Linear Classification

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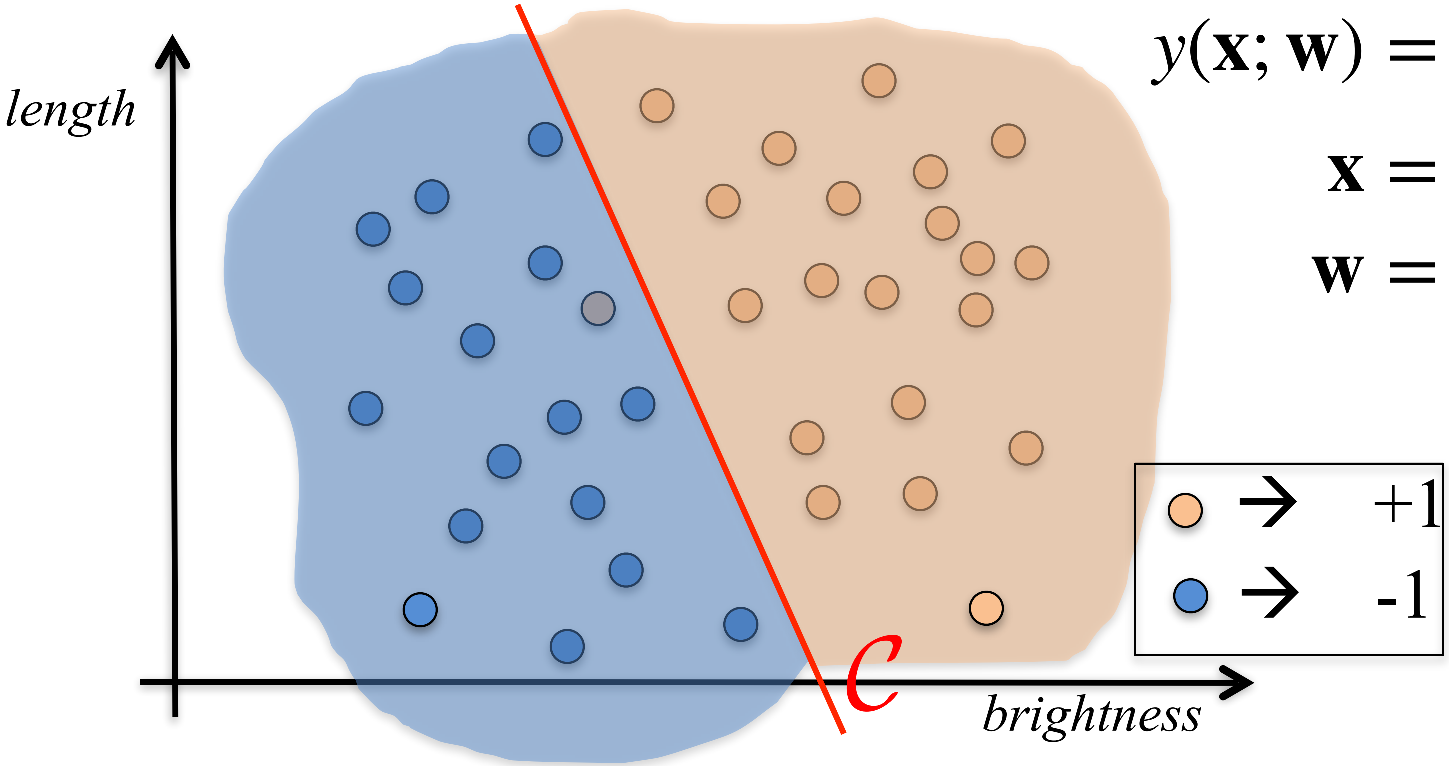
IC-CVLab

EPFL

Reminder: Linear 2D Model

Some algorithm →

$$\begin{pmatrix} brightness \\ length \end{pmatrix}$$



$$y(\mathbf{x};\mathbf{w}) = \text{sign}(\text{w}_x\text{b} + \text{w}_y\text{l} + \text{w}_0)$$

$$\mathbf{x} = [b, l]$$

$$\mathbf{w} = [w_x, w_y, w_0]$$

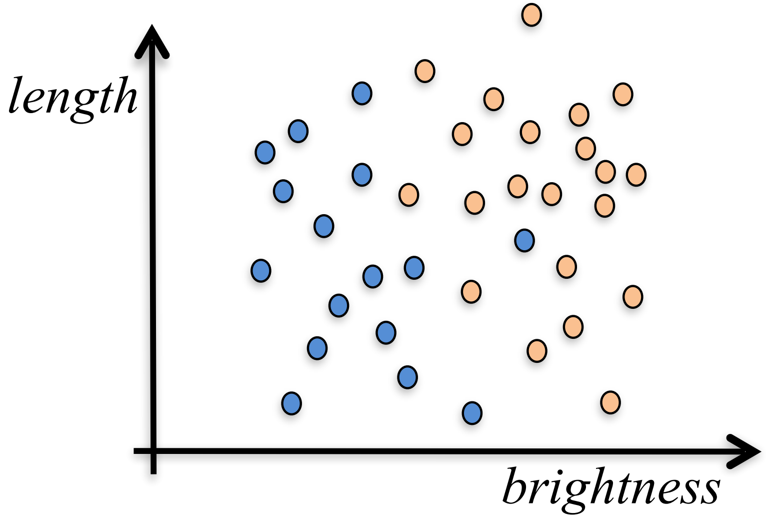
How do we find **w**?

Reminder: Training vs Testing

Supervised training:

Given a **training** set $\{(\mathbf{x}_n, t_n)_{1\leq n\leq N}\}$ minimize:

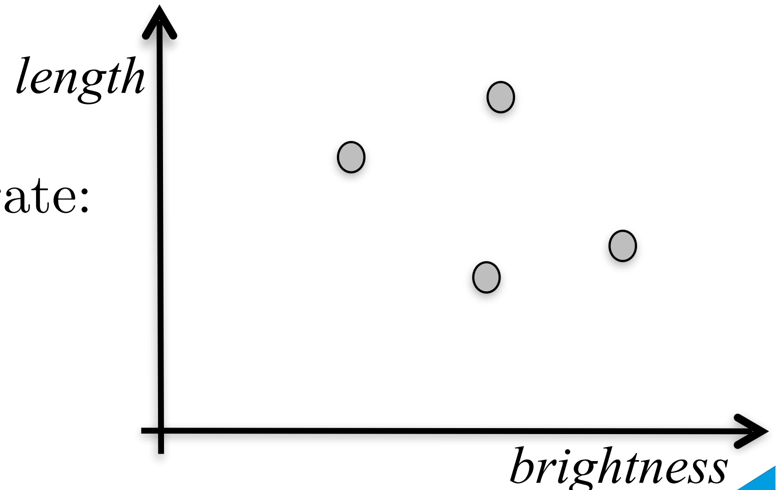
$$E(\mathbf{w}) = \sum_{n=1}^{N} L(y(\mathbf{x}_n;\mathbf{w}), t_n)$$
$$= \sum_{n=1}^{N} [y(\mathbf{x}_n;\mathbf{w}) \neq t_n]$$



Testing:

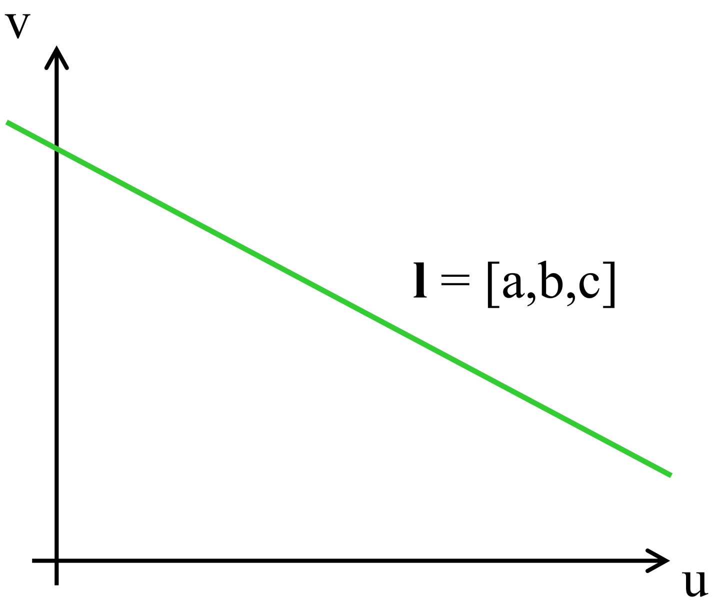
Given a **test** set $\{(\mathbf{x}_n, t_n)_{1\leq n\leq N}\}$ compute the error rate:

