

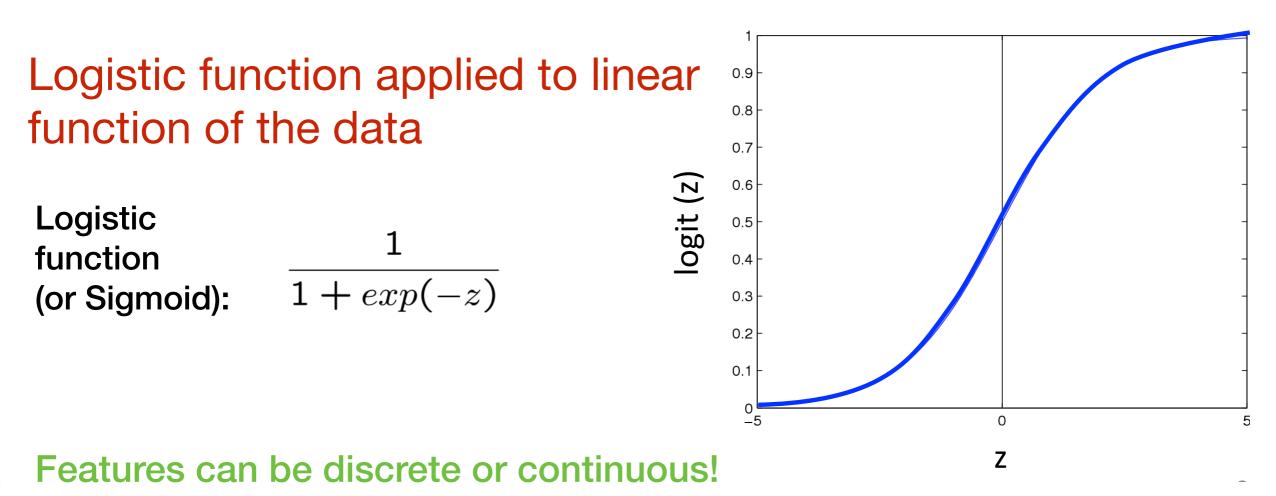


Erkut Erdem // Hacettepe University // Fall 2024

Last time... Logistic Regression

Assumes the following functional form for P(Y|X):

$$P(Y = 1|X) = \frac{1}{1 + \exp(w_0 + \sum_i w_i X_i)}$$



Last time.. Logistic Regression vs. Gaussian Naïve Bayes

- \cdot LR is a linear classifier
 - decision rule is a hyperplane
- LR optimized by maximizing conditional likelihood
 - no closed-form solution
 - concave ! global optimum with gradient ascent
- Gaussian Naïve Bayes with class-independent variances representationally equivalent to LR
 - Solution differs because of objective (loss) function
- In general, NB and LR make different assumptions
 - NB: Features independent given class! assumption on P(X|Y)
 - LR: Functional form of P(Y|X), no assumption on P(X|Y)
- Convergence rates
 - GNB (usually) needs less data
 - LR (usually) gets to better solutions in the limit

Linear Discriminant Functions

Linear Discriminant Function

• Linear discriminant function for a vector \mathbf{x}

$$y(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + w_0$$

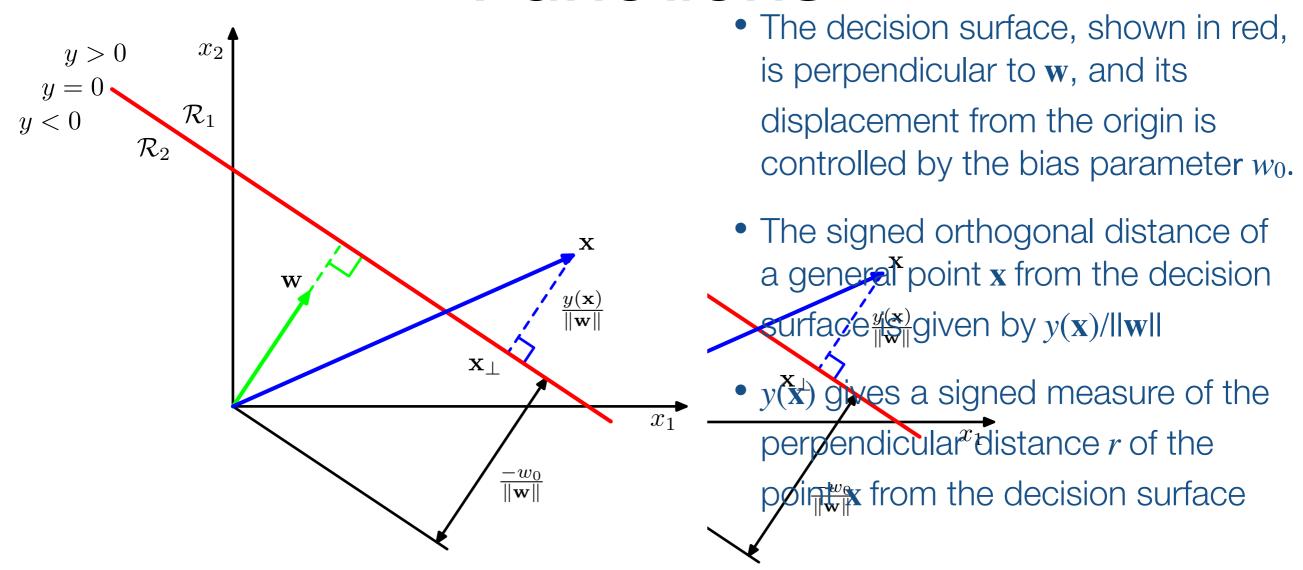
where w is called weight vector, and w_0 is a bias.

• The classification function is $C(\mathbf{x}) = \operatorname{sign}(\mathbf{w}^T \mathbf{x} + w_0)$

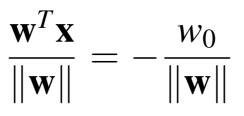
where step function $sign(\cdot)$ is defined as

$$\operatorname{sign}(a) = \begin{cases} +1, & a \ge 0\\ -1, & a < 0 \end{cases}$$

Properties of Linear Discriminant Functions



• $y(\mathbf{x}) = 0$ for \mathbf{x} on the decision surface. The normal distance from the origin to the decision surface is



So w₀ determines the location of the decision surface.

slide by C

Properties of Linear Discriminant Functions

• Let $\mathbf{x} = \mathbf{x}_{\perp} + r \frac{\mathbf{w}}{\|\mathbf{w}\|}$

where \mathbf{x}_{\perp} is the projection \mathbf{x} on the decision surface. Then

$$\mathbf{w}^{T}\mathbf{x} = \mathbf{w}^{T}\mathbf{x}_{\perp} + r\frac{\mathbf{w}^{T}\mathbf{w}}{\|\mathbf{w}\|}$$
$$\mathbf{w}^{T}\mathbf{x} + w_{0} = \mathbf{w}^{T}\mathbf{x}_{\perp} + w_{0} + r\|\mathbf{w}\|$$
$$y(\mathbf{x}) = r\|\mathbf{w}\|$$
$$r = \frac{y(\mathbf{x})}{\|\mathbf{w}\|}$$

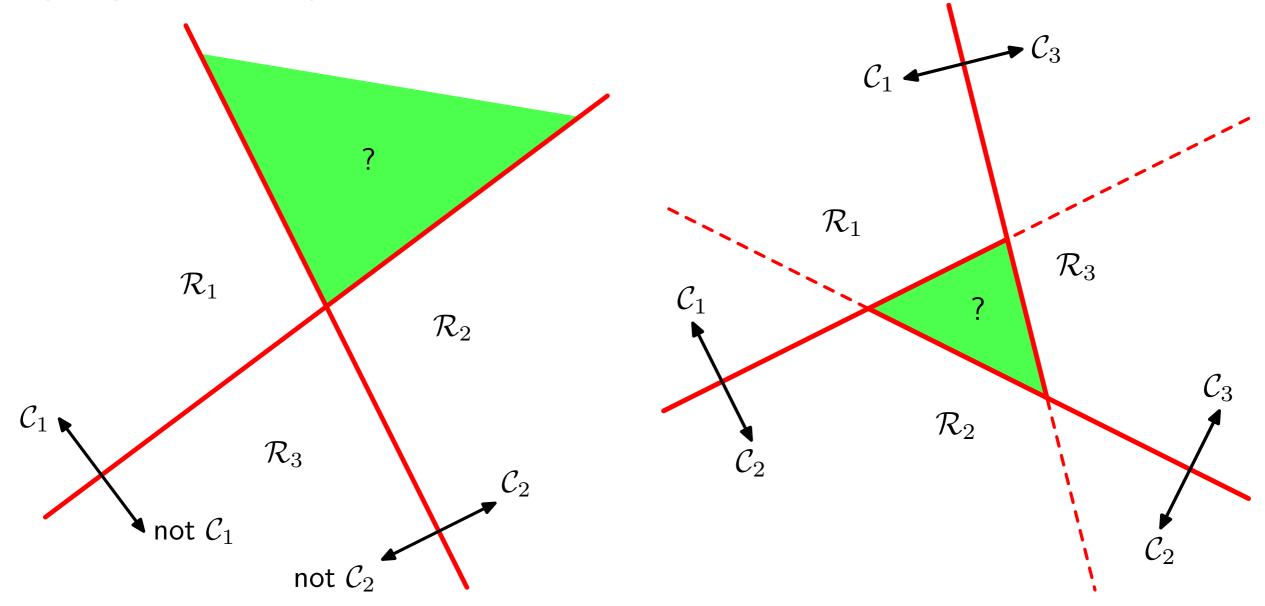
• Simpler notion: define $\widetilde{\mathbf{w}} = (w_0, \mathbf{w})$ and $\widetilde{\mathbf{x}} = (1, \mathbf{x})$ so that

$$y(\mathbf{x}) = \widetilde{\mathbf{w}}^T \widetilde{\mathbf{x}}$$

 \mathbf{X}

Multiple Classes: Simple Extension

- **One-versus-the-rest** classifier: classify C_k and samples not in C_k . (K –1 classifiers)
- One-versus-one classifier: classify every pair of classes.
 K(K 1)/2 classifiers)



Multiple Classes: K-Class Discriminant

• A single K-class discriminant comprising K linear functions

$$y_k(\mathbf{x}) = \mathbf{w}_k^T \mathbf{x} + w_{k0}$$

Decision function

$$C(\mathbf{x}) = k$$
, if $y_k(\mathbf{x}) > y_j(\mathbf{x}) \forall j \neq k$

• The decision boundary between class C_k and C_j is given by $y_k(\mathbf{x}) = y_j(\mathbf{x})$

$$(\mathbf{w}_k - \mathbf{w}_j)^T \mathbf{x} + (w_{k0} - w_{j0}) = 0$$

Property of the Decision Regions

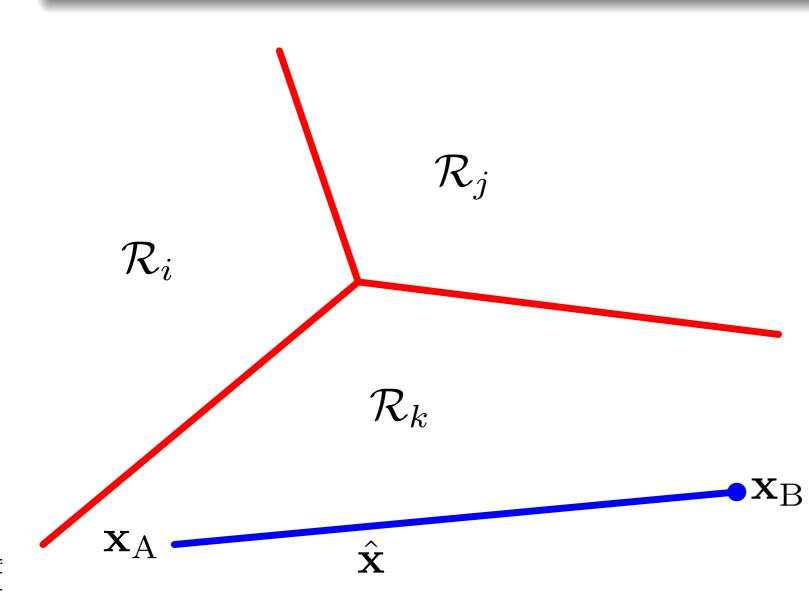
Theorem

The decision regions of the K-class discriminant $y_k(\mathbf{x}) = \mathbf{w}_k^T \mathbf{x} + w_{k0}$ are singly connected and convex.

Property of the Decision Regions

Theorem

The decision regions of the K-class discriminant $y_k(\mathbf{x}) = \mathbf{w}_k^T \mathbf{x} + w_{k0}$ are singly connected and convex.



If two points \mathbf{x}_A and \mathbf{x}_B both lie inside the same decision region R_k , then any point \mathbf{x} that lies on the line connecting these two points must also lie in R_k , and hence the decision region must be singly connected and convex.

