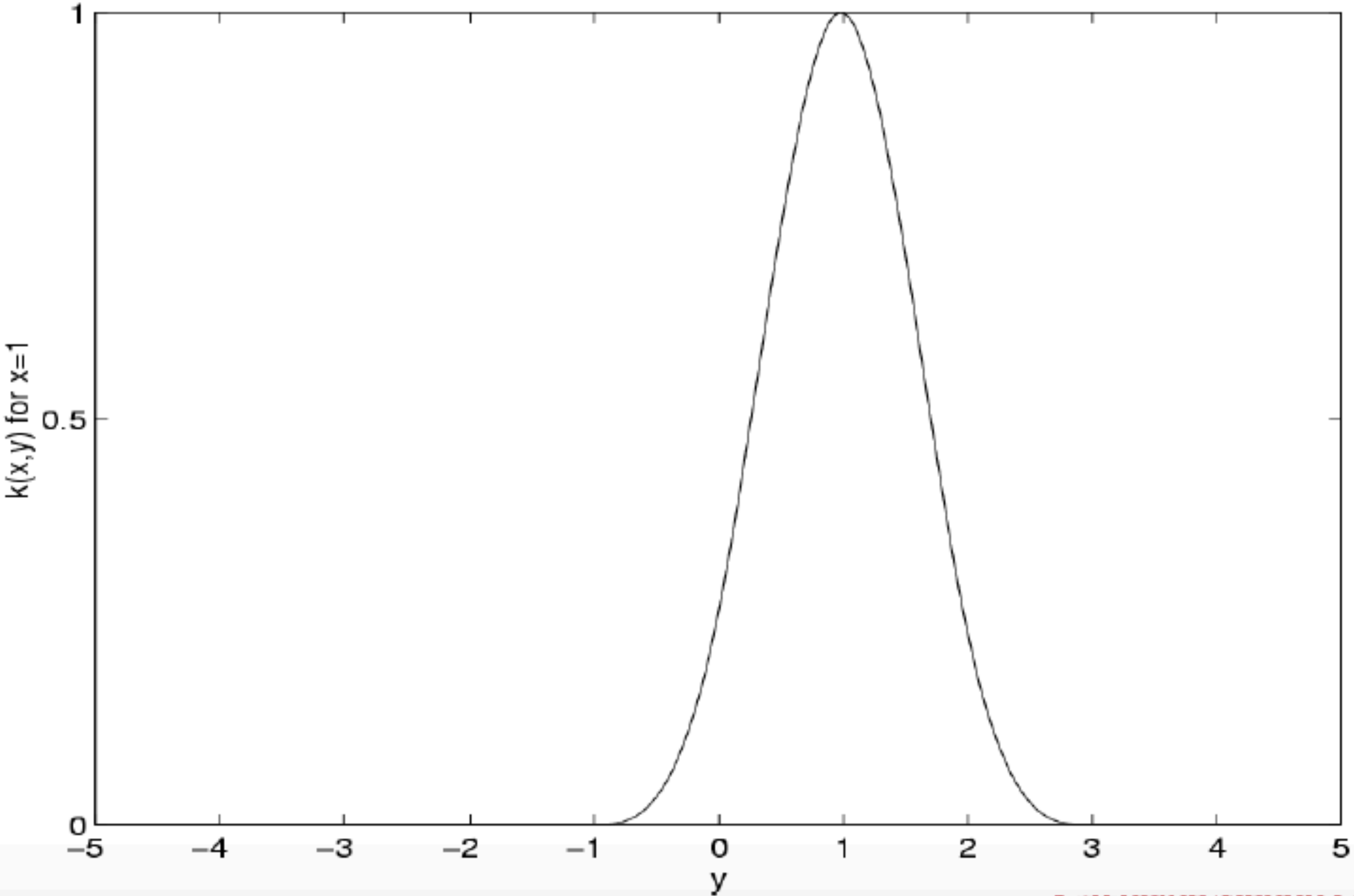
Gaussian Kernel



Polynomial of order 3



B_3 Spline Kernel



5 minutes break!

Parzen Windows

Density Estimation

- Observe some data x_i
- Want to estimate $p(x)$

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- Want to estimate p(x)
  - Find unusual observations (e.g. security)
  - Find typical observations (e.g. prototypes)

Density Estimation

- Observe some data x_i
- Want to estimate p(x)
  - Find unusual observations (e.g. security)
  - Find typical observations (e.g. prototypes)
  - Classifier via Bayes Rule

$$p(y|x) = \frac{p(x,y)}{p(x)} = \frac{p(x|y)p(y)}{\sum_{y'} p(x|y')p(y')}$$

- Need tool for computing p(x) easily

Bin Counting

- Discrete random variables, e.g.
  - English, Chinese, German, French, ...
  - Male, Female
- Bin counting (record # of occurrences)

25	English	Chinese	German	French	Spanish
male	5	2	3	1	0
female	6	3	2	2	1

Bin Counting

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25	English	Chinese	German	French	Spanish
male	0.2	0.08	0.12	0.04	0
female	0.24	0.12	0.08	0.08	0.04

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Bin Counting

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  - English, Chinese, German, French, ...
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not enough data

25	English	Chinese	German	French	Spanish
male	0.2	0.08	0.12	0.04	0
female	0.24	0.12	0.08	0.08	0.04

Curse of dimensionality (lite)

- Discrete random variables, e.g.
  - English, Chinese, German, French, ...
  - Male, Female
  - ZIP code
  - Day of the week
  - Operating system
  - ...