$$1/N \sum_{n=1}^{N} [y(\mathbf{x}_n;\mathbf{w}) \neq \mathbf{t}_n]$$



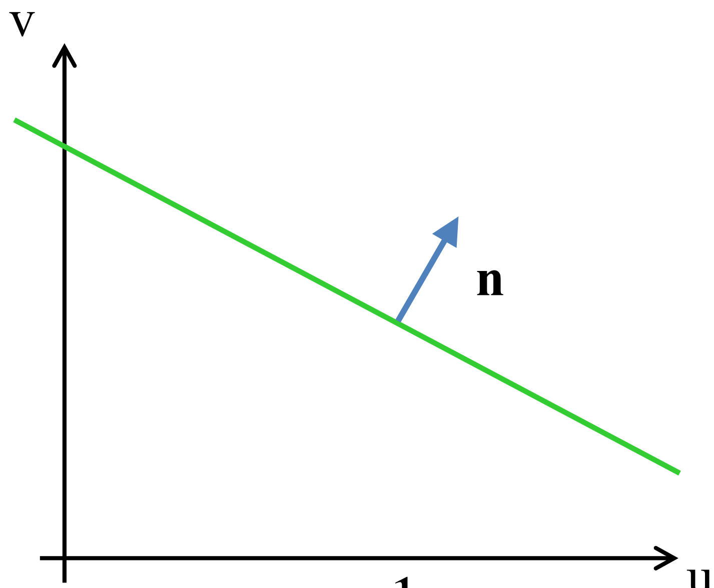
Parameterizing Lines

Equation of a line



$$(u, v) \in R^2, au + bv + c = 0$$

Normal vector

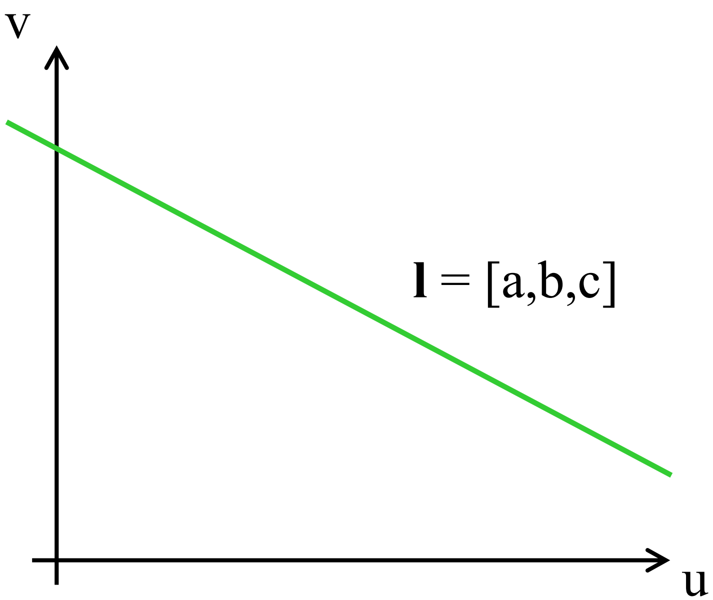


$$\mathbf{n} = \frac{1}{\sqrt{a^2 + b^2}}[a, b]$$

$[a, b, c]$ and $\frac{1}{\sqrt{a^2 + b^2}}[a, b, c]$ define the same line.

Normalized Parameterization

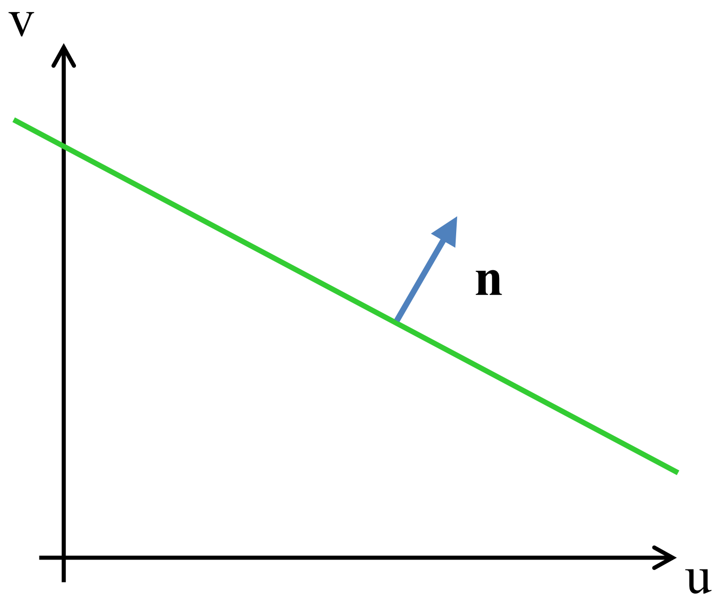
Equation of a line



$$(u, v) \in R^2, au + bv + c = 0$$

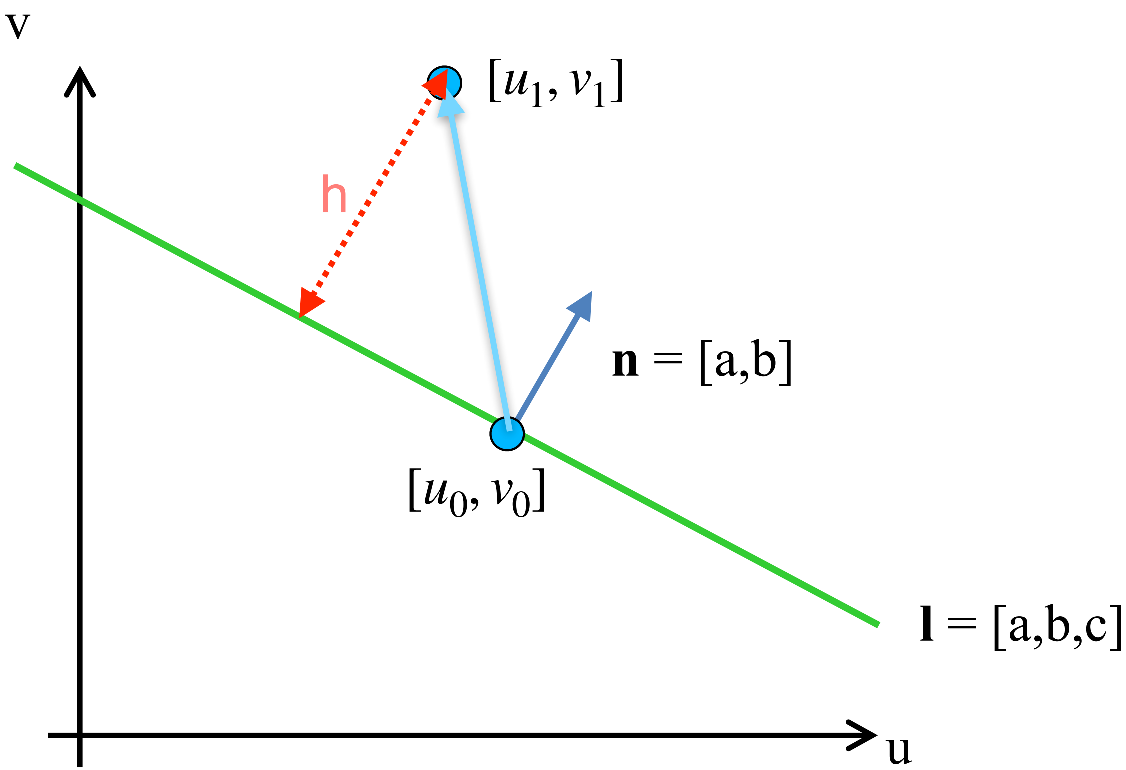
with $a^2 + b^2 = 1$

Normal vector



$$\mathbf{n} = [a, b]$$

Signed Distance to Line

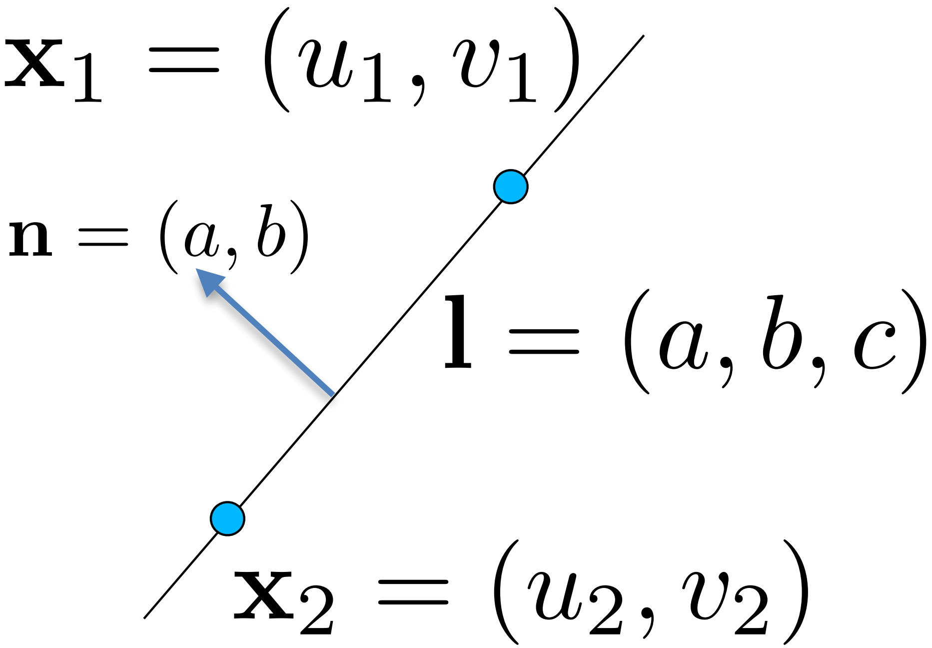


Signed distance:

$$
\begin{aligned}
h &= \mathbf{n} \cdot [u_1 - u_0, v_1 - v_0] \\
&= a(u_1 - u_0) + b(v_1 - v_0) \\
&= au_1 + bv_1 - (au_0 - bv_0) \\
&= au_1 + bv_1 + c - (au_0 - bv_0 - c) \\
&= au_1 + bv_1 + c
\end{aligned}
$$

h=0: Point is on the line.
h>0: Point on one side.
h<0: Point on the other side.