Fisher's Linear Discriminant

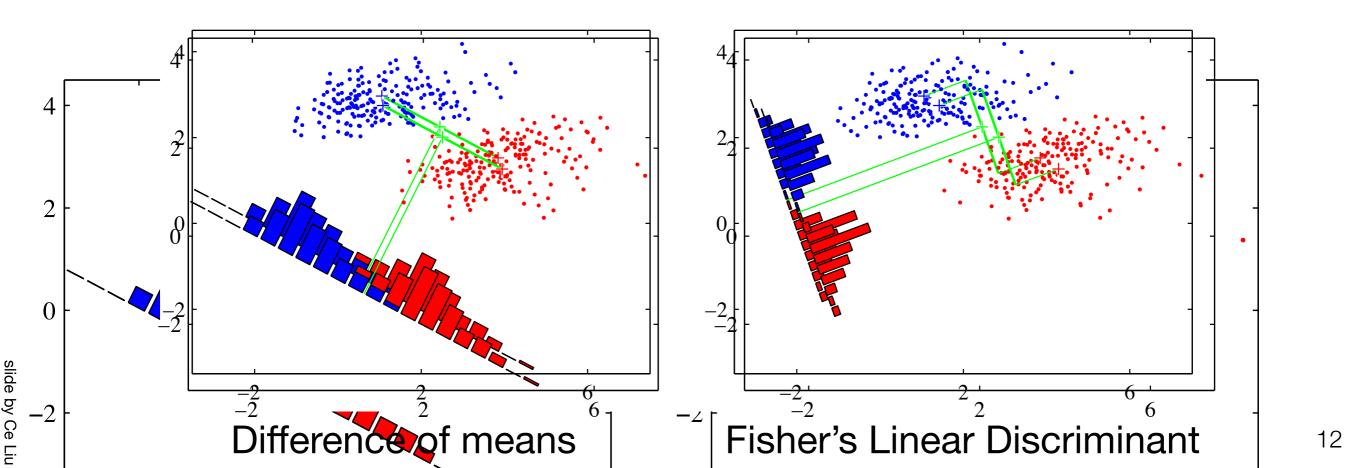
 Pursue the optimal linear projection on which the two classes can be maximally separated

$$y = \mathbf{w}^T \mathbf{x}$$

The mean vectors of the two classes

$$\mathbf{m}_1 = \frac{1}{N_1} \sum_{n \in \mathcal{C}_1} \mathbf{x}_n, \quad \mathbf{m}_2 = \frac{1}{N_2} \sum_{n \in \mathcal{C}_2} \mathbf{x}_n$$

A way to view a linear classification model is in terms of dimensionality reduction.



What's a Good Projection?

• After projection, the two classes are separated as much as possible. Measured by the distance between projected center

$$\left(\mathbf{w}^{T}(\mathbf{m}_{1} - \mathbf{m}_{2})\right)^{2} = \mathbf{w}^{T}(\mathbf{m}_{1} - \mathbf{m}_{2})(\mathbf{m}_{1} - \mathbf{m}_{2})^{T}\mathbf{w}$$

= $\mathbf{w}^{T}\mathbf{S}_{B}\mathbf{w}$

where $S_B = (m_1 - m_2)(m_1 - m_2)^T$ is called **between-class** covariance matrix.

 After projection, the variances of the two classes are as small as possible. Measured by the within-class covariance

where

$$\mathbf{w}^T \mathbf{S}_W \mathbf{w}$$

$$\mathbf{S}_W = \sum_{n \in \mathcal{C}_1} (\mathbf{x}_n - \mathbf{m}_1) (\mathbf{x}_n - \mathbf{m}_1)^T + \sum_{n \in \mathcal{C}_2} (\mathbf{x}_n - \mathbf{m}_2) (\mathbf{x}_n - \mathbf{m}_2)^T$$

Fisher's Linear Discriminant

Fisher criterion: maximize the ratio w.r.t. w

 $J(\mathbf{w}) = \frac{\text{Between-class variance}}{\text{Within-class variance}} = \frac{\mathbf{w}^T \mathbf{S}_B \mathbf{w}}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}}$

• Recall the quotient rule: for $f(x) = \frac{g(x)}{h(x)}$

$$f'(x) = \frac{g'(x)h(x) - g(x)h'(x)}{h^2(x)}$$

• Setting $\nabla J(w) = 0$, we obtain

$$(\mathbf{w}^T \mathbf{S}_B \mathbf{w}) \mathbf{S}_W \mathbf{w} = (\mathbf{w}^T \mathbf{S}_W \mathbf{w}) \mathbf{S}_B \mathbf{w}$$
$$(\mathbf{w}^T \mathbf{S}_B \mathbf{w}) \mathbf{S}_W \mathbf{w} = (\mathbf{w}^T \mathbf{S}_W \mathbf{w}) (\mathbf{m}_2 - \mathbf{m}_1) \left((\mathbf{m}_2 - \mathbf{m}_1)^T \mathbf{w} \right)$$

Terms $\mathbf{w}^T \mathbf{S}_B \mathbf{w}$, $\mathbf{w}^T \mathbf{S}_W \mathbf{w}$ and $(\mathbf{m}_2 - \mathbf{m}_1)^T \mathbf{w}$ are scalars, and we only care about directions. So the scalars are dropped. Therefore

$$\mathbf{w} \propto \mathbf{S}_W^{-1}(\mathbf{m}_2 - \mathbf{m}_1)$$

From Fisher's Linear Discriminant to Classifiers

- Fisher's Linear Discriminant is not a classifier; it only decides on an optimal projection to convert high-dimensional classification problem to 1D.
- A bias (threshold) is needed to form a linear classifier (multiple thresholds lead to nonlinear classifiers). The final classifier has the form

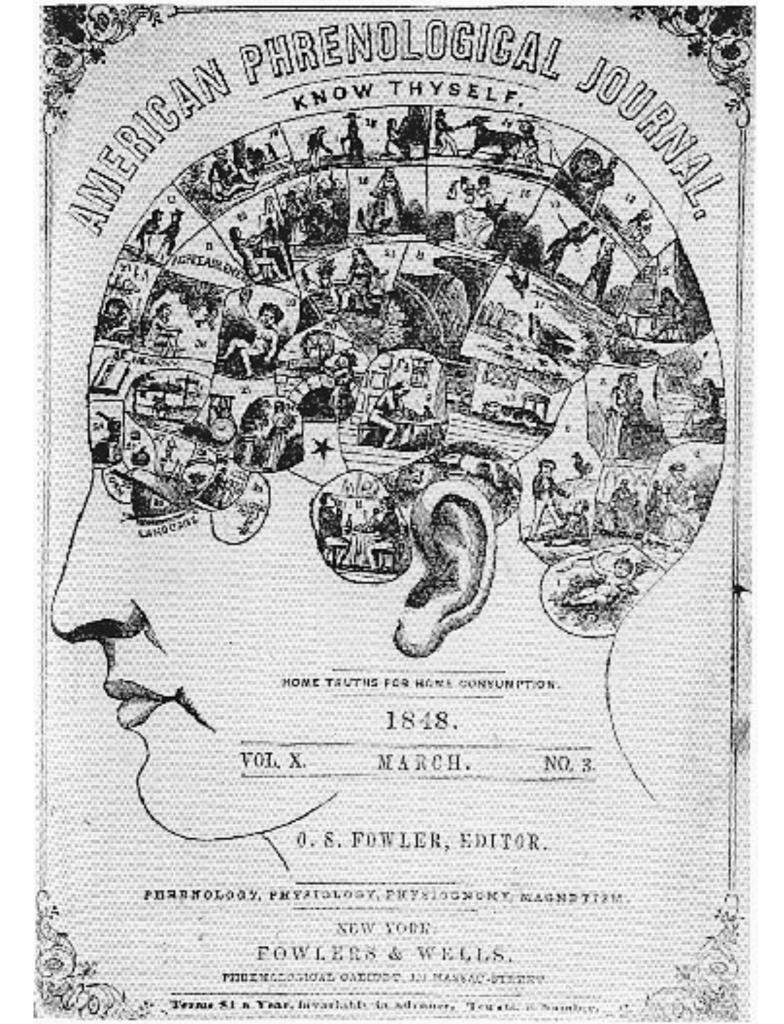
$$y(\mathbf{x}) = \operatorname{sign}(\mathbf{w}^T \mathbf{x} + w_0)$$

where the nonlinear activation function sign(\cdot) is a step function

$$\operatorname{sign}(a) = \begin{cases} +1, & a \ge 0\\ -1, & a < 0 \end{cases}$$

• How to decide the bias w_0 ?

Perceptron

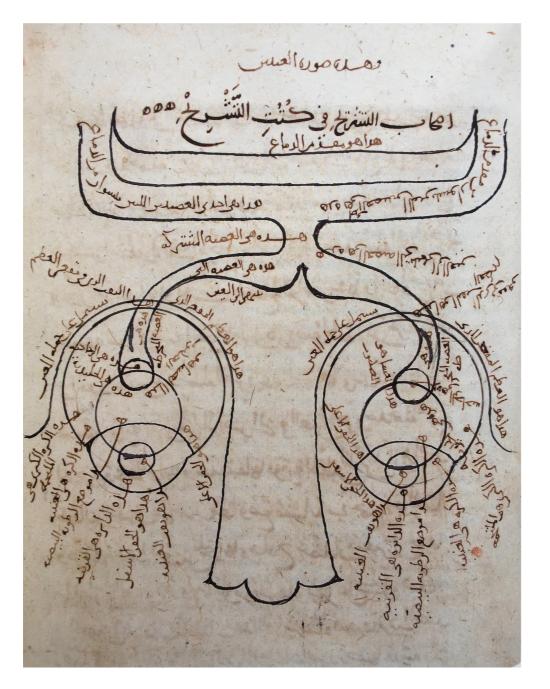


early theories of the brain

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.
- 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.

Nervous System



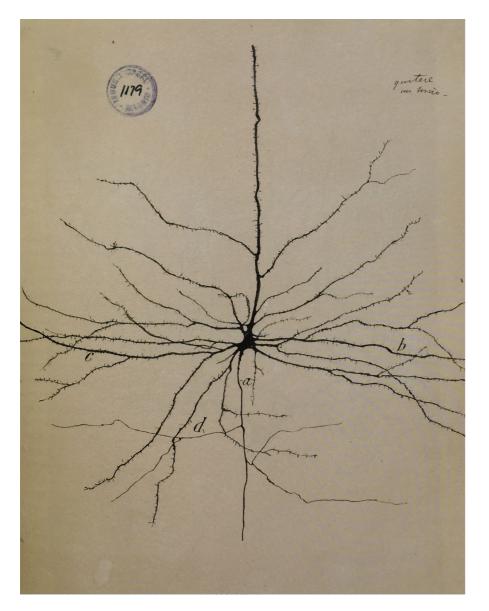
The oldest known drawing of the nervous system by Ibn al-Haytham (published in 1083)



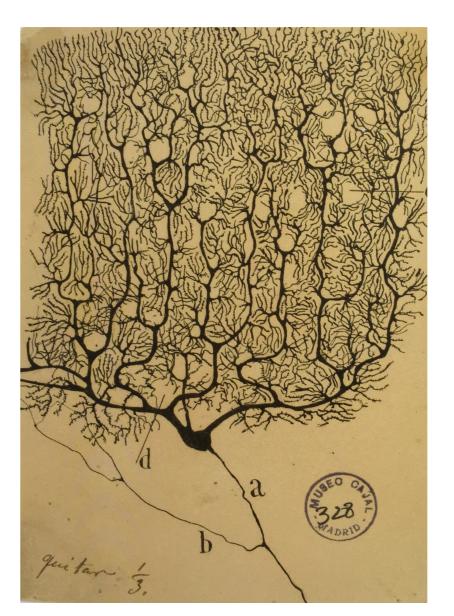
Olfactory bulb, Camillo Golgi, 1875

Santiago Ramón Y Cajal & The Neuron Doctrine

 Neuron as the discrete distinct entities in the brain as opposed to a continuous network.



pyramidal neuron. Cajal, 1899



purkinje neuron. Cajal, 1899

Santiago Ramón Y Cajal & The Neuron Doctrine

The Nobel Prize in Physiology or Medicine 1906

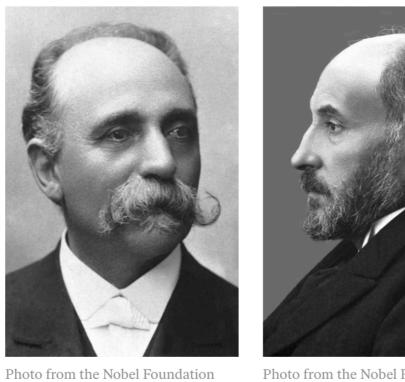


Photo from the Nobel Foundation archive. Camillo Golgi Prize share: 1/2

Photo from the Nobel Foundation archive. Santiago Ramón y Cajal Prize share: 1/2

The Nobel Prize in Physiology or Medicine 1906 was awarded jointly to Camillo Golgi and Santiago Ramón y Cajal "in recognition of their work on the structure of the nervous system"

Network of Neurons: Axons, Dendrites, and Synapses



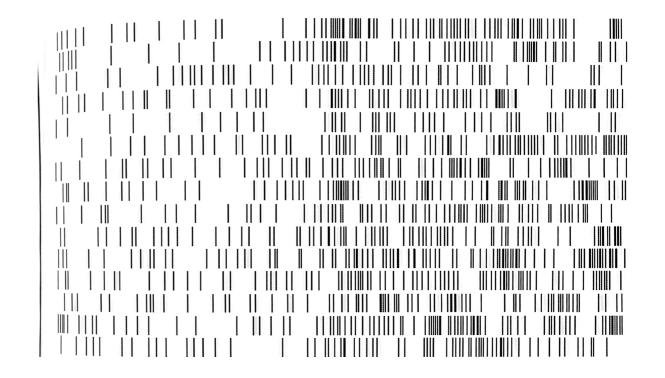
network of neurons. Cajal, 1899



Synapse. Spacek and Harris, 2000

Electricity in the brain

Whole-cell recording in an awake rat. Contantinople and Bruno, 2009

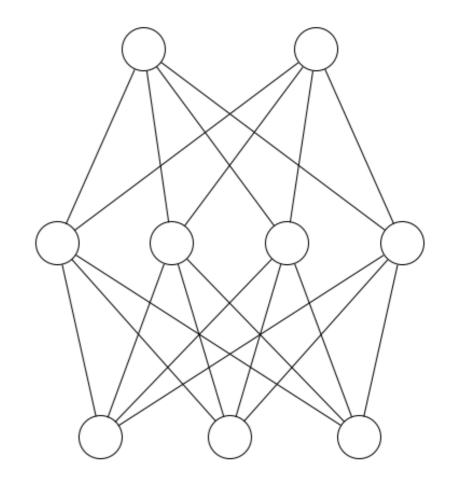


Action potentials in a live monkey brain. Saez and Salzman, 2009. (Each row, 4 seconds.)