#bins grows exponentially

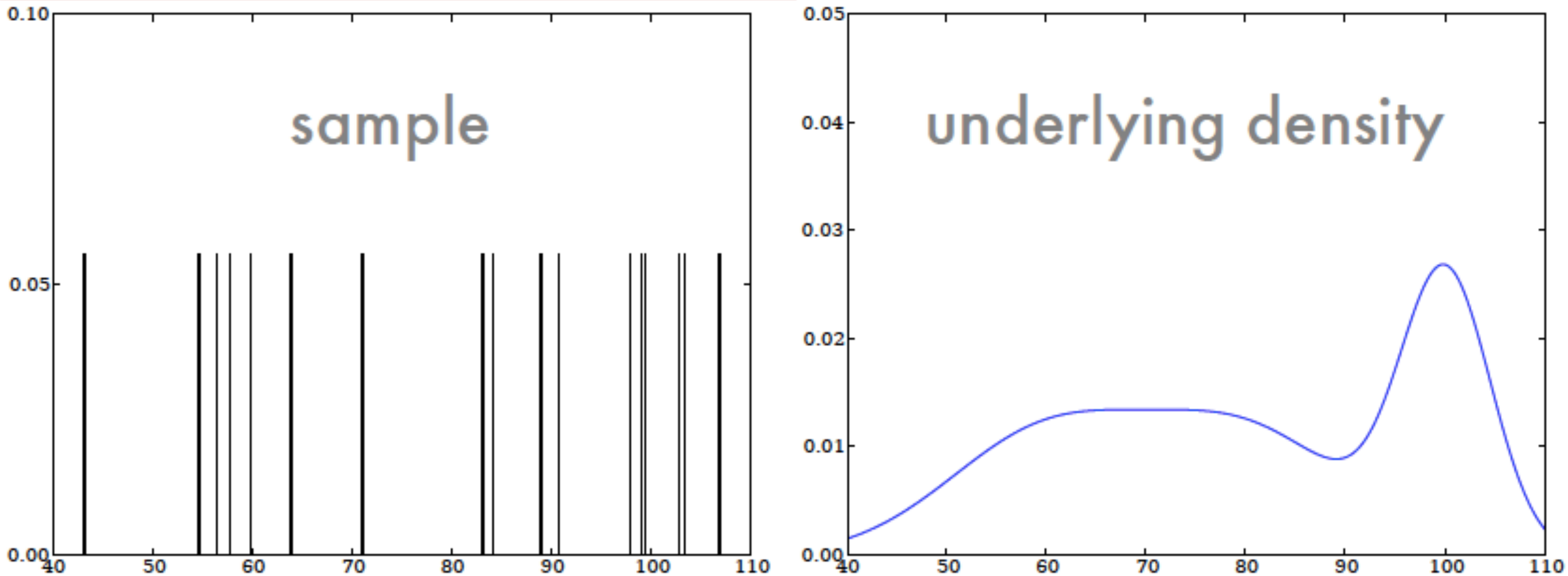
Curse of dimensionality (lite)

- Discrete random variables, e.g.
  - English, Chinese, German, French, ...
  - Male, Female
  - ZIP code
  - Day of the week
  - Operating system
  - ...
- Continuous random variables
  - Income
  - Bandwidth
  - Time