Line Going Through 2 Points



Points belong to line:

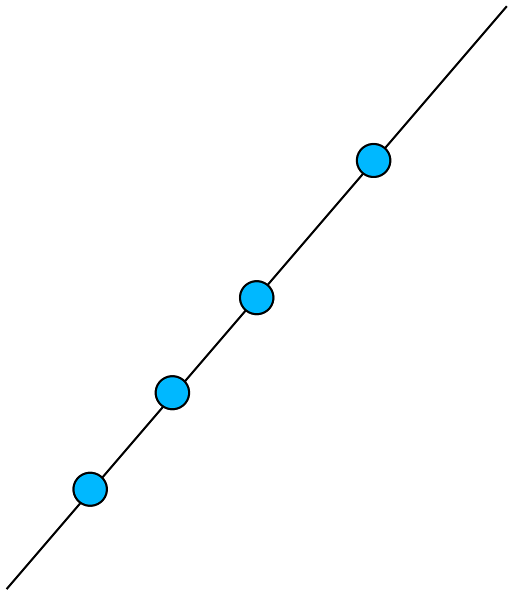
$$\begin{aligned} au_1 + bv_1 + c &= 0 \\ au_2 + bv_2 + c &= 0 \end{aligned}$$

subject to:

$$a^2 + b^2 = 1$$

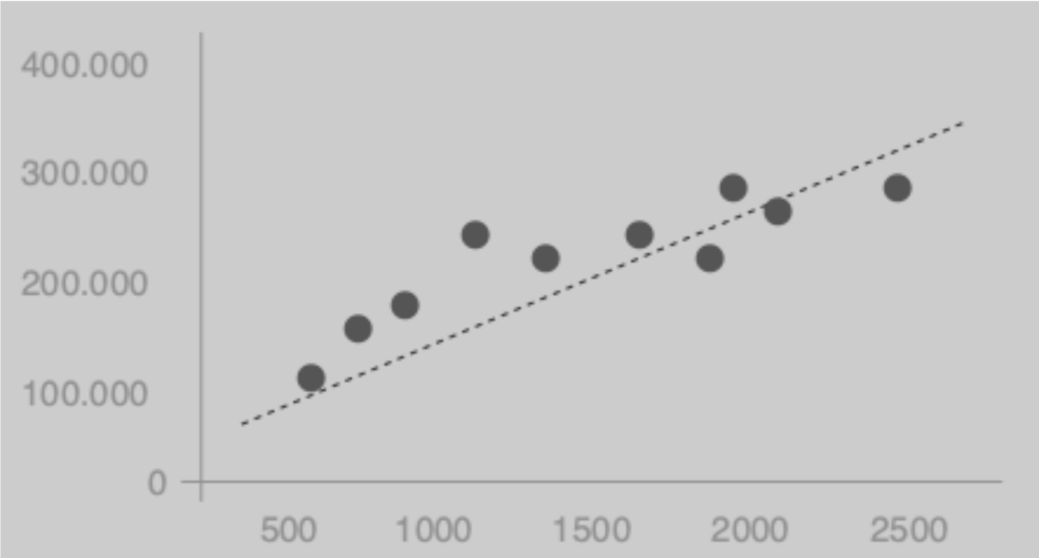
Line Going Through N Points

$$\mathbf{x}_i = (u_i, v_i)$$



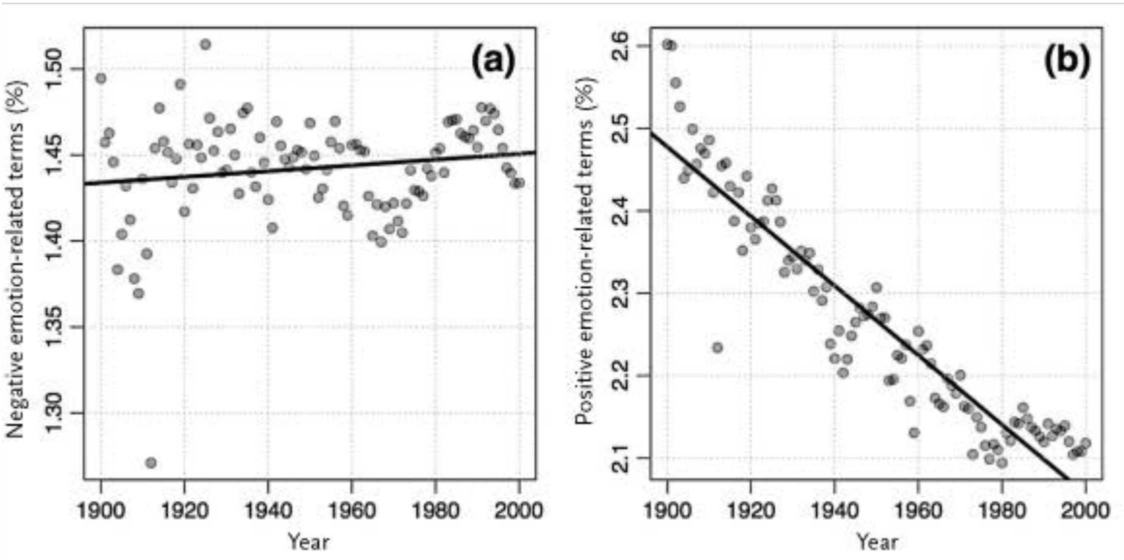
In practice, this never happens due to noise.

In Real Life



https://www.internalpointers.com/post/linear-regression-one-variable

- Price of a house a function of its size

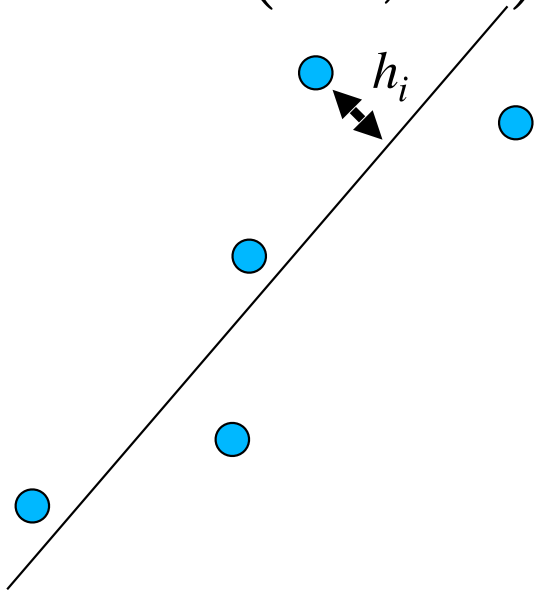


Moretti & Sobchuk, 2019

- Proportion of negative and positive emotions in anglophone fiction.

Fitting a Line to N Points

$$\mathbf{x}_i = (u_i, v_i)$$

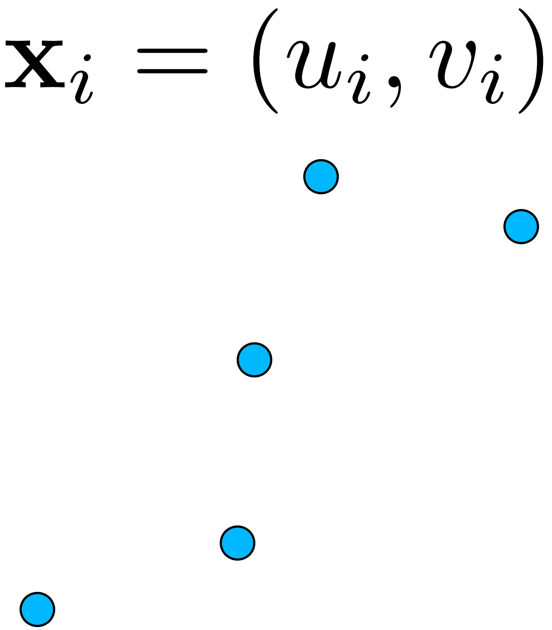


Orthogonal distance to line:

$$h_i = au_i + bv_i + c \text{ if } a^2 + b^2 = 1$$

$\rightarrow$ We want to minimize $\sum_i (au_i + bv_i + c)^2$ w.r.t. a, b, and c, subject to $a^2 + b^2 = 1$.

Centering the Coordinates



Original points:

$$\mathbf{x}_i = (u_i, v_i)_{1 \le i \le n}$$

$$\bar{\mathbf{x}} = \frac{1}{N} \sum_i \mathbf{x}_i$$

Centered points:

$$\mathbf{x}_i^c = \mathbf{x}_i - \bar{\mathbf{x}}$$

$$\overline{\mathbf{x}^c} = \mathbf{0}$$

—> The points can always be translated so that their center of gravity is at the origin.

Minimization using Centered Points

Minimize $\sum_i (au_i + bv_i + c)^2$ w.r.t. a, b, and c, subject to $a^2 + b^2 = 1$.

Minimize $\sum_i (au_i + bv_i)^2 + 2c(a\sum_i u_i + b\sum_i v_i) + \sum_i c^2$.