Electricity in the brain



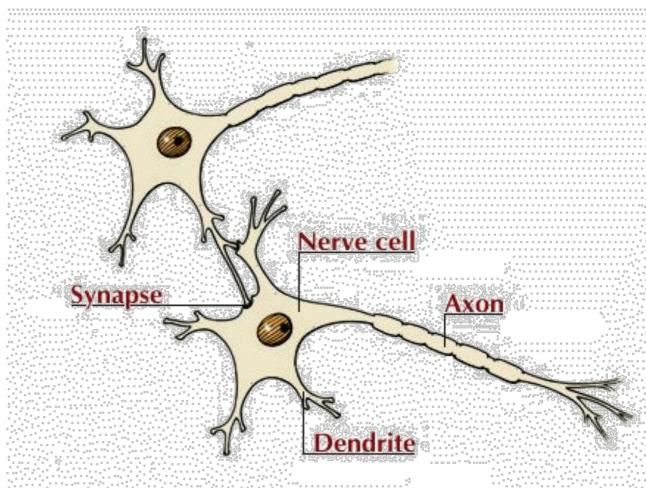
human brain: 10¹¹ neurons, 10¹⁵ synapses



GPT-4: 10⁶ neurons, 10¹¹ parameters (weights), 100 layers

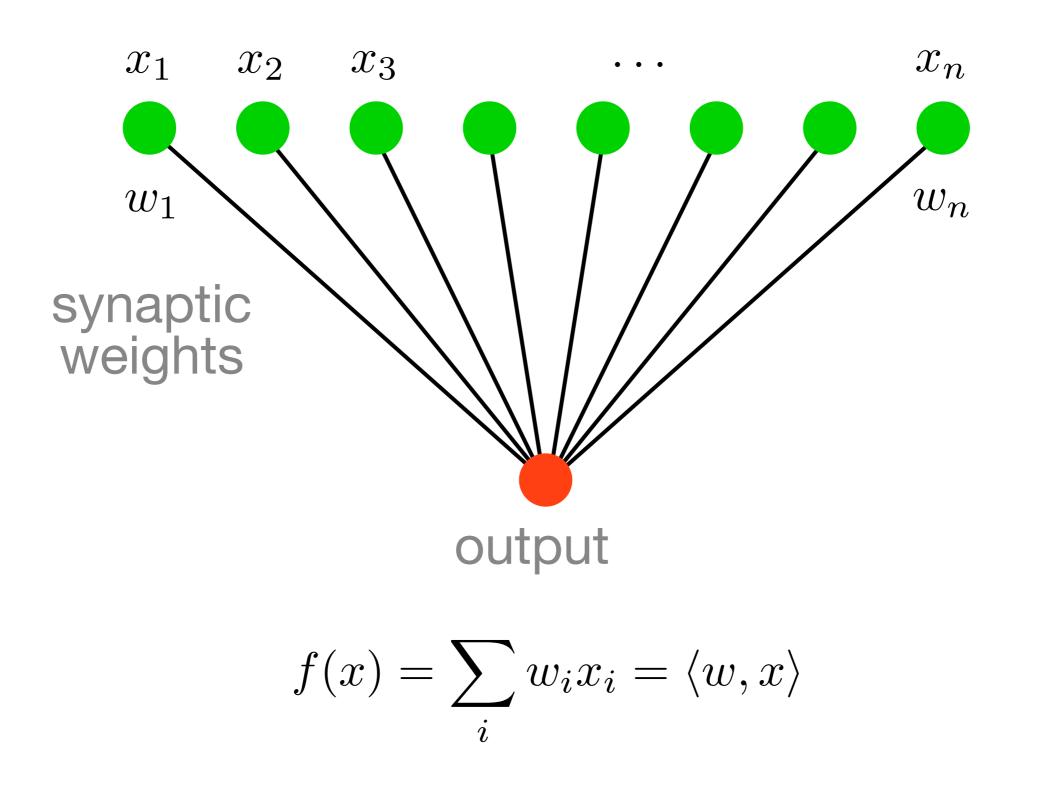
Neurons

- Soma (CPU)
 Cell body combines signals
- Dendrite (input bus)
 Combines the inputs from several other nerve cells



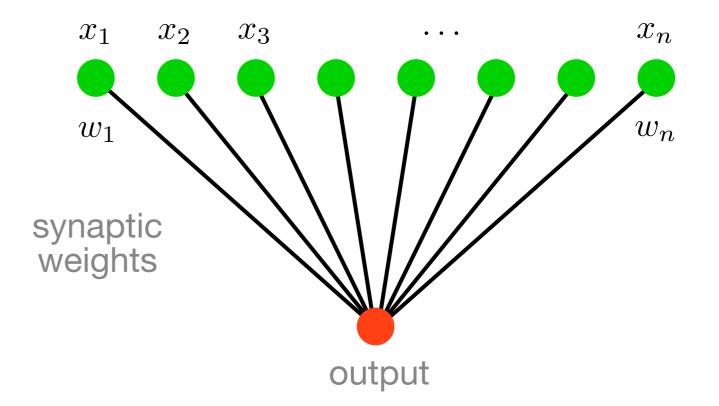
- Synapse (interface)
 Interface and parameter store between neurons
- Axon (cable)
 May be up to 1m long and will transport the activation signal to neurons at different locations

Neurons



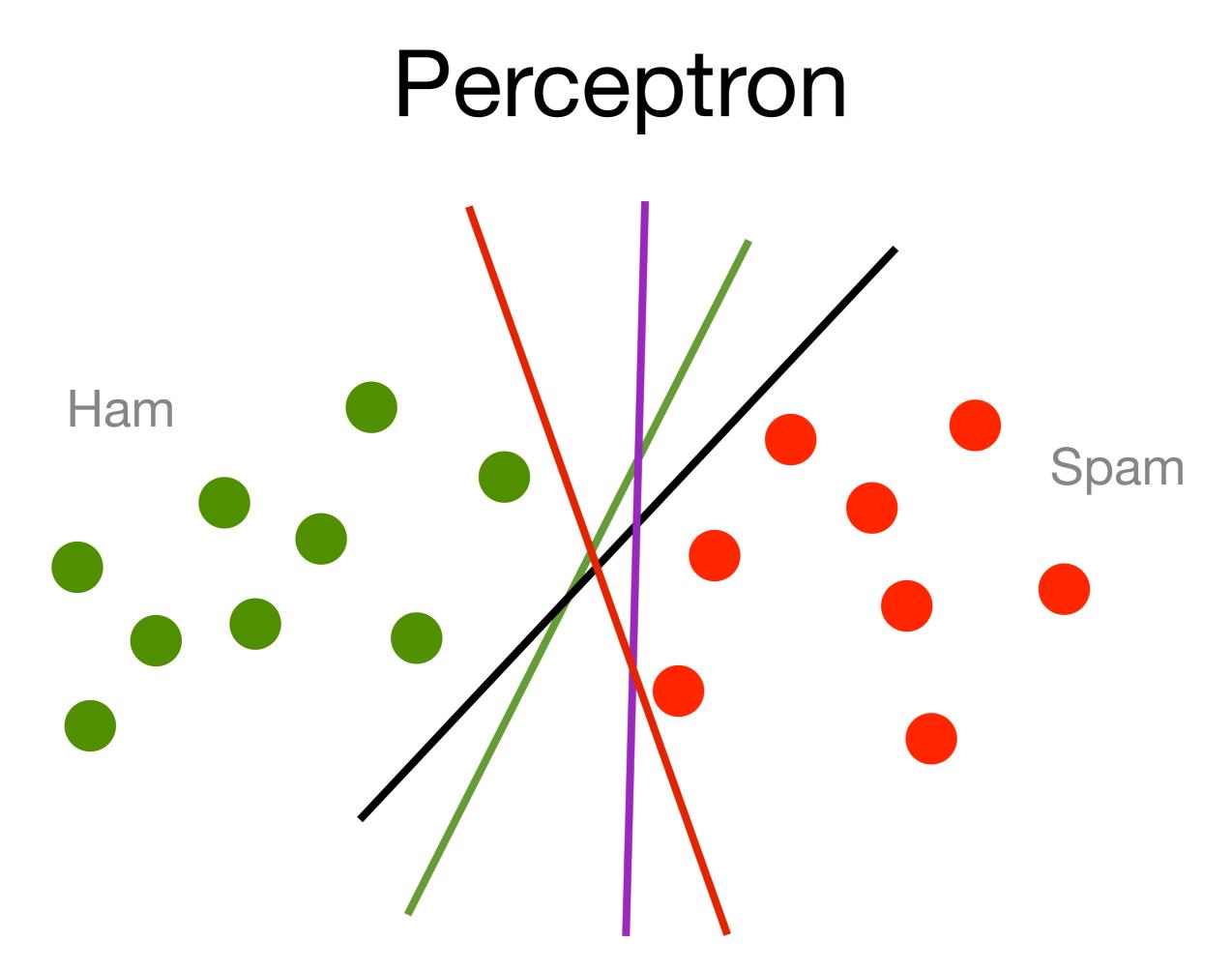
Perceptron

- 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

Widom

Rosenblatt

Perceptron Inductive Bias

 Decision boundary should be linear
 Most recent mistakes are most important (and should be corrected)

Background: Hyperplanes

Notation Trick: fold the bias b and the weights w into a single vector $\boldsymbol{\theta}$ by prepending a constant to value increasing dimensionality by one to get x'!

Hyperplane (Definition 1): Hyperplane (Definition 2): $\mathcal{H} = \{\mathbf{x}': \boldsymbol{\theta}^T \mathbf{x}' = 0$ and $x_1^2 = 1$ $\boldsymbol{\theta} = [b, w_1, \dots, w_M]^T$

Half-spaces:

$$\mathcal{H}^{+} = \{ \mathbf{x} : \boldsymbol{\theta}^{T} \mathbf{x} > 0 \text{ and } x_{1} = 1 \}$$
$$\mathcal{H}^{-} = \{ \mathbf{x} : \boldsymbol{\theta}^{T} \mathbf{x} < 0 \text{ and } x_{1} = 1 \}$$

(Online) Perceptron Algorithm

Data: Inputs are continuous vectors of length *M*. Outputs are discrete. $(\mathbf{x}^{(1)}, y^{(1)}), (\mathbf{x}^{(2)}, y^{(2)}), \dots$ where $\mathbf{x} \in \mathbb{R}^M$ and $y \in \{+1, -1\}$

Prediction: Output determined by hyperplane.

 $\hat{y} = h_{\theta}(\mathbf{x}) = \operatorname{sign}(\boldsymbol{\theta}^T \mathbf{x}) \qquad \operatorname{sign}(a) = \begin{cases} 1, & \text{if } a \ge 0\\ -1, & \text{otherwise} \end{cases}$

Assume $\boldsymbol{\theta} = [b, w_1, \dots, w_M]^T$ and $x_1 = 1$

Learning: Iterative procedure:

- initialize parameters to vector of all zeroes
- while not converged
 - receive next example (x⁽ⁱ⁾, y⁽ⁱ⁾)
 - predict y' = h(x⁽ⁱ⁾)
 - if positive mistake: add x⁽ⁱ⁾ to parameters
 - **if** negative mistake: **subtract x**⁽ⁱ⁾ from parameters

(Online) Perceptron Algorithm

Data: Inputs are continuous vectors of length *M*. Outputs are discrete. $(\mathbf{x}^{(1)}, y^{(1)}), (\mathbf{x}^{(2)}, y^{(2)}), \dots$ where $\mathbf{x} \in \mathbb{R}^M$ and $y \in \{+1, -1\}$

Prediction: Output determined by hyperplane.