#bins grows exponentially

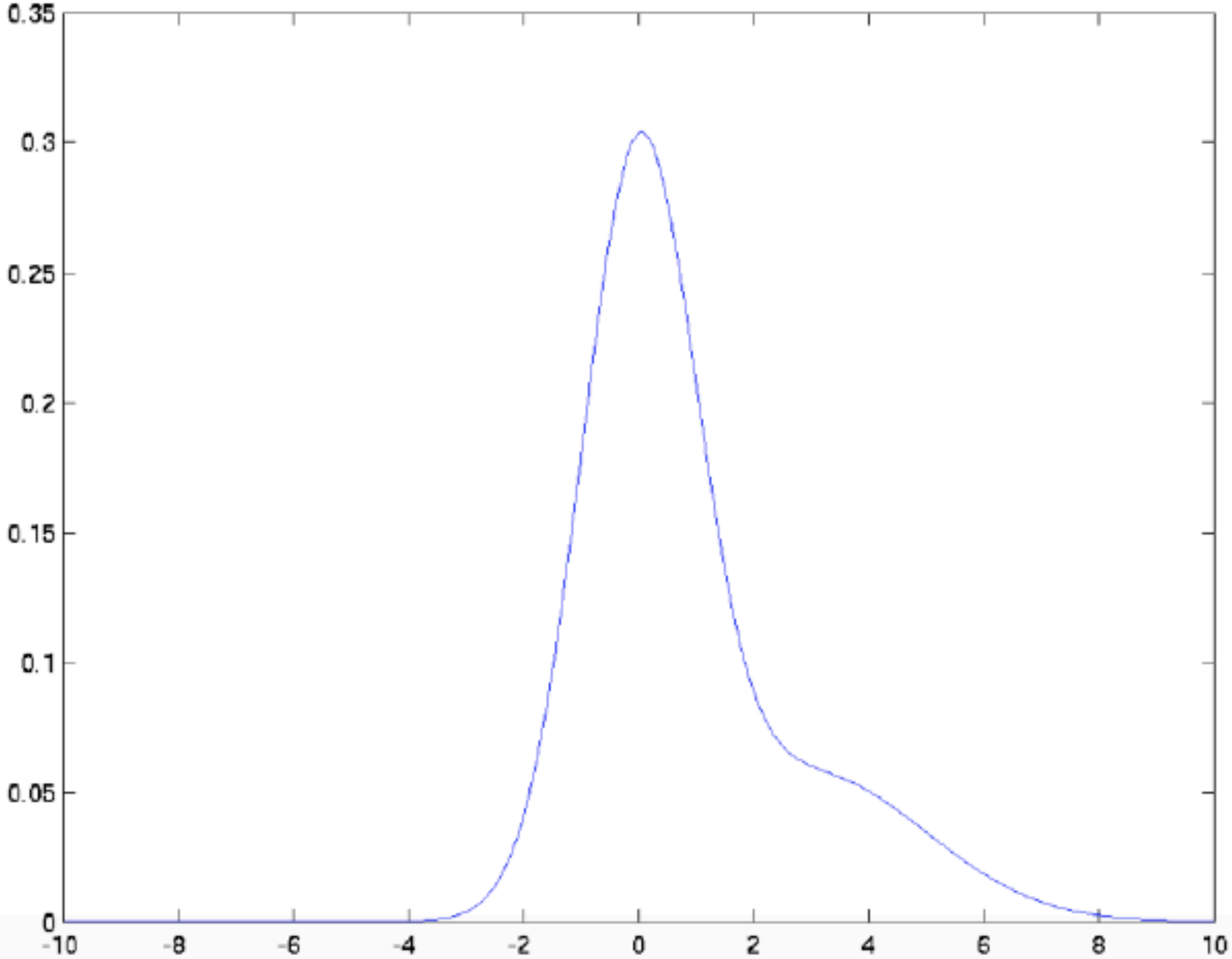
need many bins per dimension

Density Estimation

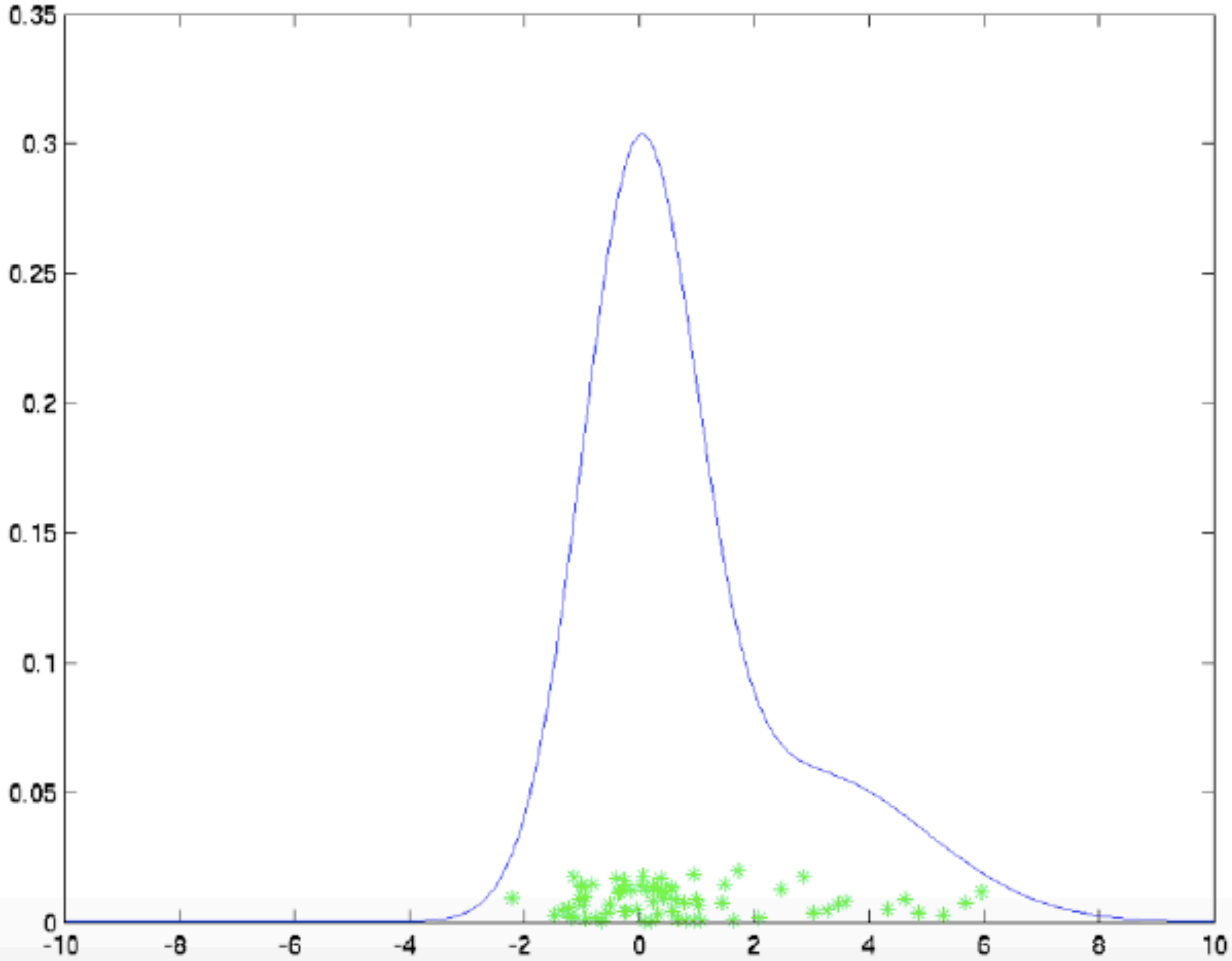


- Continuous domain = infinite number of bins
- Curse of dimensionality
  - 10 bins on [0, 1] is probably good
  - 10^{10} bins on $[0, 1]^{10}$ requires high accuracy in estimate: probability mass per cell also decreases by 10^{10}