Zero if coordinates are centered. c=0

Minimize $\|\mathbf{M}\begin{bmatrix} a \\ b \end{bmatrix}\|^2$ subject to $a^2 + b^2 = 1$, with $\mathbf{M} = \begin{bmatrix} u_1 & v_1 \\ u_2 & v_2 \\ .. & .. \\ u_n & v_n \end{bmatrix}$.

$\rightarrow \begin{bmatrix} a \\ b \end{bmatrix}$ is the eigenvector associated to the smallest eigenvalue of $\mathbf{M}^T\mathbf{M}$.

Optional: Proof Sketch

Let us consider the symmetric matrix $\mathbf{A} = \mathbf{M}^T\mathbf{M}$ of size N x N:

- We can write $A = R^T DR$ where D is diagonal and $R^T R = I$, therefore

$$\forall X \in R^N, \quad \|AX\|^2 = X^T A^T AX = X^T MX = (RX)^T D(RX).$$

- R is a rotation matrix and

$$\forall X \in R^N, \|RX\| = \|X\|.$$

- Let $X \in R^N$, $\|X\| = 1$ and $Y = RX$, we have

$$\|AX\|^2 = Y^T DY \text{ with } \|Y\| = 1.$$

- D is a diagonal matrix, therefore we have

$$D = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \lambda_N \end{bmatrix},$$

$$\Rightarrow \lambda_1 \leq \|DY\| \leq \lambda_N \text{ if } \|Y\| = 1 .$$

This result applies in any dimension.

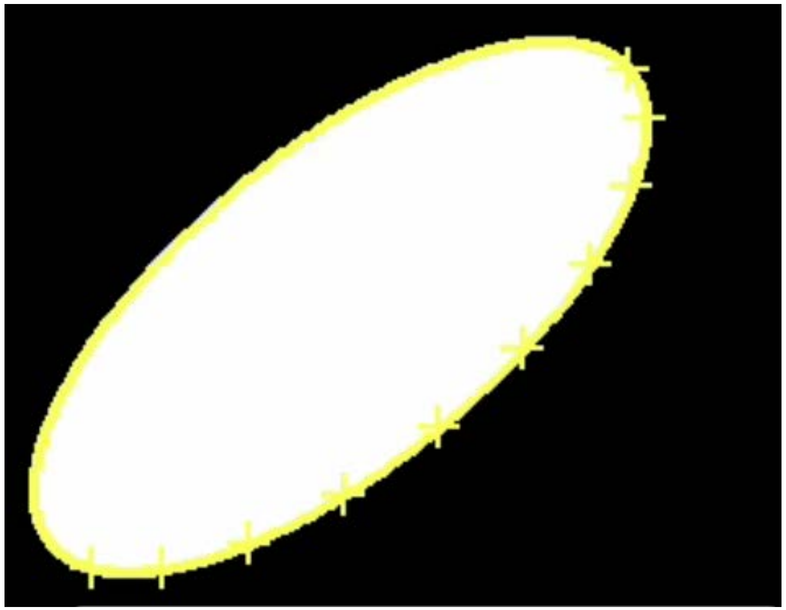
Optional: Fitting Ellipses

For each point :

$$d_a(\mathbf{x}_i, \mathbf{X}) = au_i^2 + bu_iv_i + cv_i^2 + du_i + ev_i + f$$
$$= \begin{bmatrix} u_i^2 & u_iv_i & v_i^2 & u_i & v_i & 1 \end{bmatrix} \bullet \mathbf{X}$$

Minimize :

$$\sum_{\mathrm{i}} d_a(\mathbf{x}_i, \mathbf{X})^2 = \|\mathbf{AX}\|^2 \text{ subject to } \|\mathbf{X}\| = 1$$



$$\text{where } \mathbf{A} = \begin{bmatrix} u_1^2 & u_1v_1 & v_1^2 & u_1 & v_1 & 1 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ u_n^2 & u_nv_n & v_n^2 & u_n & v_n & 1 \end{bmatrix}$$

The line and ellipse fitting algorithms we showed are examples of an important technique known as the Direct Linear Transform.

Optional: Generalization

Line:

$$\begin{aligned} \mathbf{x}_i &= [u_i, v_i] \\ \mathbf{w} &= [a, b] \\ \phi(\mathbf{x}) &= [u, v, 1] \\ t_i &= 0 \end{aligned}$$

Ellipse :

$$\begin{aligned} \mathbf{x}_i &= [u_i, v_i] \\ \mathbf{w} &= [a, b, c, d, e, f] \\ \phi(\mathbf{x}) &= [u^2, uv, v^2, u, v, 1] \\ t_i &= 0 \end{aligned}$$

Feature Vector

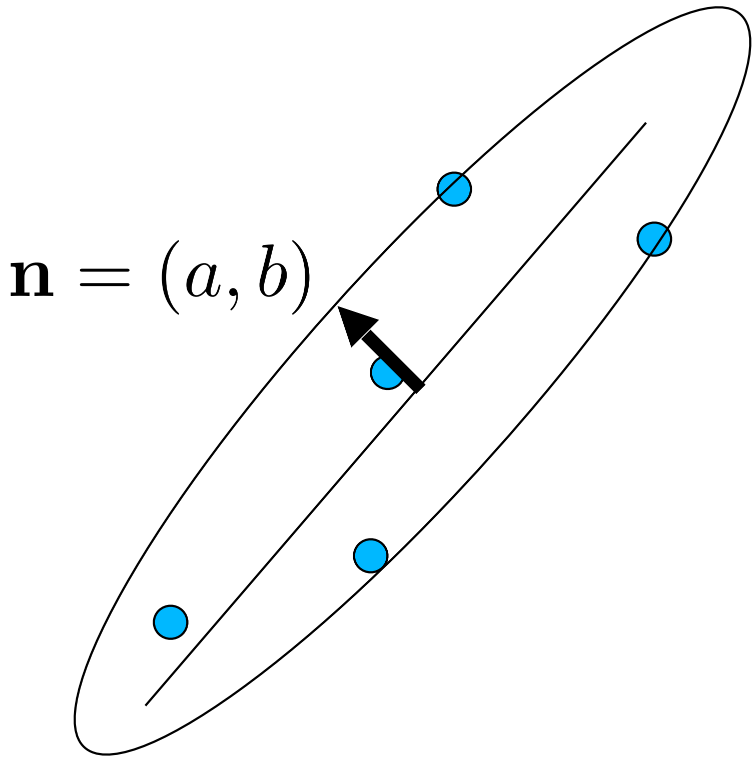
In both case we minimize:

$$\sum_i d_a(\mathbf{x}_i, \mathbf{X})^2 = \sum_i (\mathbf{w}^T \phi(\mathbf{x}_i) - t_i)^2$$

$$\Rightarrow \forall i, \mathbf{w}^T \phi(\mathbf{x}_i) \approx t_i$$

We will encounter this formulation again later in the class.

Back to 2D Lines

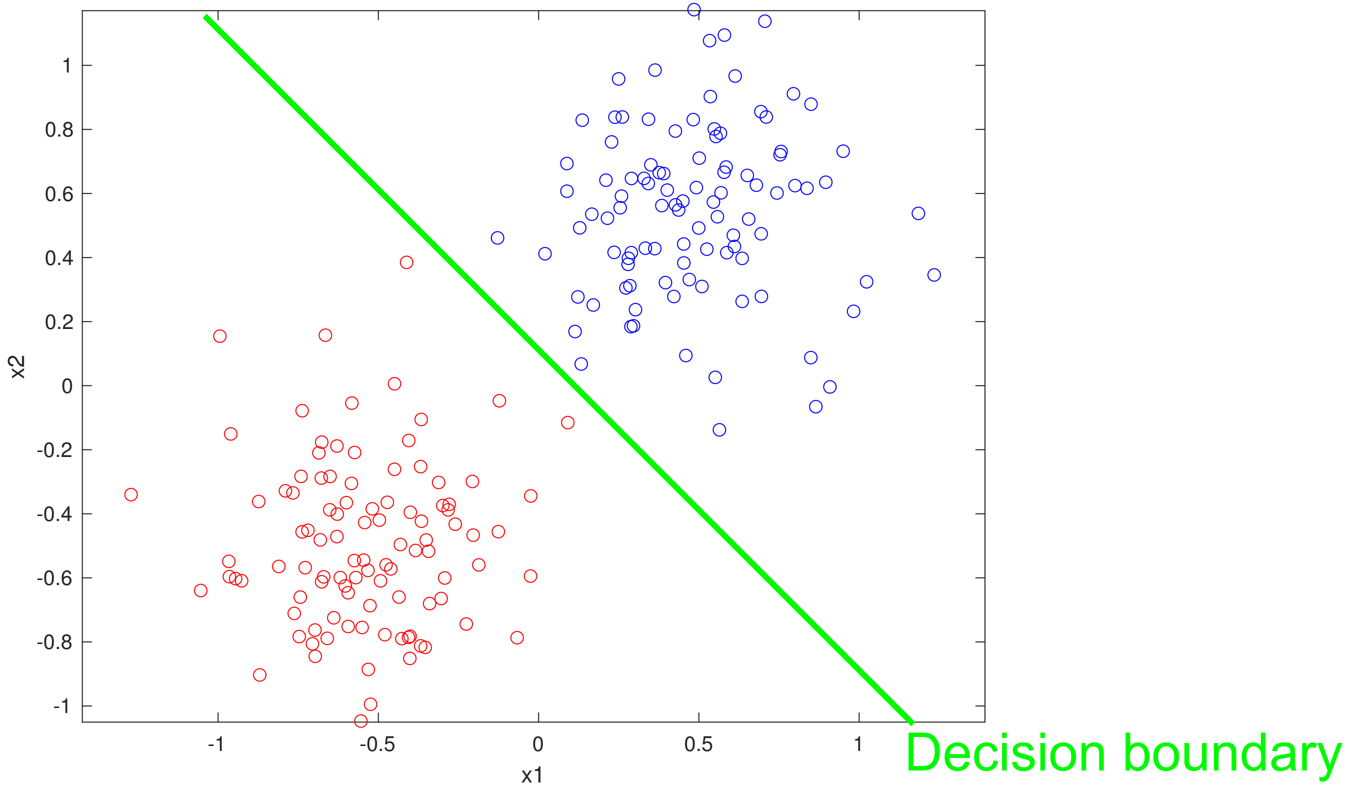


$$\mathbf{M}^T\mathbf{M} = \begin{bmatrix} \sum u_i^2 & \sum u_i v_i \\ \sum u_i v_i & \sum v_i^2 \end{bmatrix}$$