 $\hat{y} = h_{\boldsymbol{\theta}}(\mathbf{x}) = \operatorname{sign}(\boldsymbol{\theta}^{T}\mathbf{x}) \qquad \text{sign}(a) = \begin{cases} 1, & \text{if } a \ge 0\\ -1, & \text{otherwise} \end{cases}$ Assume $\boldsymbol{\theta} = [b, w_1, \dots, w_M]^T$ and $x_1 = 1$

Learning:

Algorithm 1 Perceptron Learning Algorithm (Online)

1: **procedure** PERCEPTRON($\mathcal{D} = \{(\mathbf{x}^{(1)}, y^{(1)}), (\mathbf{x}^{(2)}, y^{(2)}), \ldots\})$ 2: $\theta \leftarrow 0$ \triangleright Initialize parameters 3: **for** $i \in \{1, 2, \ldots\}$ **do** \triangleright For each example 4: $\hat{y} \leftarrow \text{sign}(\theta^T \mathbf{x}^{(i)})$ \triangleright Predict 5: **if** $\hat{y} \neq y^{(i)}$ **then** \triangleright If mistake 6: $\theta \leftarrow \theta + y^{(i)} \mathbf{x}^{(i)}$ \triangleright Update parameters 7: **return** θ

(Online) Perceptron Algorithm

Data: Inputs are continuous vectors of length M. Outputs $(\mathbf{x}^{(1)}, y^{(1)}), (\mathbf{x}^{(2)}, y^{(2)}), \dots$ are discrete. where $\mathbf{x} \in \mathbb{R}^M$ and $y \in \{+1, -1\}$

Prediction: Output determine

 $\hat{y} = h_{\boldsymbol{\theta}}(\mathbf{x}) = \operatorname{sign}(\boldsymbol{\theta}^T \mathbf{x})$

Assume $\boldsymbol{\theta} = [b, w_1, \dots, w_M]$

Learning:

Algorithm 1 Perceptron Learning Alg

- 1: **procedure** PERCEPTRON($\mathcal{D} = \{(\mathbf{x} \in \mathcal{D}) \mid \mathbf{x} \in \mathcal{D}\}$ $\theta \leftarrow 0$ 2: $\begin{array}{l} \text{for } i \in \{1,2,\ldots\} \text{ do} \\ \hat{y} \leftarrow \text{sign}(\boldsymbol{\theta}^T \mathbf{x}^{(i)}) \\ \text{if } \hat{y} \neq y^{(i)} \text{ then} \end{array}$ 3: 4: 5: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + y^{(i)} \mathbf{x}^{(i)}$
- 6:
 - return θ 7:

Implementation Trick: same behavior as our "add on positive mistake and subtract on negative mistake" version, because y⁽ⁱ⁾ takes care of the sign

> Initialize parameters ▷ For each example Predict If mistake Update parameters

(Batch) Perceptron Algorithm

Learning for Perceptron also works if we have a fixed training dataset, D. We call this the "batch" setting in contrast to the "online" setting that we've discussed so far.

Algorithm 1 Perceptron Learning Algorithm (Batch)

1: procedure PERCEPTRON($\mathcal{D} = \{(\mathbf{x}^{(1)}, y^{(1)}), \dots, (\mathbf{x}^{(N)}, y^{(N)})\}$) $oldsymbol{ heta} \leftarrow \mathbf{0}$ Initialize parameters 2: while not converged do 3: for $i \in \{1, 2, ..., N\}$ do ▷ For each example 4: $\hat{y} \leftarrow \operatorname{sign}(\boldsymbol{\theta}^T \mathbf{x}^{(i)})$ ▷ Predict 5: if $\hat{y} \neq y^{(i)}$ then ▷ If mistake 6: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + y^{(i)} \mathbf{x}^{(i)}$ ▷ Update parameters 7: return θ 8:

(Batch) Perceptron Algorithm

Learning for Perceptron also works if we have a fixed training dataset, D. We call this the "batch" setting in contrast to the "online" setting that we've discussed so far.

Discussion:

The Batch Perceptron Algorithm can be derived in two ways.

- 1. By extending the online Perceptron algorithm to the batch setting (as mentioned above)
- 2. By applying **Stochastic Gradient Descent (SGD)** to minimize a so-called **Hinge Loss** on a linear separator

The Perceptron

- initialize w = 0 and b = 0repeat if $y_i [\langle w, x_i \rangle + b] \le 0$ 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 $w = \sum y_i x_i$
- Classifier is linear combination of inner products $f(x) = \sum_{i \in I} y_i \langle x_i, x \rangle + b$

 $i \in I$

Convergence Theorem

• If there exists some (w^*, b^*) with unit length and $y_i [\langle x_i, w^* \rangle + b^*] \ge \rho$ for all *i*

then the perceptron converges to a linear separator after a number of steps bounded by

$$(b^{*2}+1)(r^2+1)\rho^{-2}$$
 where $||x_i|| \le r$

- Dimensionality independent
- Order independent (i.e. also worst case)
- Scales with 'difficulty' of problem

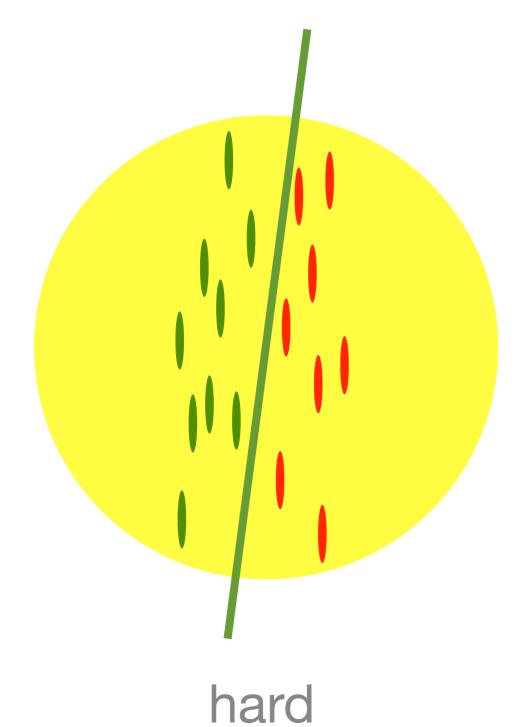
Consequences

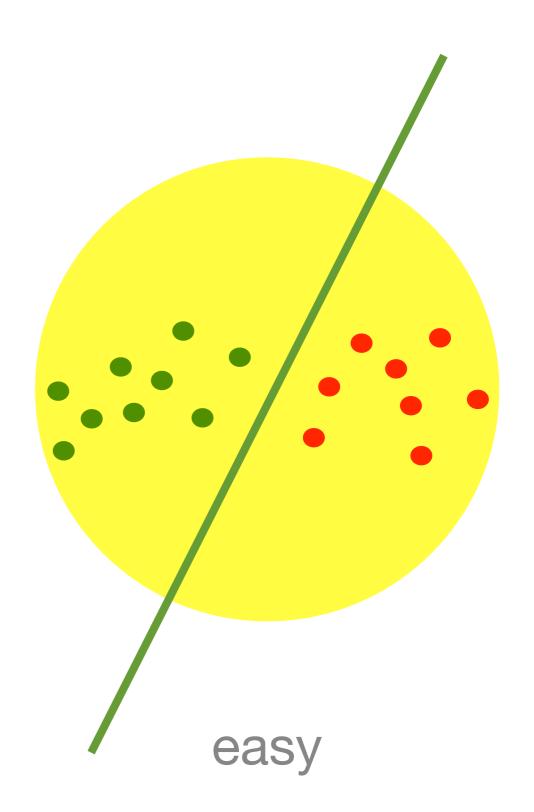
- Only need to store errors.
 This gives a compression bound for perceptron.
- Stochastic gradient descent on hinge loss $l(x_i, y_i, w, b) = \max(0, 1 - y_i [\langle w, x_i \rangle + b])$
- Fails with noisy data

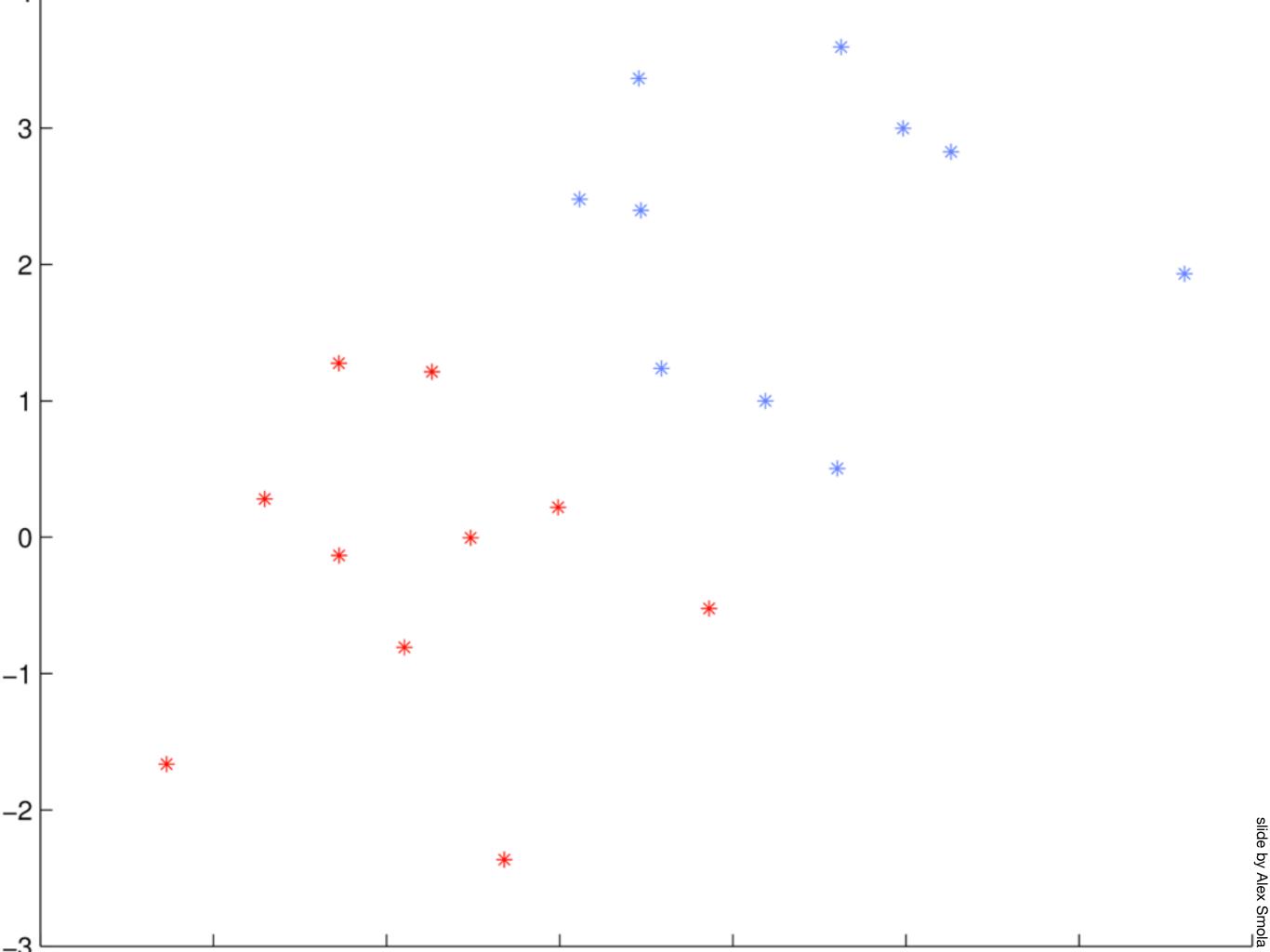
do NOT train your avatar with perceptrons