Bin Counting



Bin Counting



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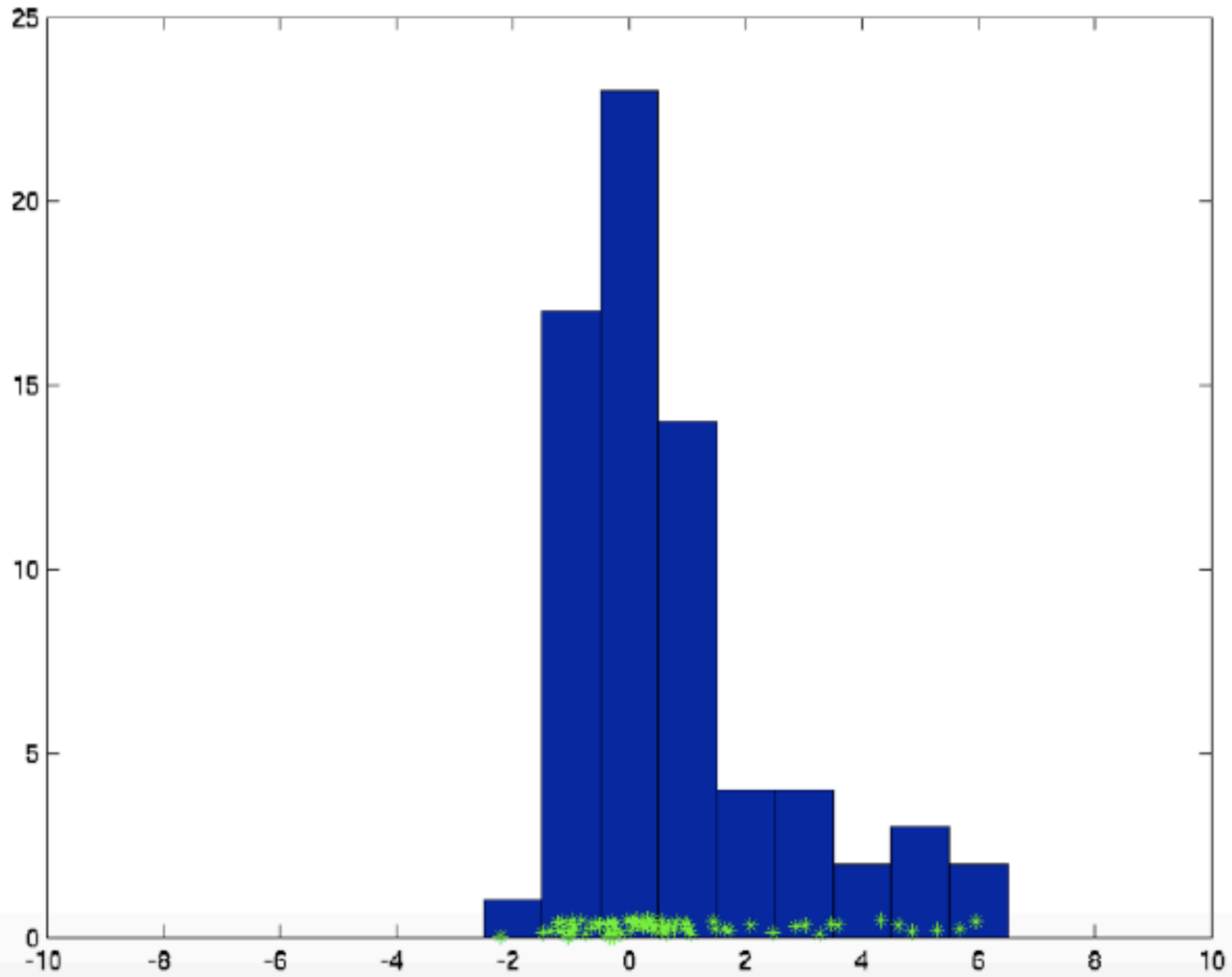
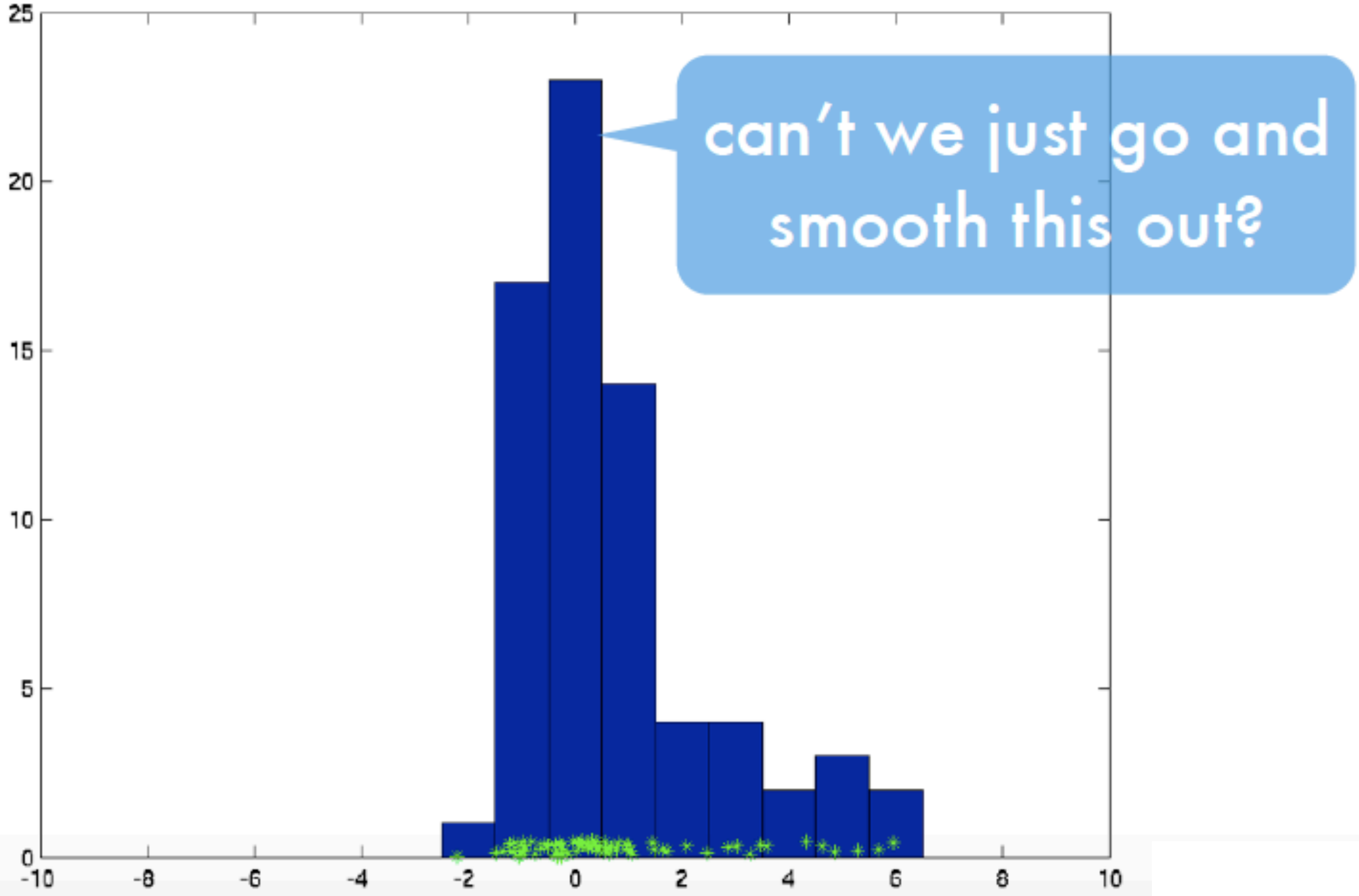


Bin Counting



Parzen Windows

- Naive approach
  Use empirical density (delta distributions)

$$p_{\text{emp}}(x) = \frac{1}{m} \sum_{i=1}^{m} \delta_{x_i}(x)$$

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- This breaks if we see slightly different instances
- Kernel density estimate