Moment Matrix

- The eigenvector corresponding to the largest eigenvalue of $\mathbf{M}^T\mathbf{M}$ is the direction of the fitted line.
- The eigenvector corresponding to the smallest eigenvalue is its normal.
- The ratio of the two eigenvalues indicates how much noise there is:
  - zero without noise,
  - close to one if the points are randomly distributed.

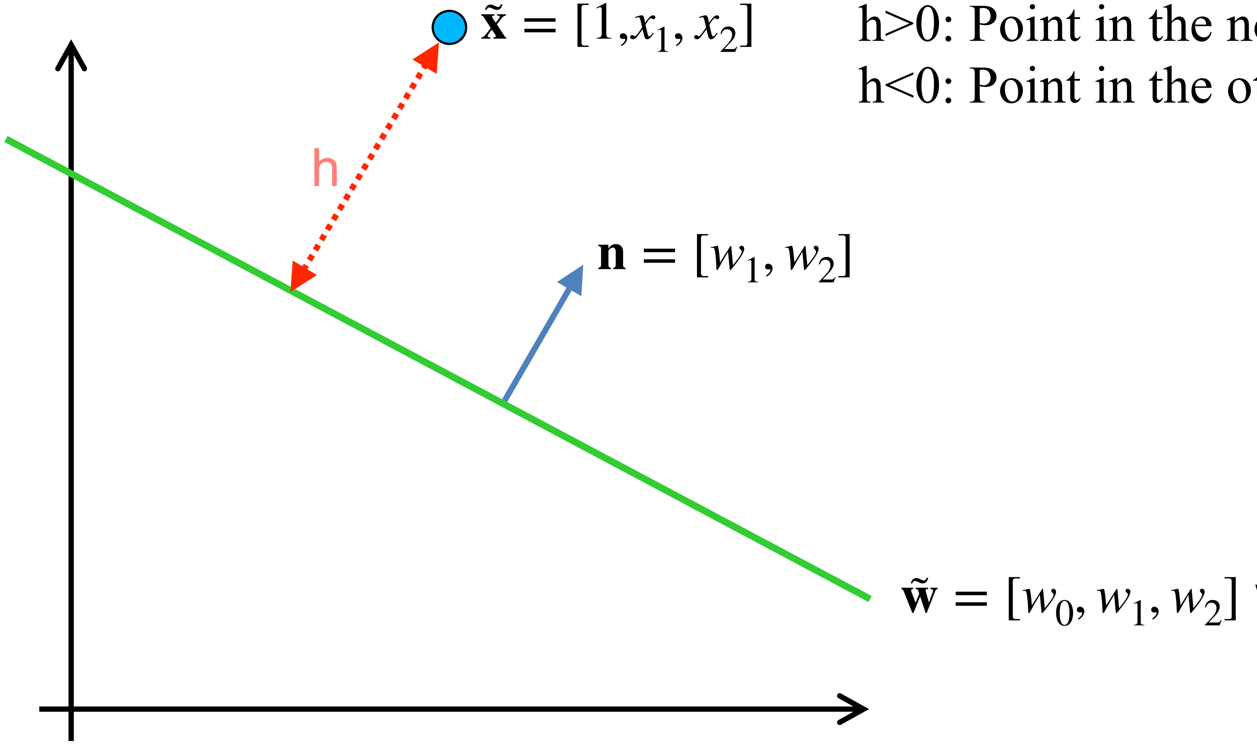
Binary Classification



Two classes shown as different colors:

- The label $y \in \{-1,1\}$ or $y \in \{0,1\}$.
- The samples with label 1 are called positive samples.
- The samples with label -1 or 0 are called negative samples.

Signed Distance Reformulated



h=0: Point is on the line.
h>0: Point in the normal's direction.
h<0: Point in the other direction.

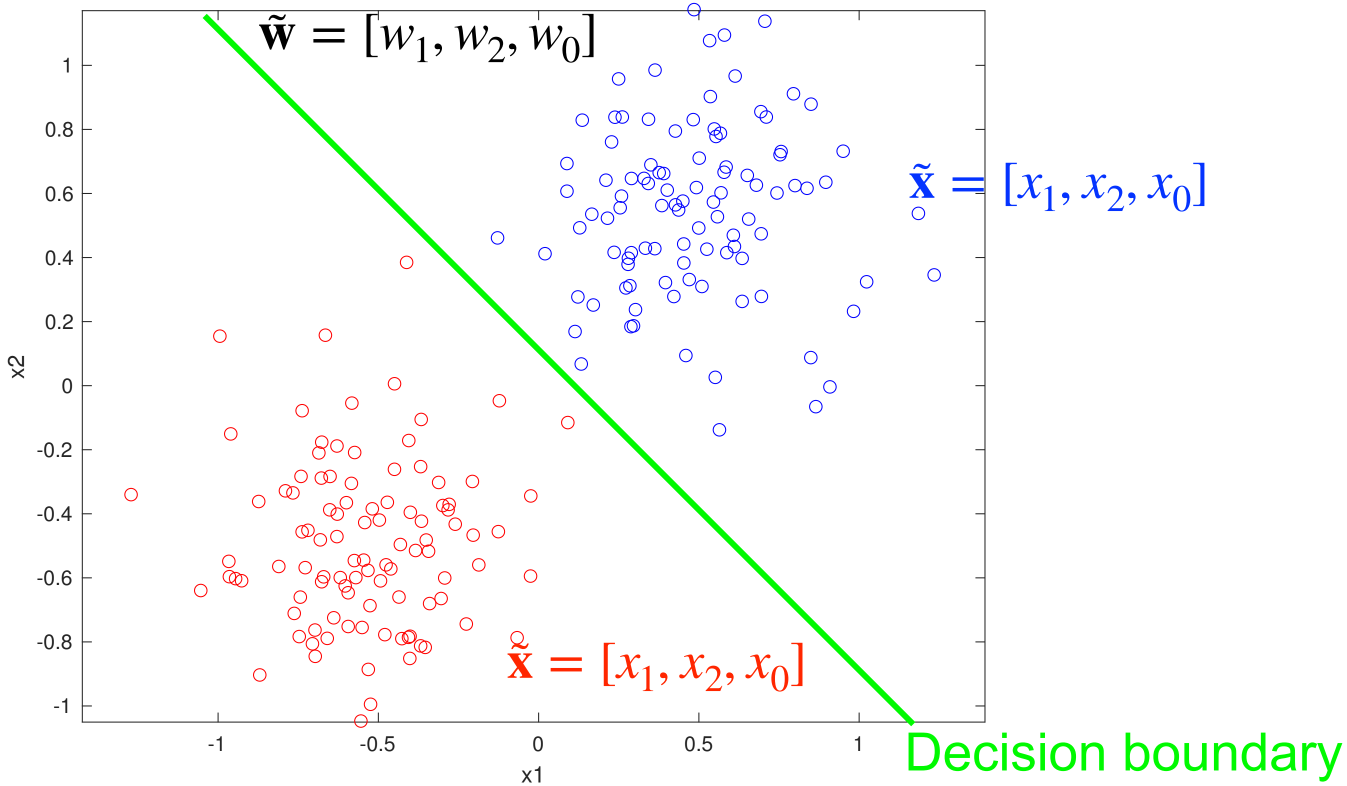
Notation:

$$\mathbf{x} = [x_1, x_2]$$
$$\tilde{\mathbf{x}} = [1, x_1, x_2]$$

Signed distance:

$$h = w_0 + w_1 x_1 + w_2 x_2$$
$$= \tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}}$$