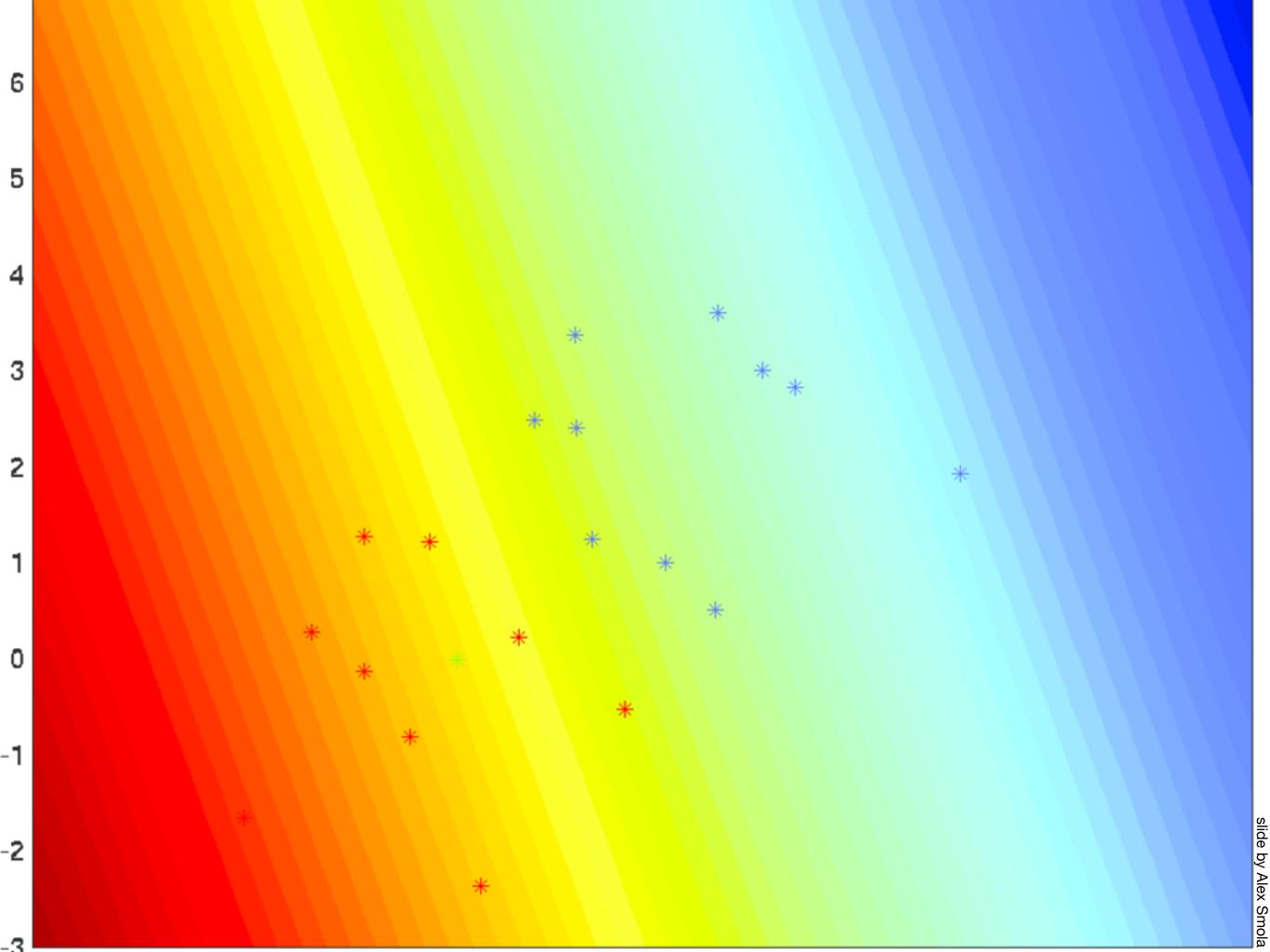


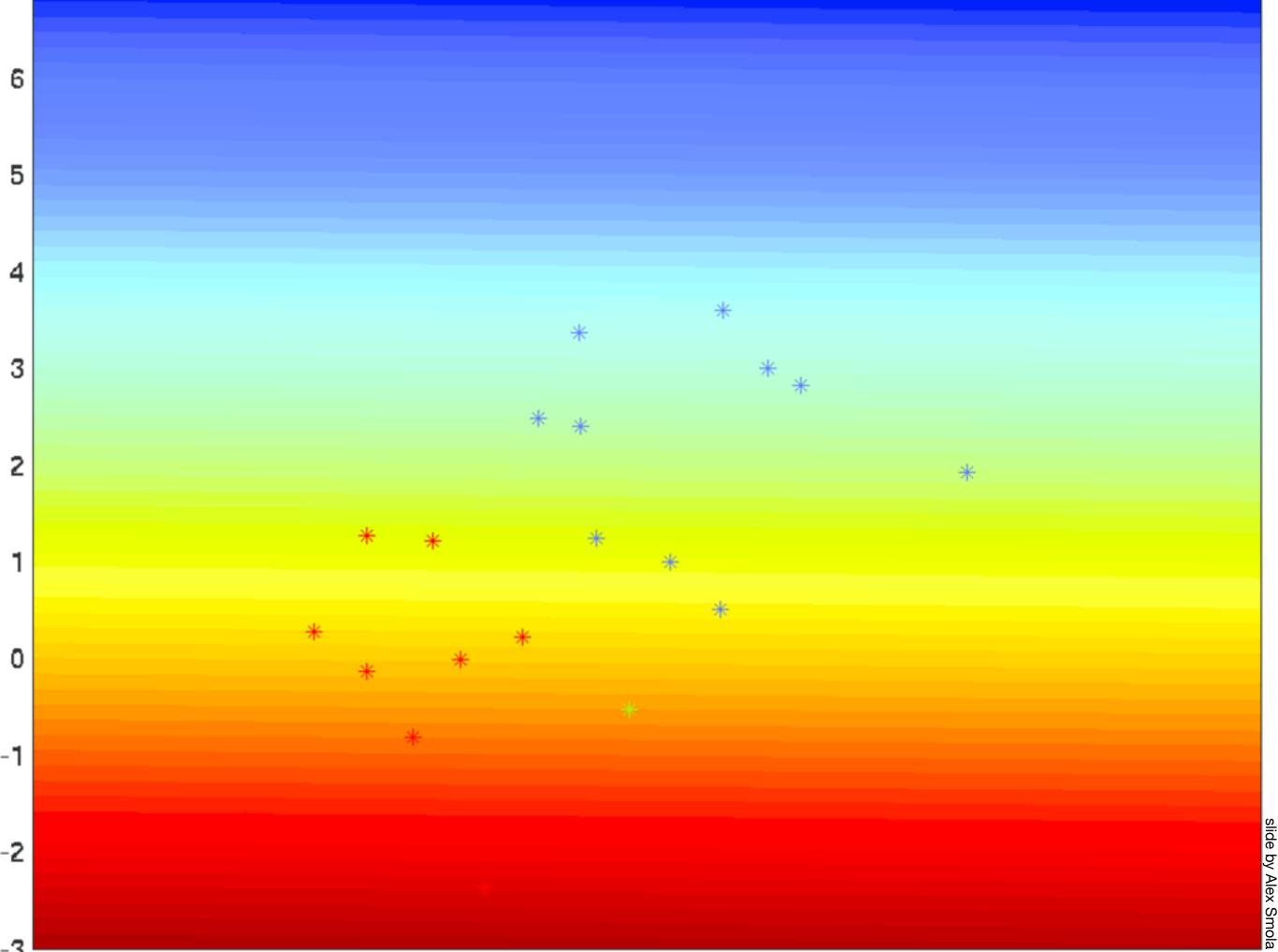
Hardness: margin vs. size



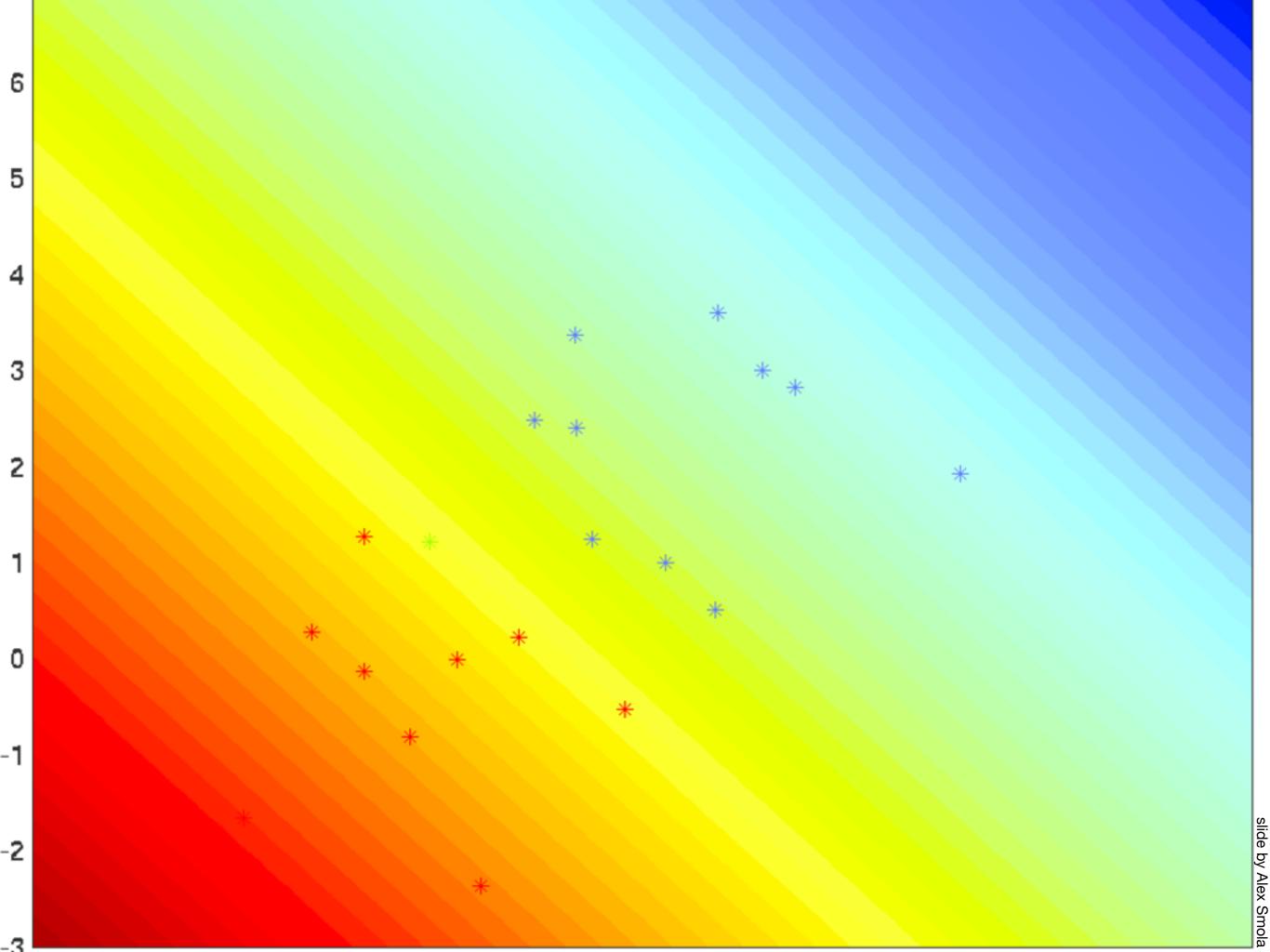


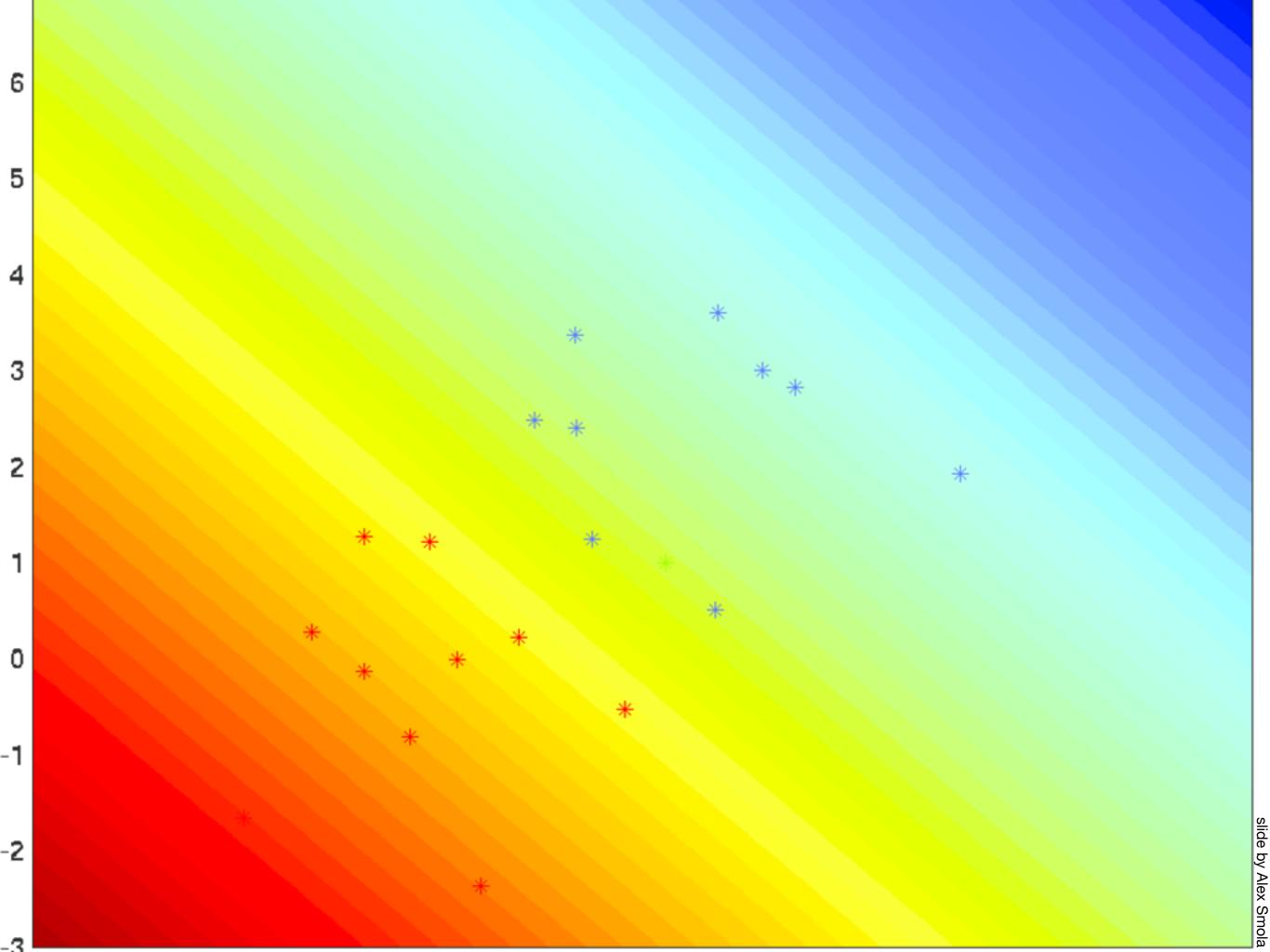