Parzen Windows

- Naive approach
  Use empirical density (delta distributions)

$$p_{\text{emp}}(x) = \frac{1}{m} \sum_{i=1}^{m} \delta_{x_i}(x)$$

- This breaks if we see slightly different instances
- Kernel density estimate
  Smear out empirical density with a nonnegative smoothing kernel $k_x(x')$ satisfying

$$\int_{\mathcal{X}} k_x(x') dx' = 1 \text{ for all } x$$

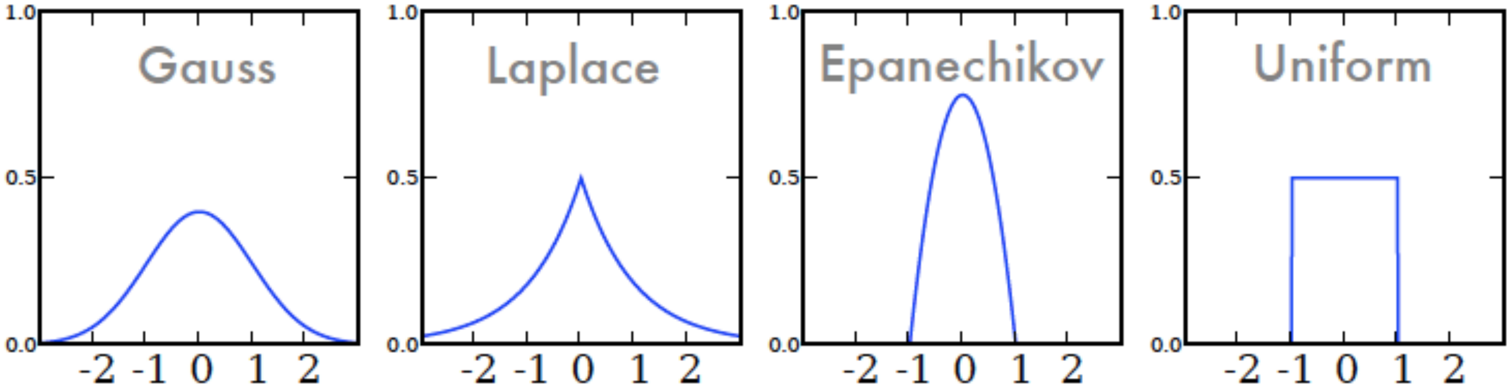
Parzen Windows

- **Density estimate**

$$p_{\text{emp}}(x) = \frac{1}{m}\sum_{i=1}^{m}\delta_{x_i}(x)$$

$$\hat{p}(x) = \frac{1}{m}\sum_{i=1}^{m}k_{x_i}(x)$$

- **Smoothing kernels**



$(2\pi)^{-\frac{1}{2}}e^{-\frac{1}{2}x^2}$ $\quad$ $\frac{1}{2}e^{-|x|}$ $\quad$ $\frac{3}{4}\max(0, 1-x^2)$ $\quad$ $\frac{1}{2}\chi_{[-1,1]}(x)$

Nearest Neighbor

Nearest Neighbors

- Table lookup
  For previously seen instance remember label

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  For previously seen instance remember label
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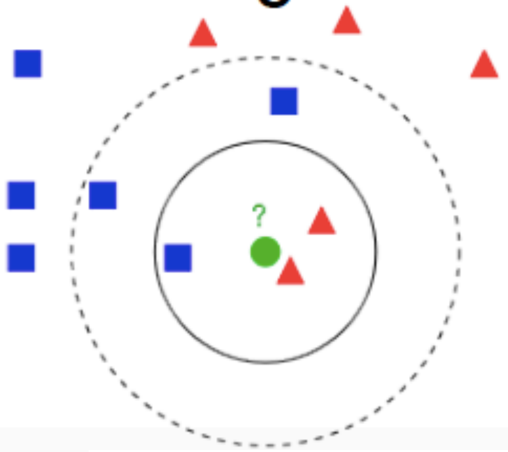