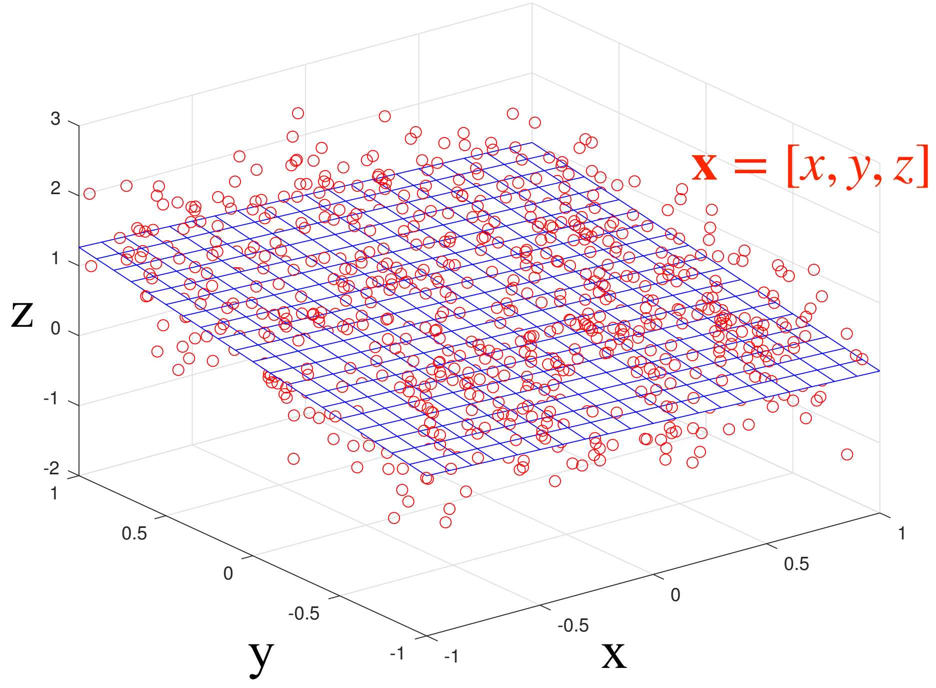
Problem Statement in 2D

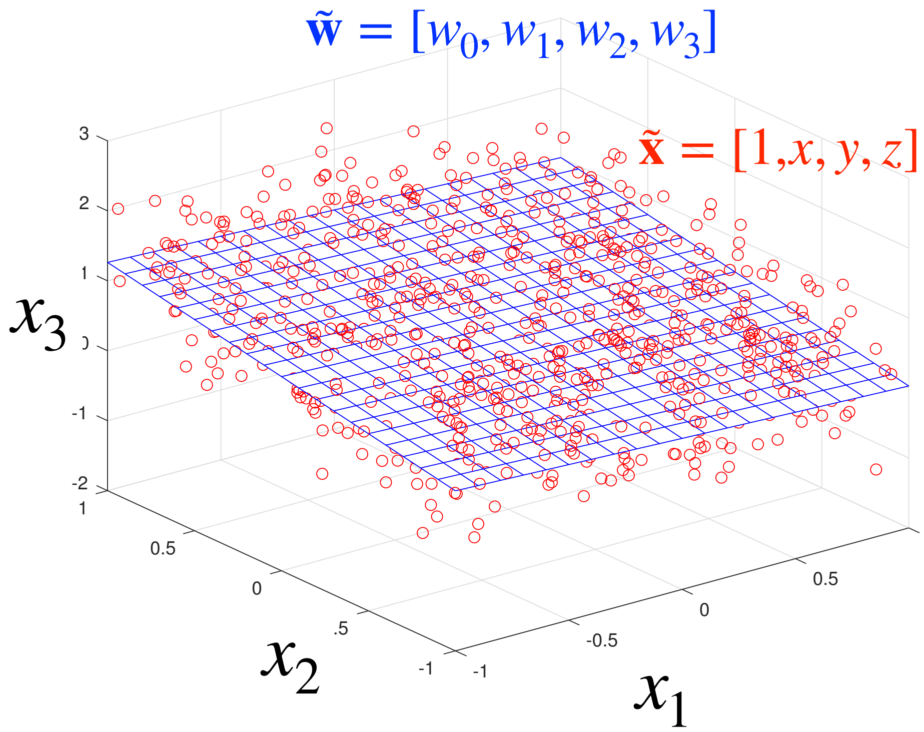


Find $\tilde{\mathbf{w}}$ such that:

- For all or most positive samples $\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}} > 0$.
- For all or most negative samples $\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}} < 0$.

Signed Distance in 3D



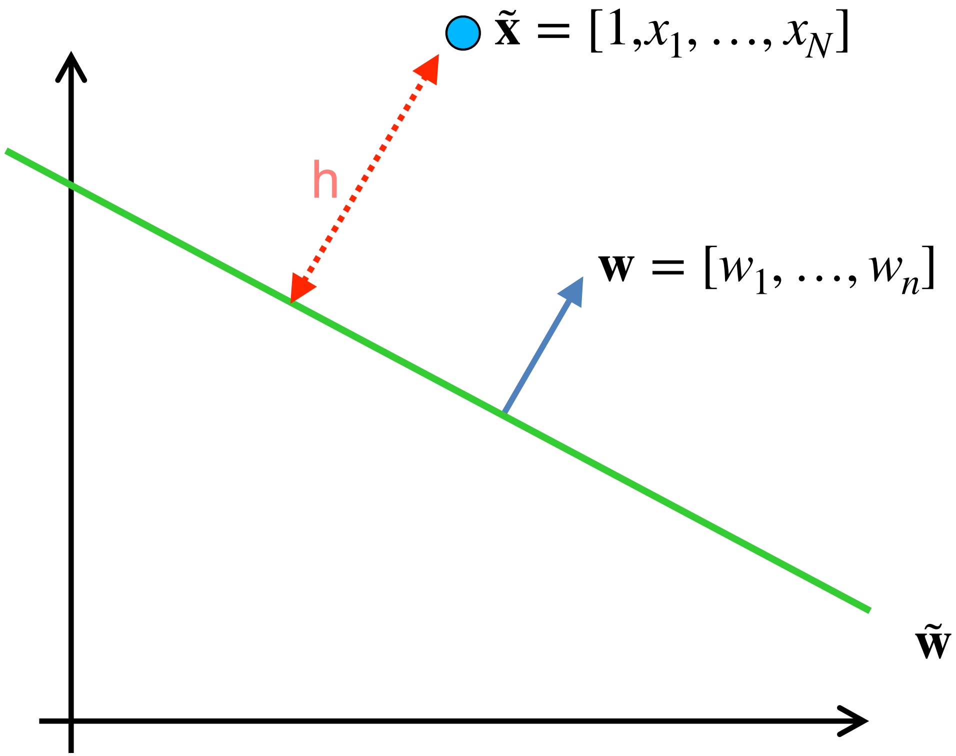


$\mathbf{x} \in R^3, 0 = ax + by + cz + d$

$\tilde{\mathbf{x}} \in R^4, \tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}} = 0$

Signed distance $h = \tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}}$ if $w_1^2 + w_2^2 + w_3^2 = 1$.

Signed Distance in N Dimensions



h=0: Point is on the decision boundary.
h>0: Point on one side.
h<0: Point on the other side.

$\tilde{\mathbf{w}} = [w_0, w_1, \ldots, w_n]$ with $\sum_{i=1}^{N} w_i^2 = 1$

Notation: $\mathbf{x} = [x_1, \ldots, x_n]$

$\tilde{\mathbf{x}} = [1, x_1, \ldots, x_n]$

Hyperplane: $\mathbf{x} \in R^n, \quad 0 = \tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}}$

$$= w_0 + w_1 x_1 + \ldots w_n x_n$$

Signed distance: $h = \tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}}$

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Problem Statement in N Dimensions

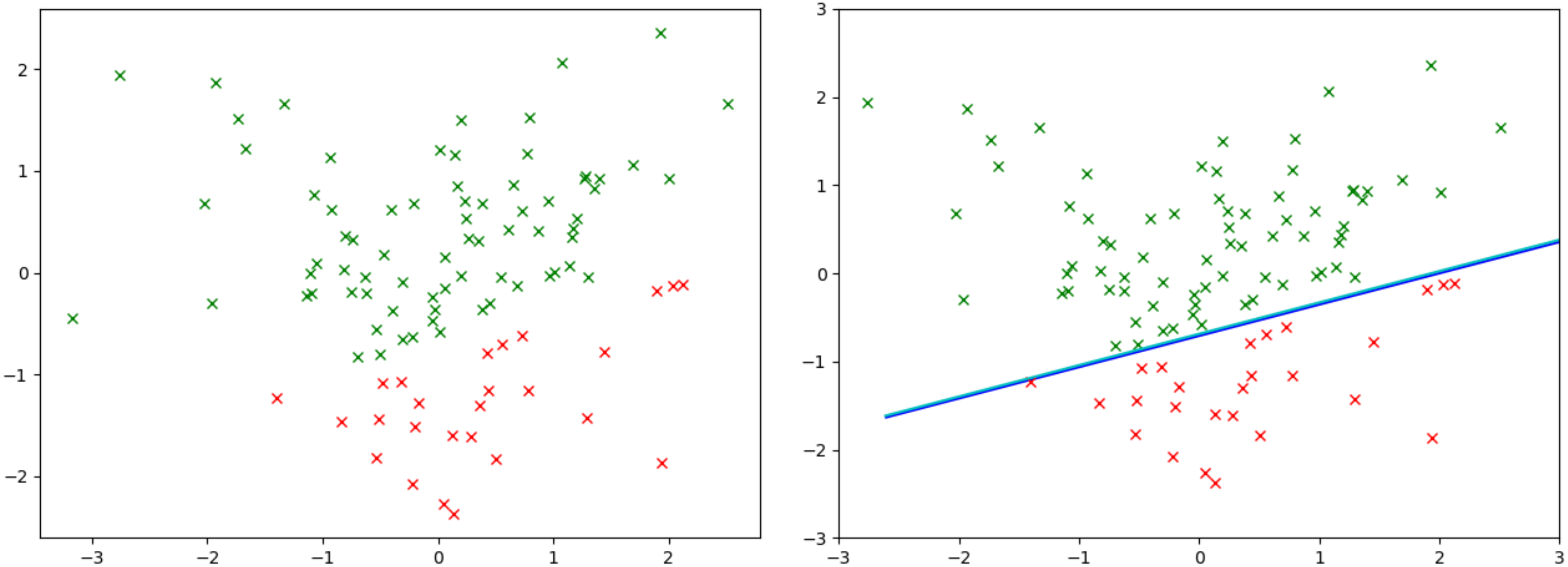
Hyperplane: $\mathbf{x} \in R^N, \tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}} = 0$, with $\tilde{\mathbf{x}} = [1 \mid \mathbf{x}]$.