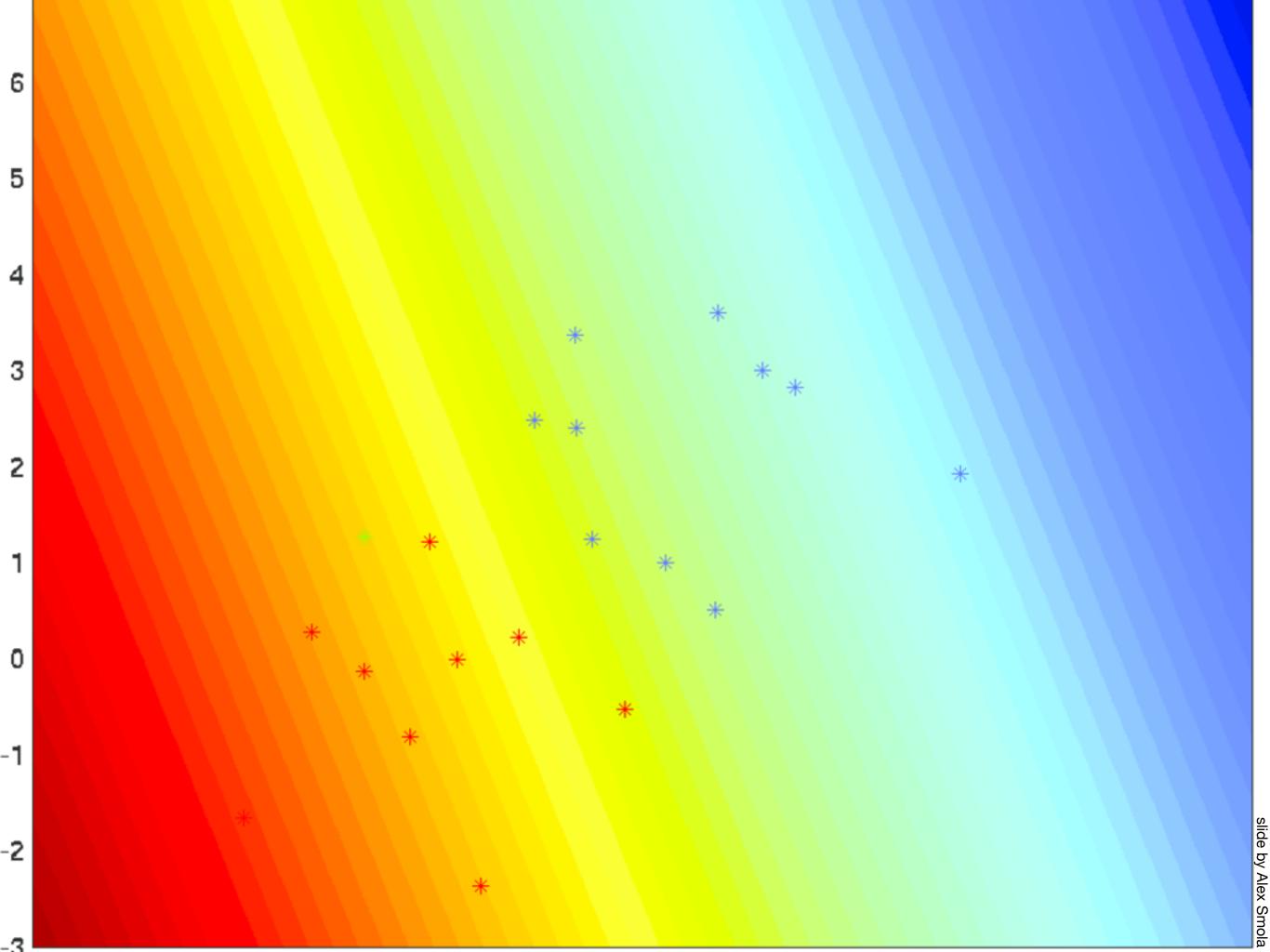


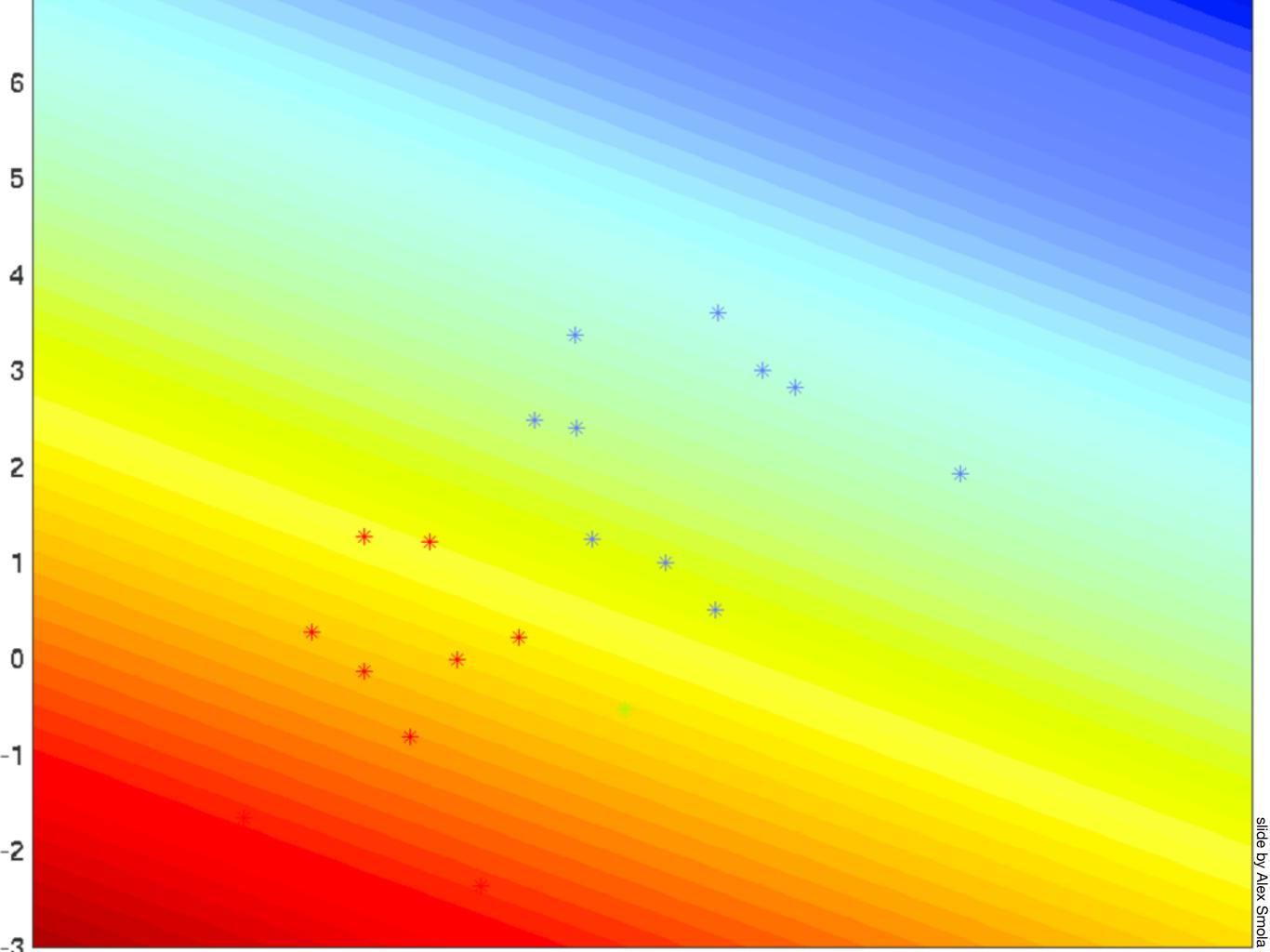


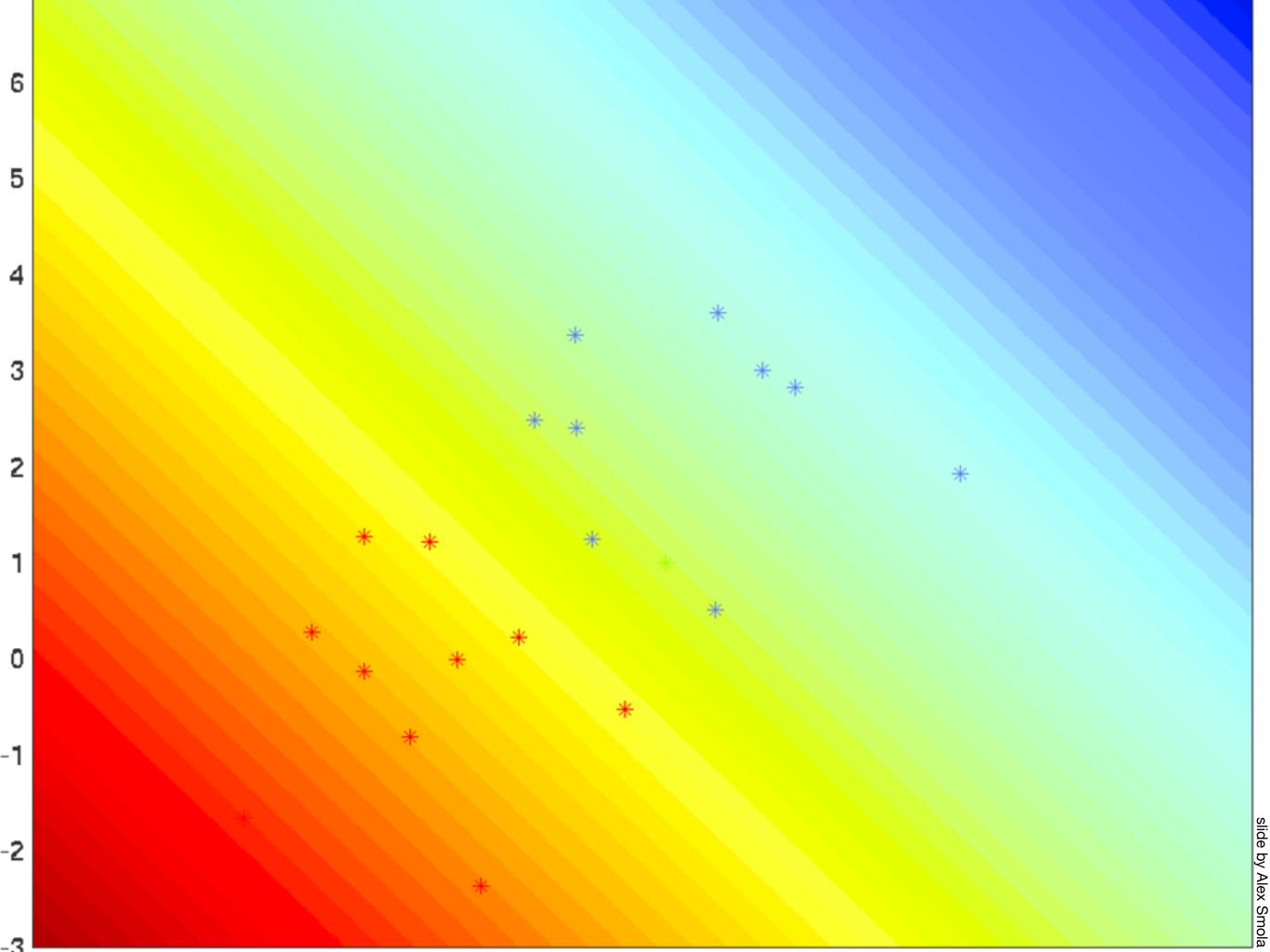
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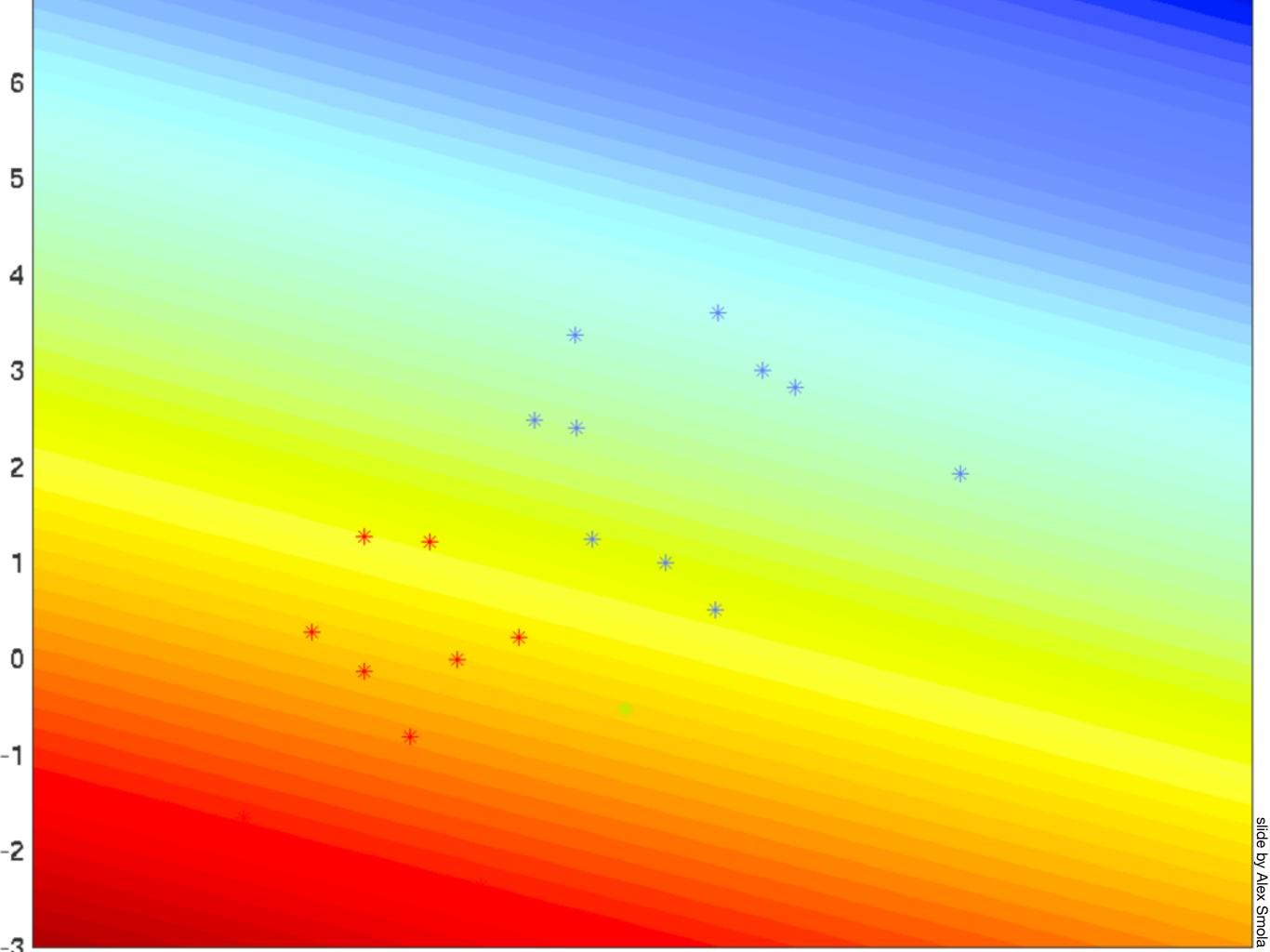