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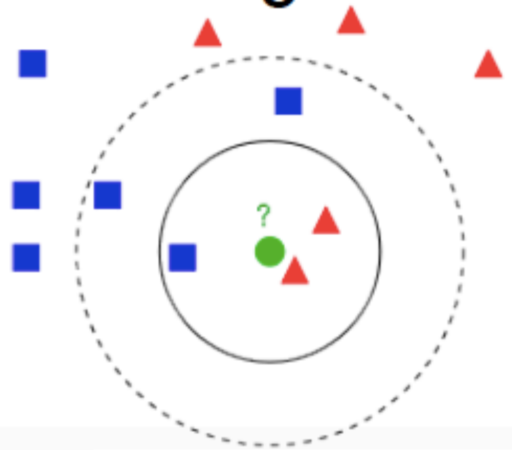
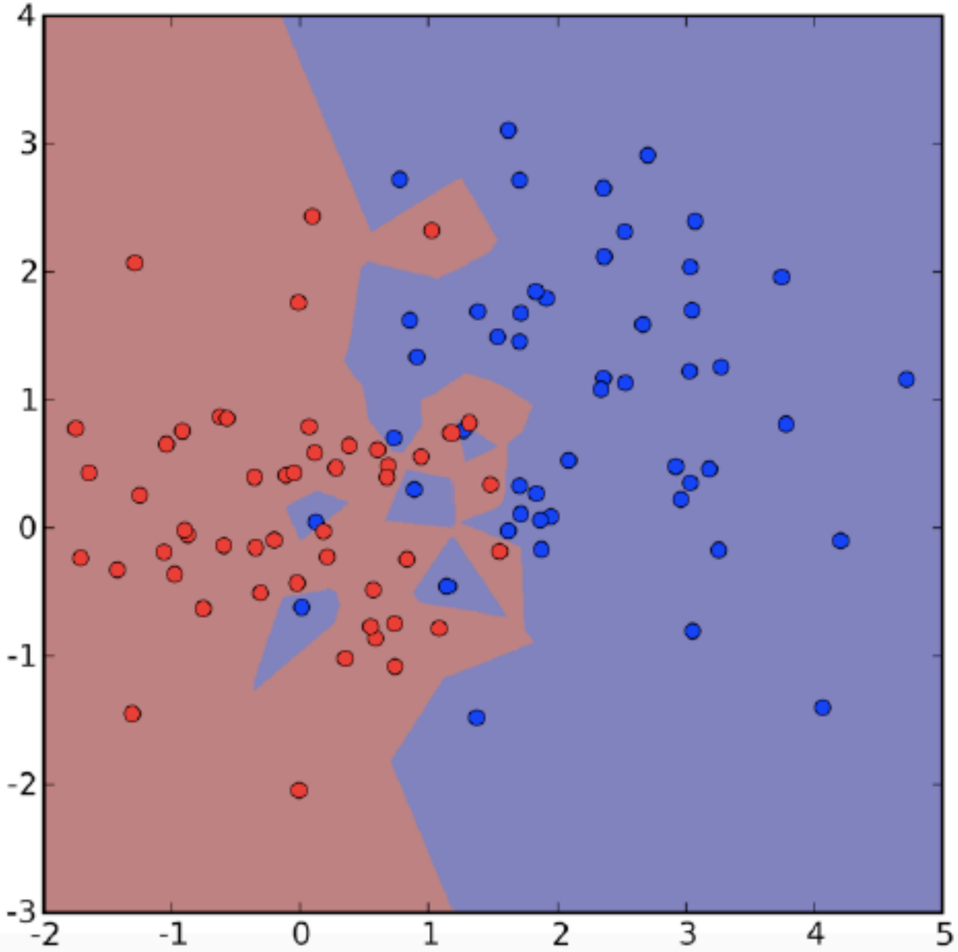
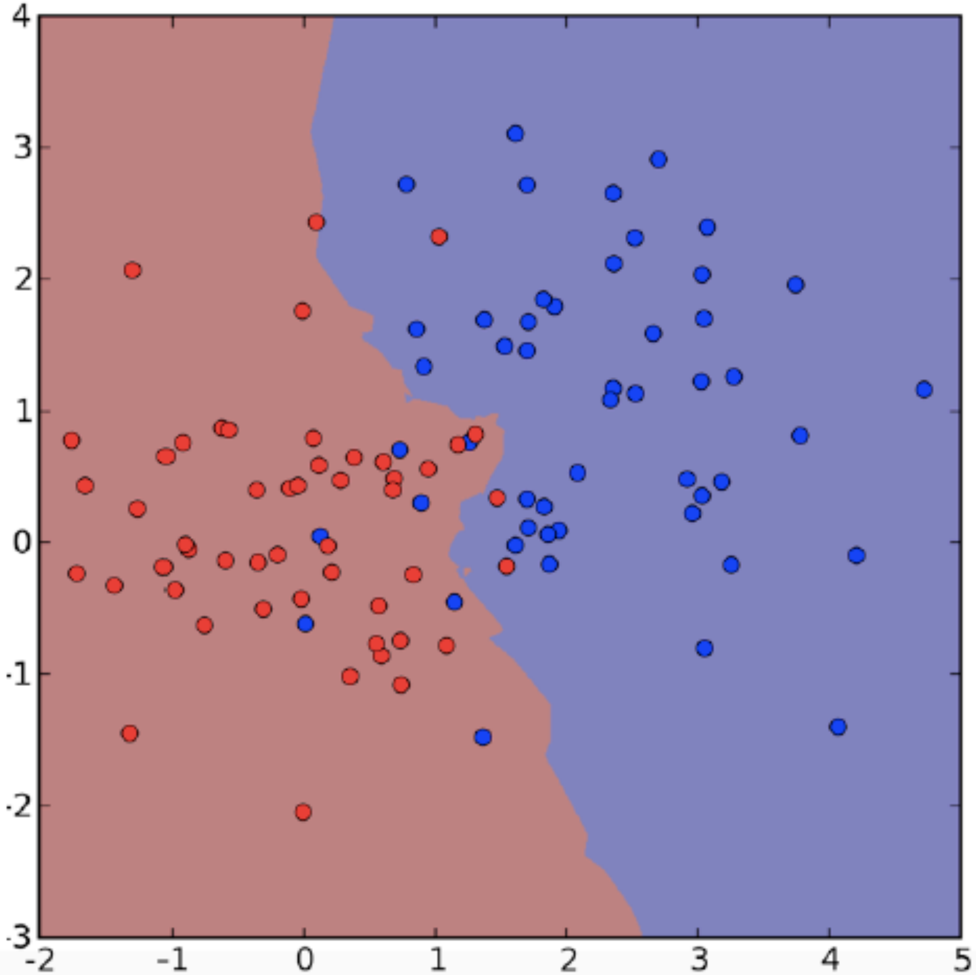


- Really useful baseline!
- Easy to implement for small amounts of data.