Signed distance: $\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}}$, with $\tilde{\mathbf{w}} = [w_0 \mid \mathbf{w}]$ and $\|\mathbf{w}\| = 1$.

Find $\tilde{\mathbf{w}}$ such that

- for all or most positive samples $\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}} > 0$,
- for all or most negative samples $\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}} < 0$.

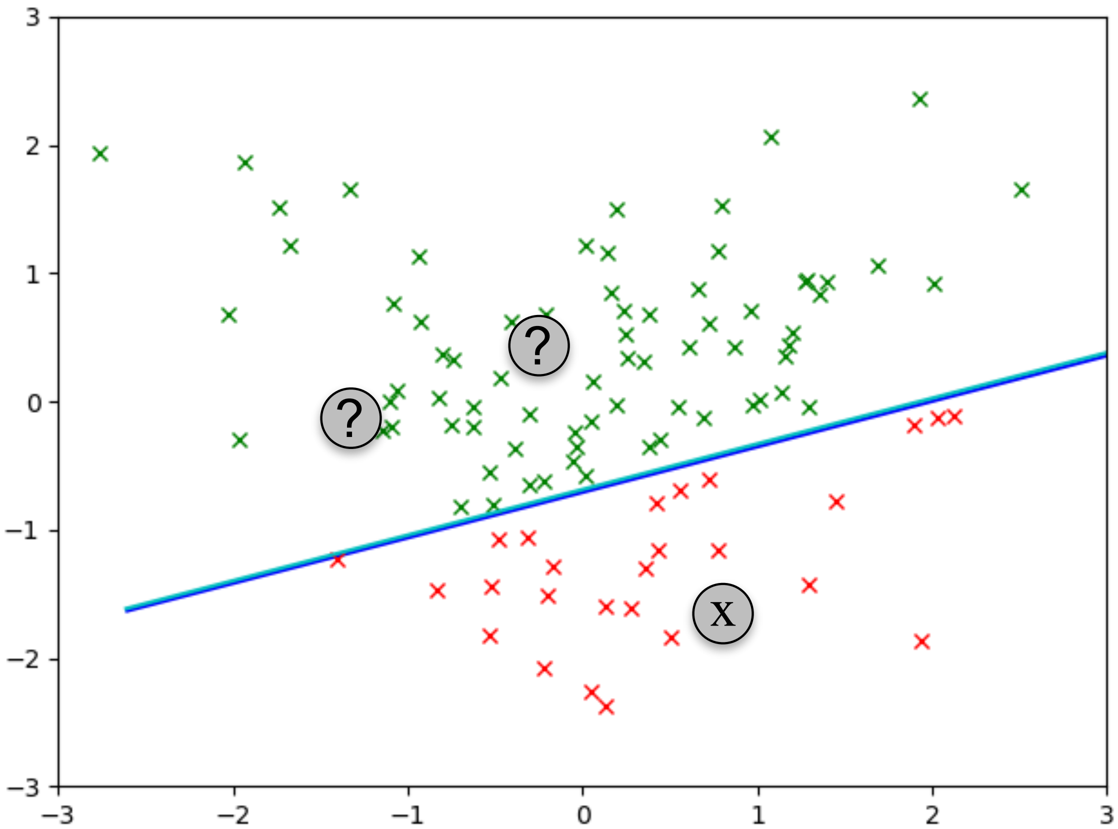
Perceptron



$$\text{Minimize: } E(\tilde{\mathbf{w}}) = -\sum_{n=1}^{N} \text{sign}(\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}}_n) t_n$$

- Set $\tilde{\mathbf{w}}_1$ to $\mathbf{0}$.
- Iteratively, pick a random index n.
  - If $\tilde{\mathbf{x}}_n$ is correctly classified, do nothing.
  - Otherwise, $\tilde{\mathbf{w}}_{t+1} = \tilde{\mathbf{w}}_t + t_n \tilde{\mathbf{x}}_n$.

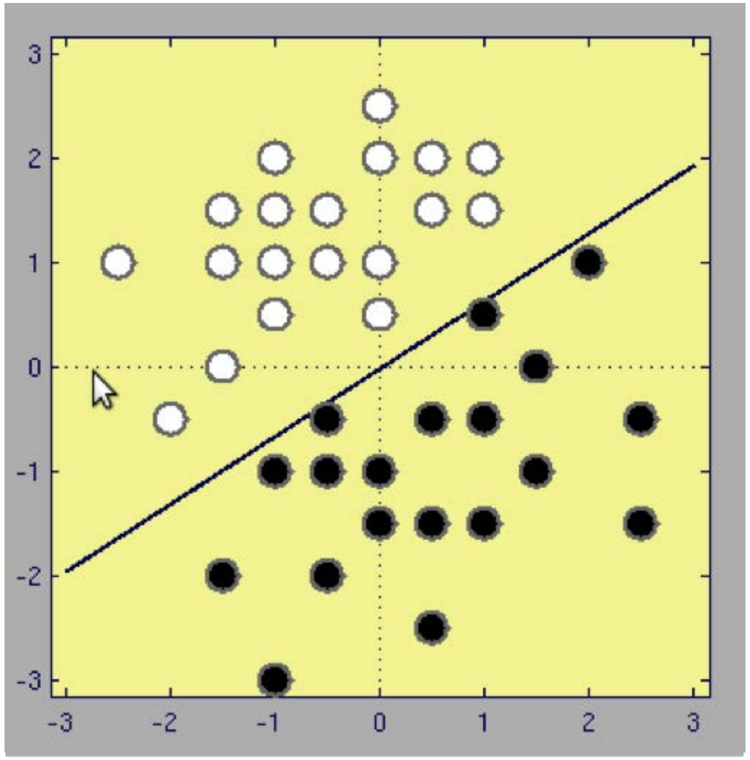
Test Time



$$y(\mathbf{x}; \tilde{\mathbf{w}}) = \begin{cases} 1 & \text{if} \quad \tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}} \geq 0\ , \\ -1 & \text{otherwise.} \end{cases}$$

$$\tilde{\mathbf{x}} = [1, x_1, ..., x_n]$$

Centered Perceptron



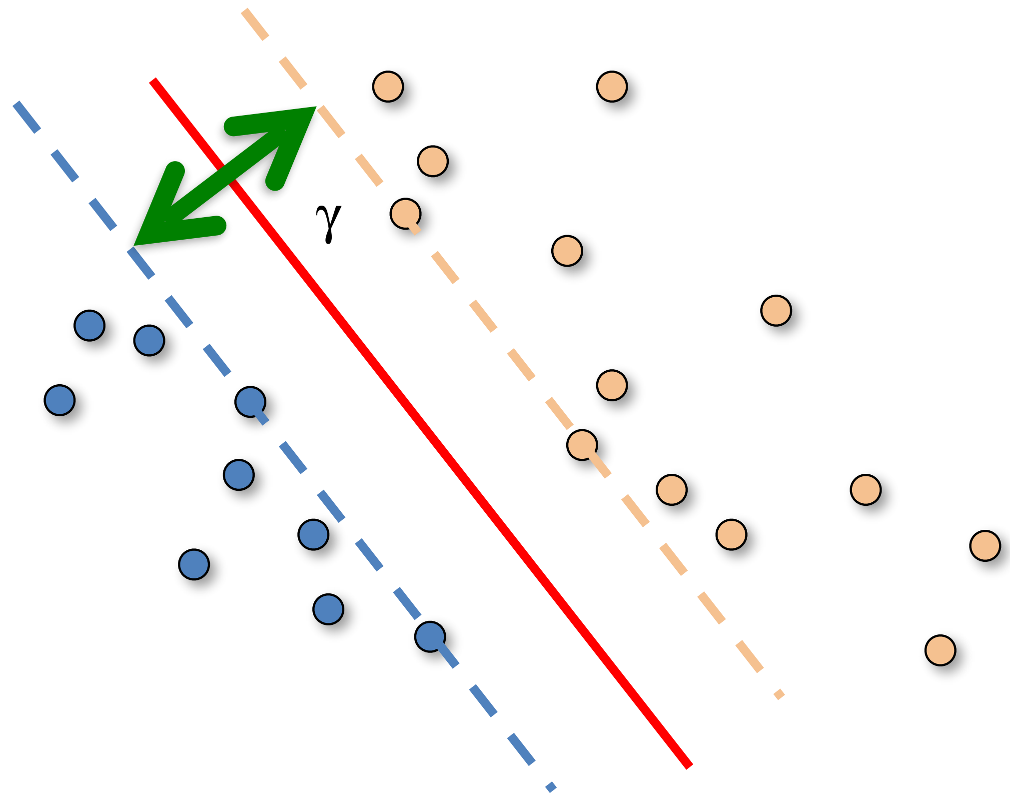
If the two populations are of the same size, the decision boundary can be assumed to go through the center of gravity.