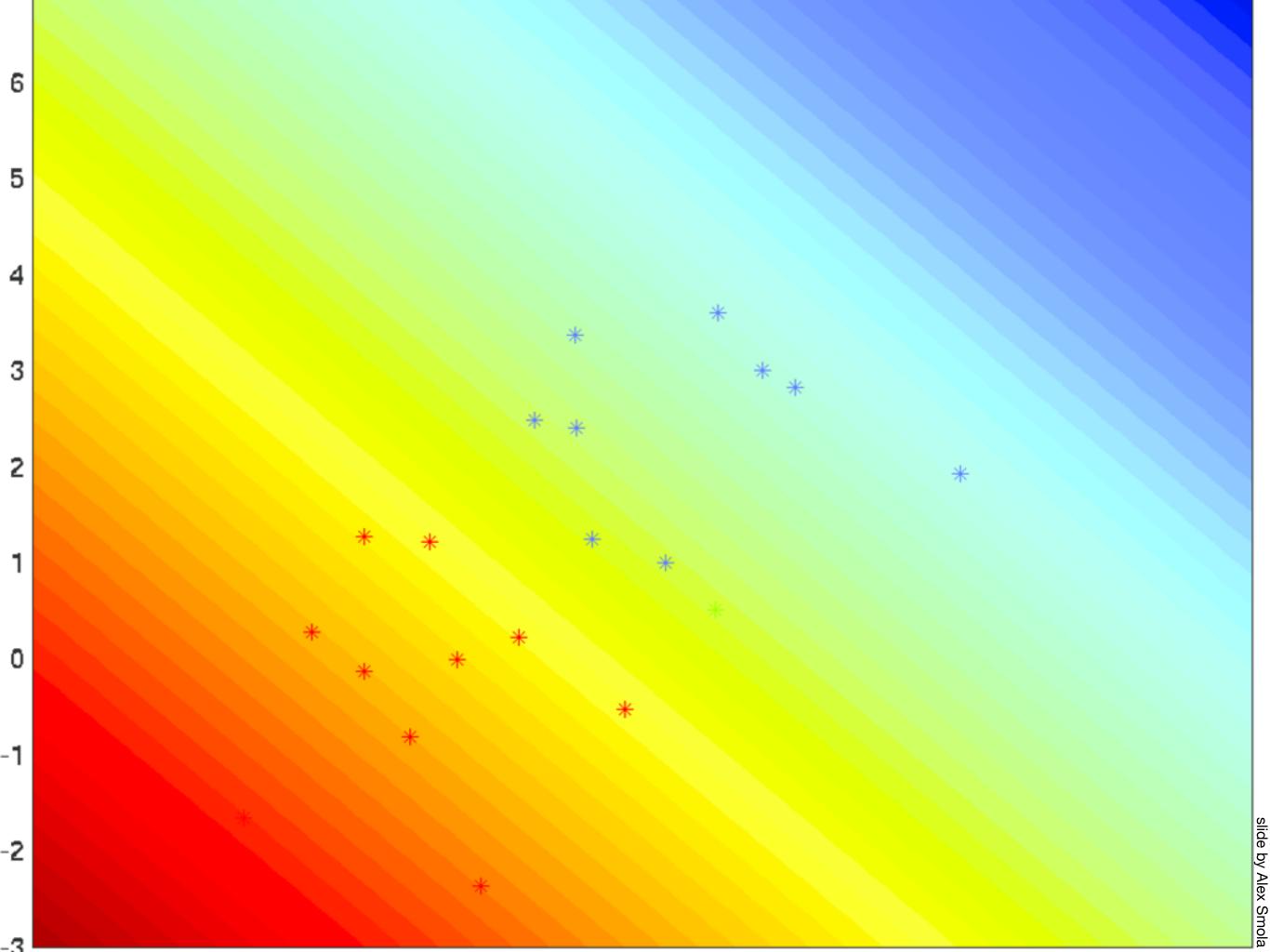


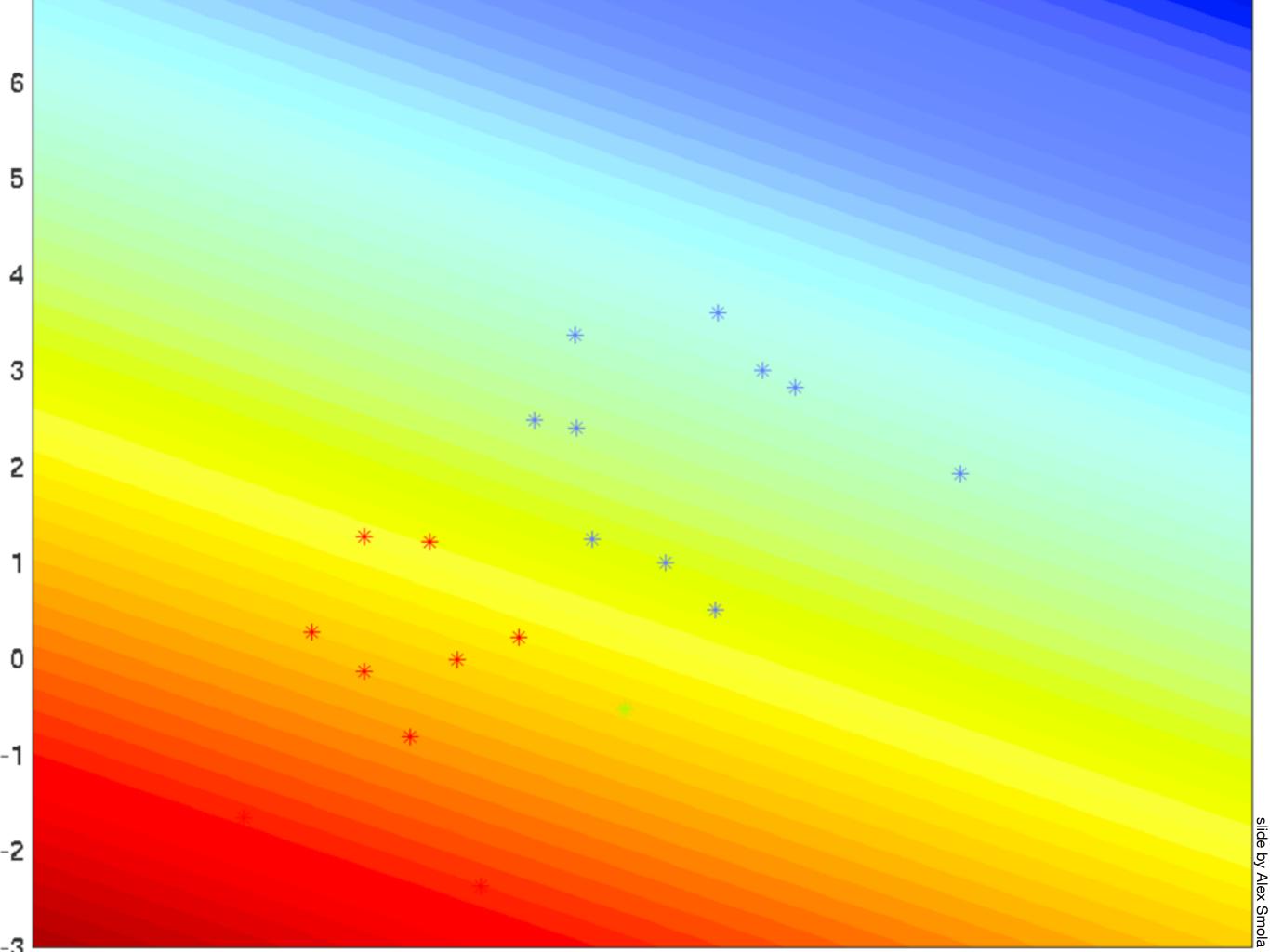


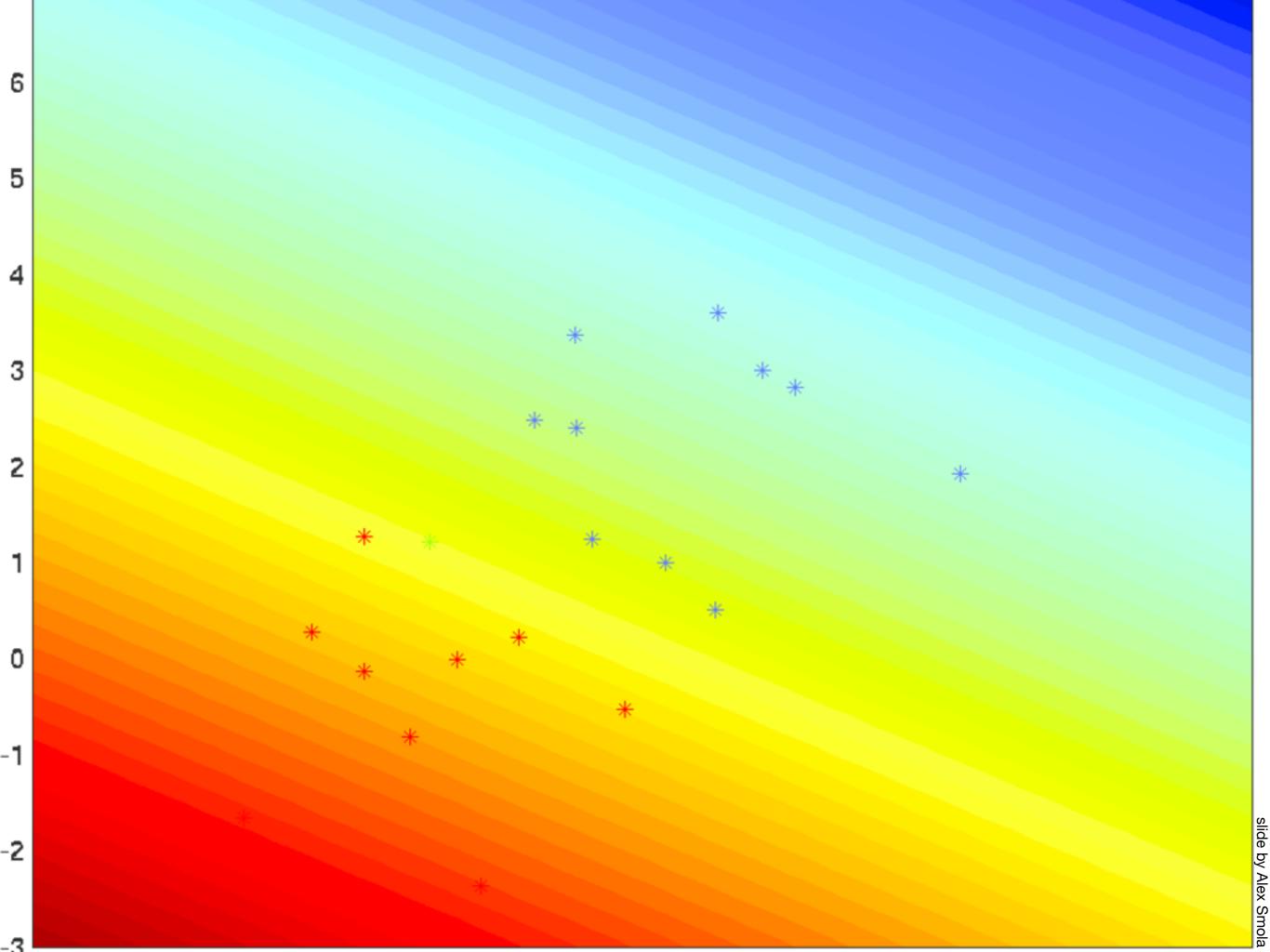






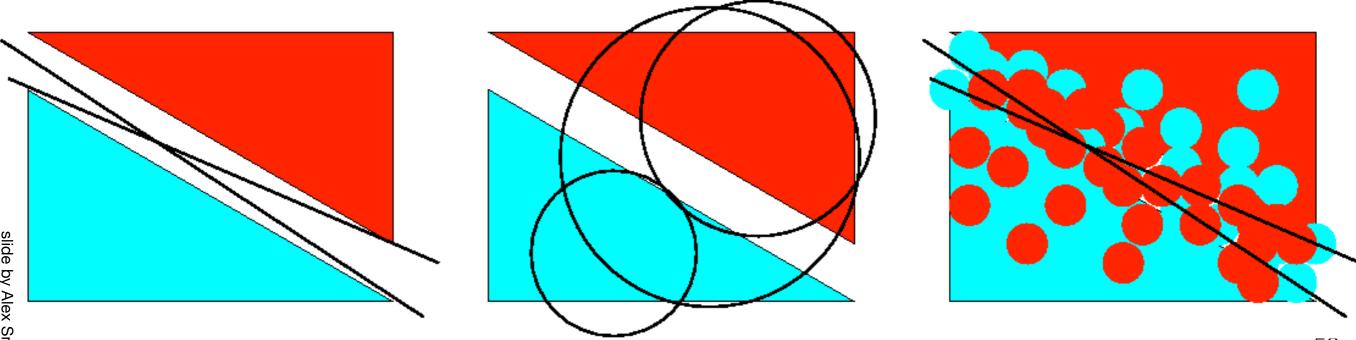


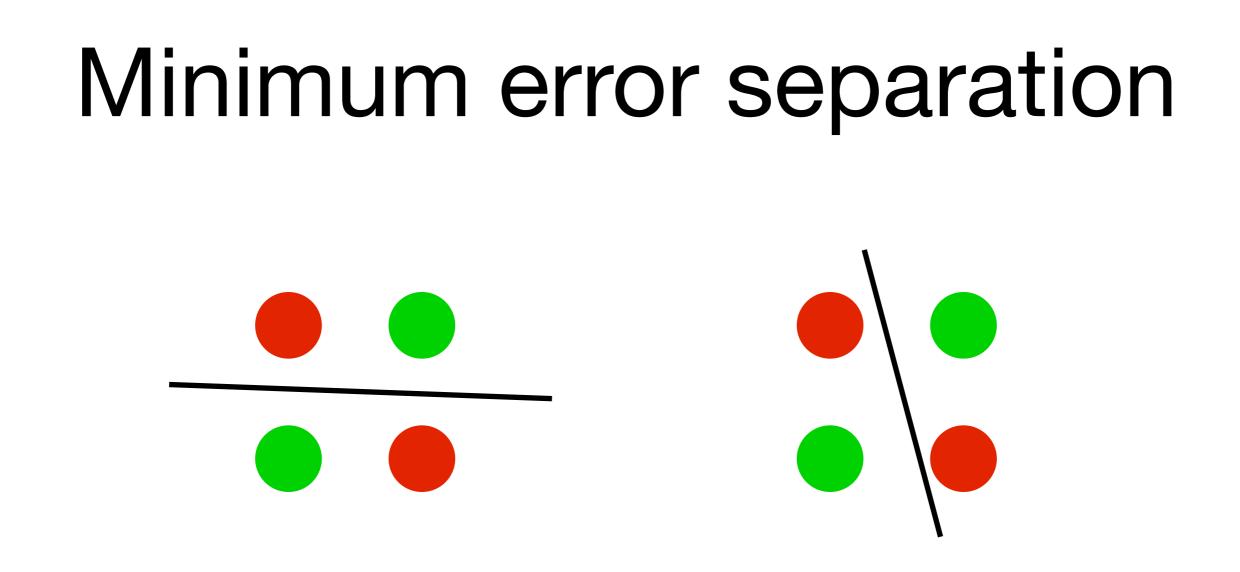




Concepts & version space

- 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)





- 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).

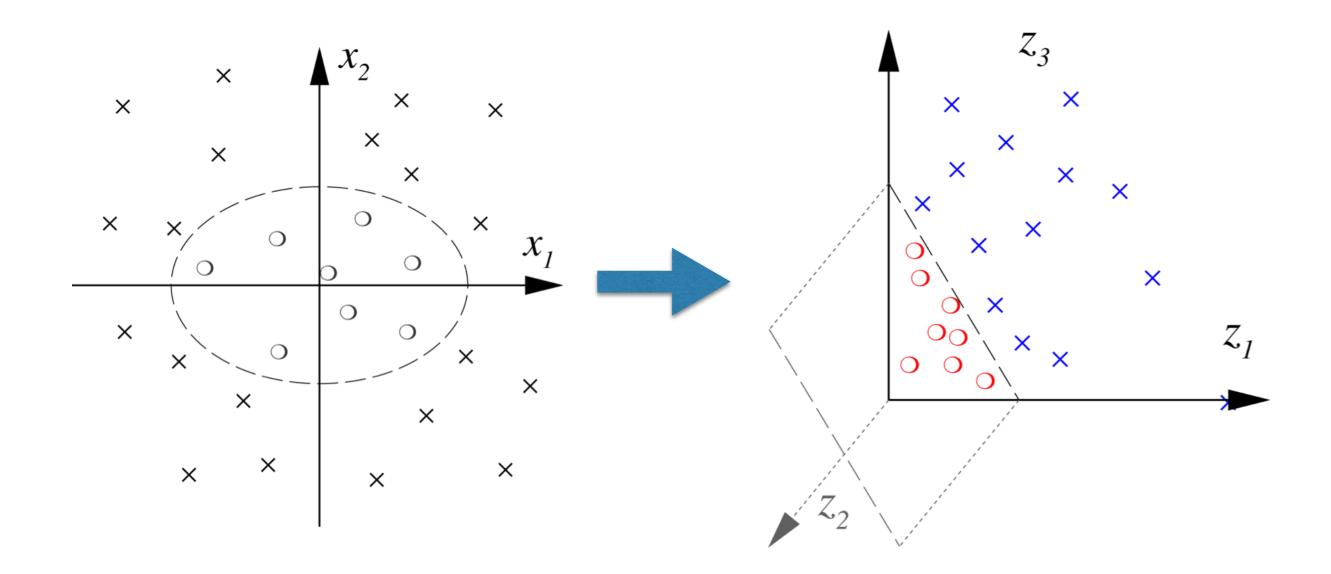
Nonlinear Features

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)

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

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Feature Engineering for Spam Filtering

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

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lide

More feature engineering

Two Interlocking Spirals
 Transform the data into a radial and angular part

 $(x_1, x_2) = (r\sin\phi, r\cos\phi)$

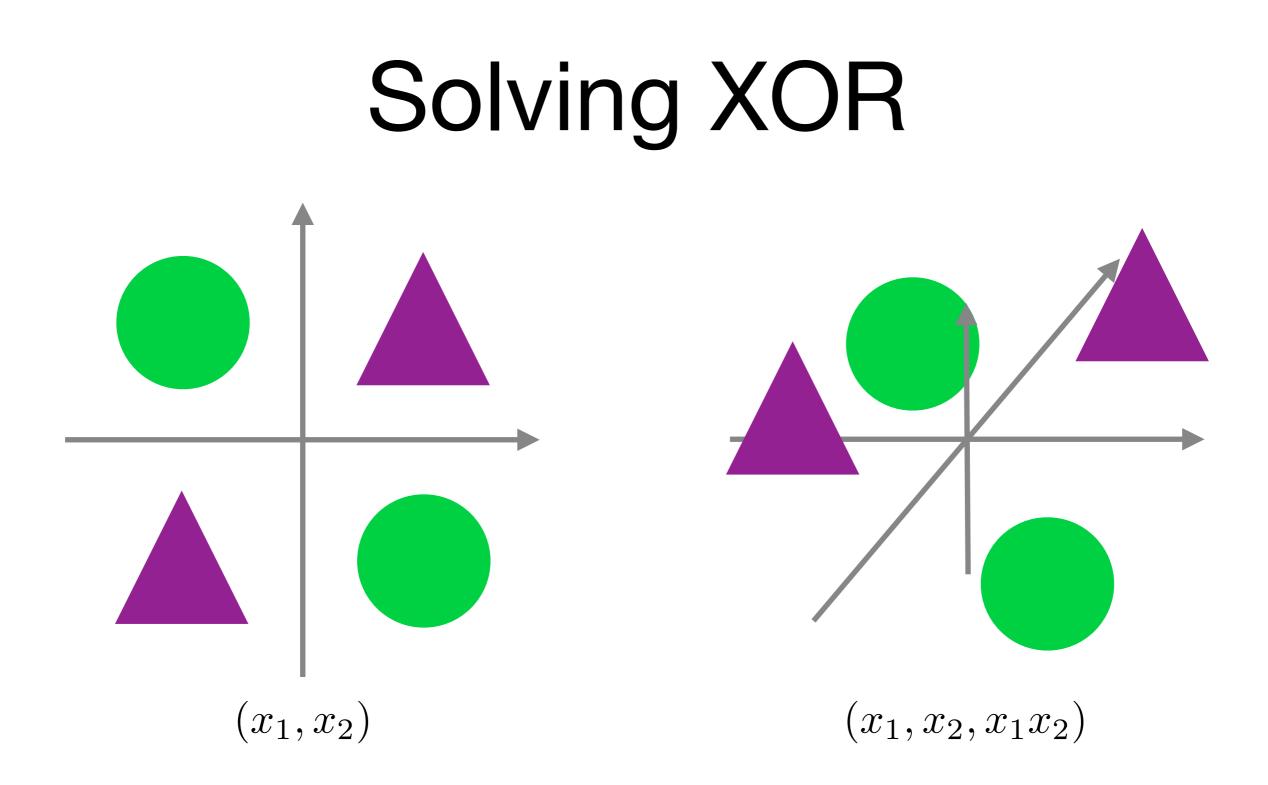
- Handwritten Japanese Character Recognition
 - Break down the images into strokes and recognize it
 - Lookup based on stroke order
- Medical Diagnosis
 - Physician's comments
 - Blood status / ECG / height / weight / temperature ...
 - Medical knowledge
- Preprocessing
 - Zero mean, unit variance to 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
 $w' = w + y_i \Phi(x_i)$
 $b' = b + y_i$
until $y_i(w \cdot \Phi(x_i) + b) > 0$ for all i

- Nothing happens if classified correctly
- Weight vector is linear combination $w = \sum y_i \phi(x_i)$
- Classifier is linear combination of $i \in I$ inner products $f(x) = \sum_{i \in I} y_i \langle \phi(x_i), \phi(x) \rangle + b$



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

Extensions of Perceptron

Voted Perceptron

- generalizes better than (standard) perceptron
- memory intensive (keeps around every weight vector seen during training, so each one can vote)

Averaged Perceptron

- empirically similar performance to voted perceptron
- can be implemented in a memory efficient way (running averages are efficient)

Extensions of Perceptron

Kernel Perceptron

- Choose a kernel K(x', x)
- Apply the kernel trick to Perceptron
- Resulting algorithm is still very simple

Structured Perceptron

- Basic idea can also be applied when **y** ranges over an exponentially large set
- Mistake bound does not depend on the size of that set

Summary: Perceptron

- Perceptron is a linear classifier
- Simple learning algorithm: when a mistake is made, add / subtract the features
- Perceptron will converge if the data are linearly separable, it will not converge if the data are linearly inseparable
- For linearly separable and inseparable data, we can **bound the number of mistakes** (geometric argument)
- Extensions support nonlinear separators and structured prediction

Next Lecture: Multi-layer Perceptron