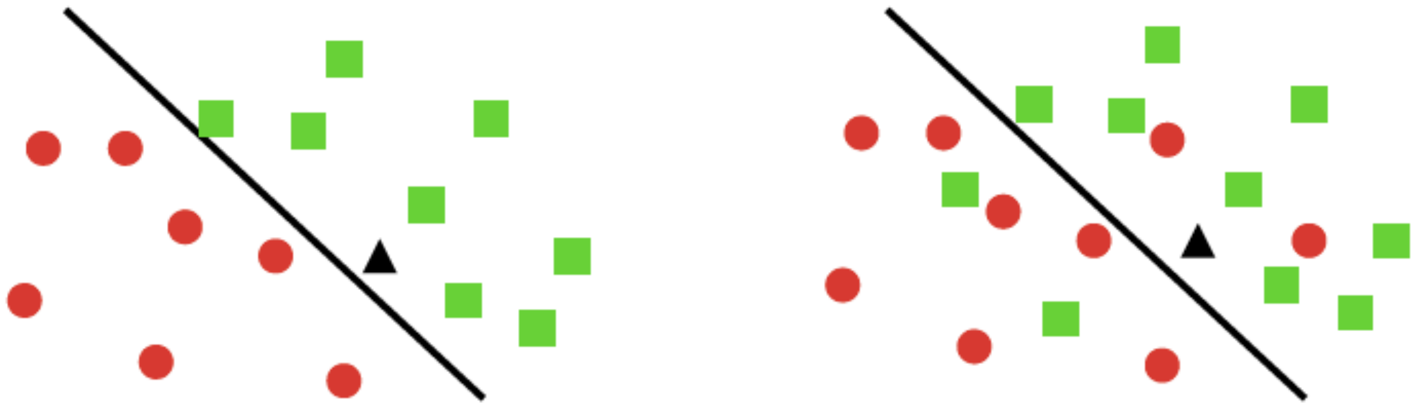
1-Nearest Neighbor



4-Nearest Neighbors Sign

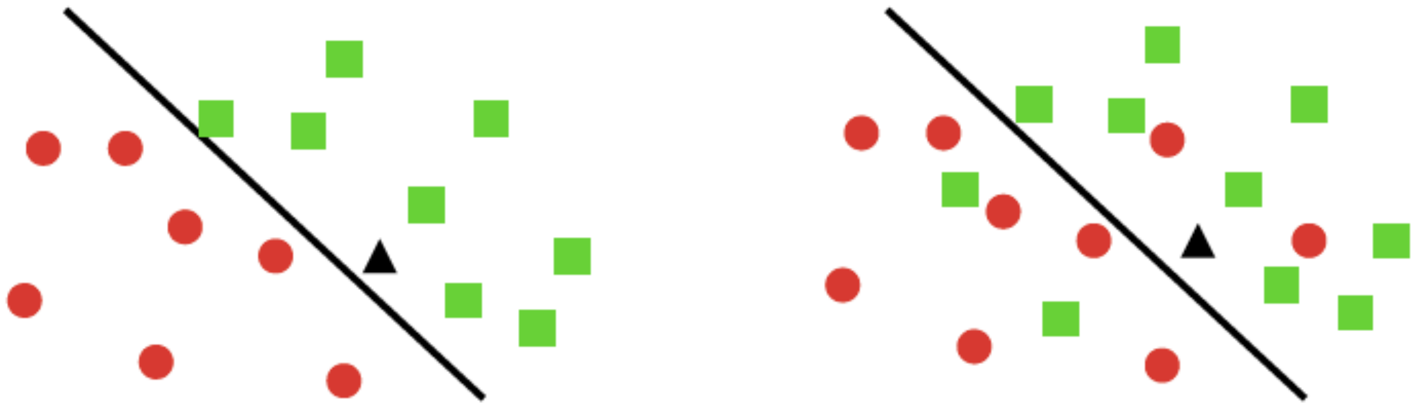


If we get more data



- 1 Nearest Neighbor
  - Converges to perfect solution if separation
  - Twice the minimal error rate 2p(1-p) for noisy problems

If we get more data



- 1 Nearest Neighbor
  - Converges to perfect solution if separation
  - Twice the minimal error rate 2p(1-p) for noisy problems
- k-Nearest Neighbor
  - Converges to perfect solution if separation (but needs more data)
  - Converges to minimal error min(p,1-p) for noisy problems (use increasing k)

That's all