Given a **training** set $\{(\mathbf{x}_n, t_n)_{1 \leq n \leq N}\}$ minimize:

$$E(\mathbf{w}) = -\sum_{n=1}^{N} \text{sign}(\mathbf{w} \cdot \mathbf{x}_n) t_n$$

- Center the $\mathbf{x}_n$s so that $w_0 = 0$.
- Set $\mathbf{w}_1$ to $\mathbf{0}$.
- Iteratively, pick a random index n.
  - If $\mathbf{x}_n$ is correctly classified, do nothing.
  - Otherwise, $\mathbf{w}_{t+1} = \mathbf{w}_t + t_n \mathbf{x}_n$.

Convergence Theorem



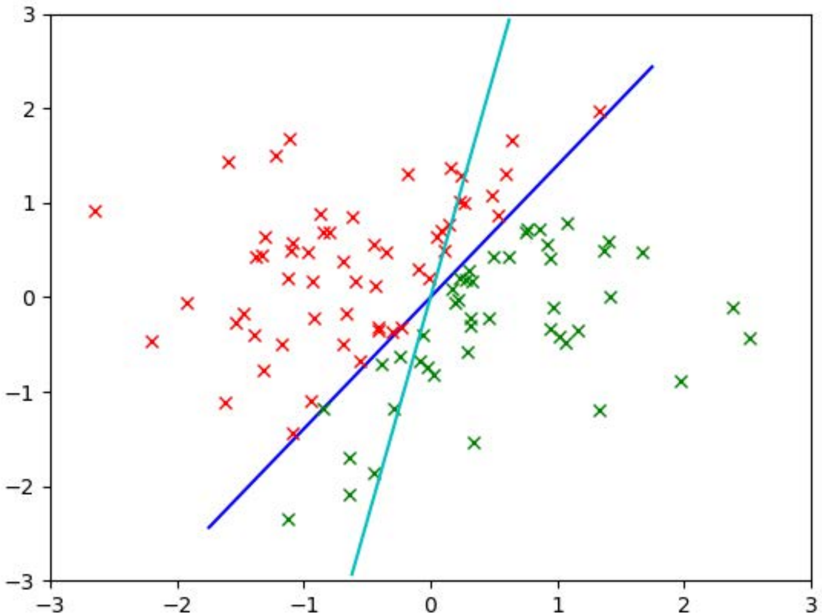
γ is the margin

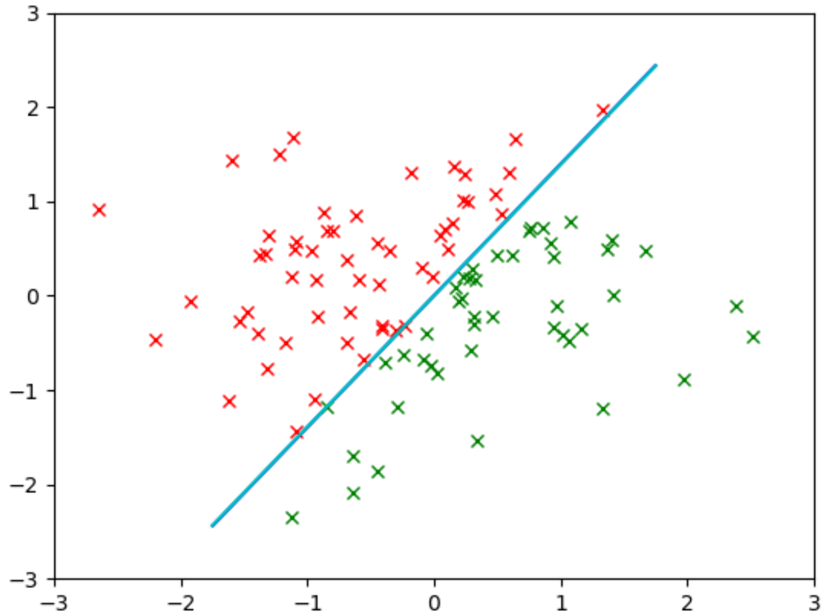
If there exists a number $\gamma > 0$ and a parameter vector $\mathbf{w},^*$ with $\|\mathbf{w}\| = 1$, such that

$$\forall n \quad t_n(\mathbf{x}_n \cdot \mathbf{w}^*) \geq \gamma \ ,$$

then the perceptron algorithm makes at most $\frac{R^2}{\gamma^2}$ errors, where $R = max_n \|\mathbf{x}_n\|$.

What if γ is Small?






```
for n in range(nIt):
  for i in range(ns):
```

- If $\mathbf{x}_n$ is correctly classified, do nothing.
- Otherwise, $\mathbf{w}_{t+1} = \mathbf{w}_t + t_n \mathbf{x}_n$.

```
for n in range(nIt):
  inds=list(range(ns))
  random.shuffle(inds)
  for i in range(inds):
```

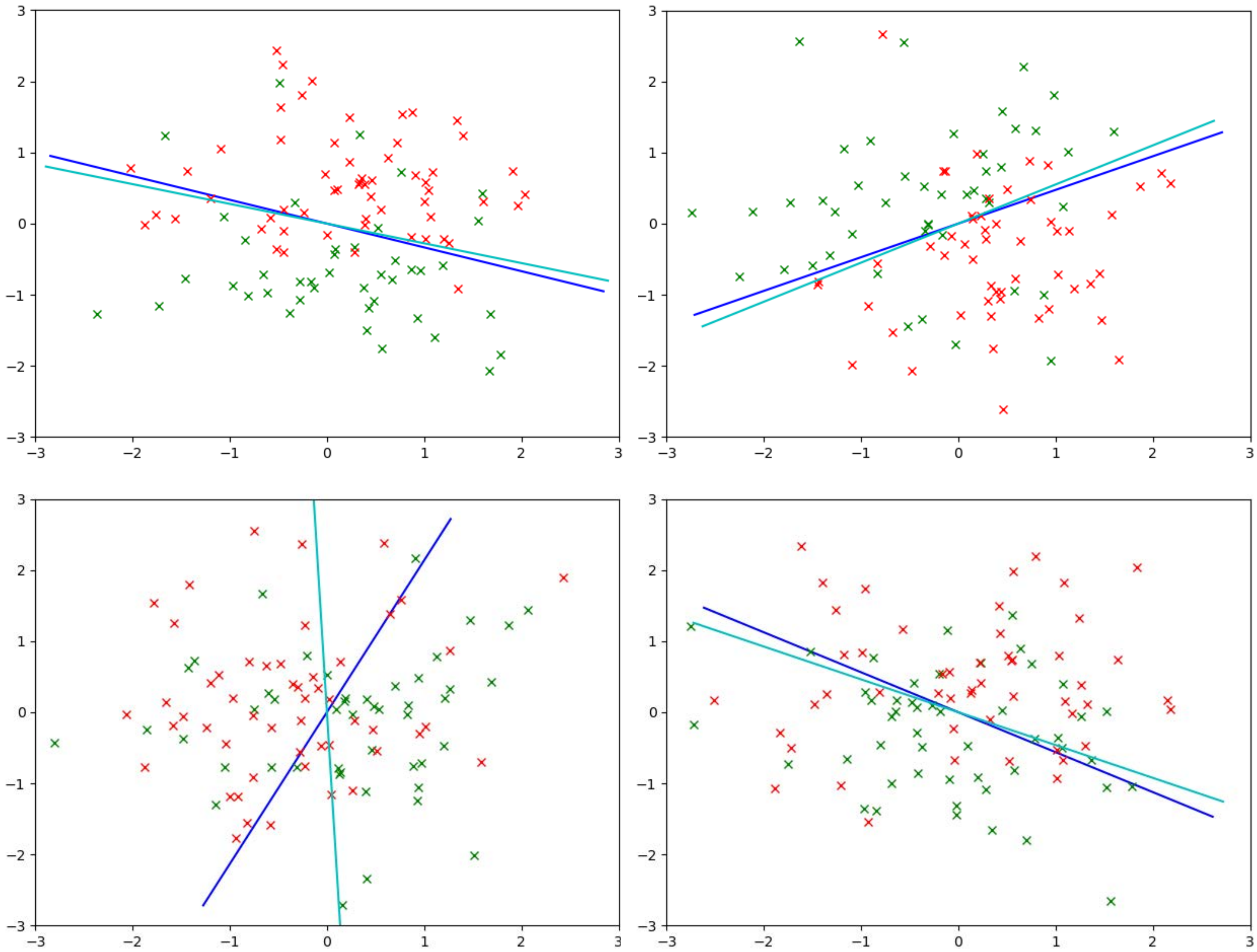
- If $\mathbf{x}_n$ is correctly classified, do nothing.
- Otherwise, $\mathbf{w}_{t+1} = \mathbf{w}_t + t_n \mathbf{x}_n$.

Randomizing helps!

What if γ Does Not Exist?

20% of outliers

30% of outliers



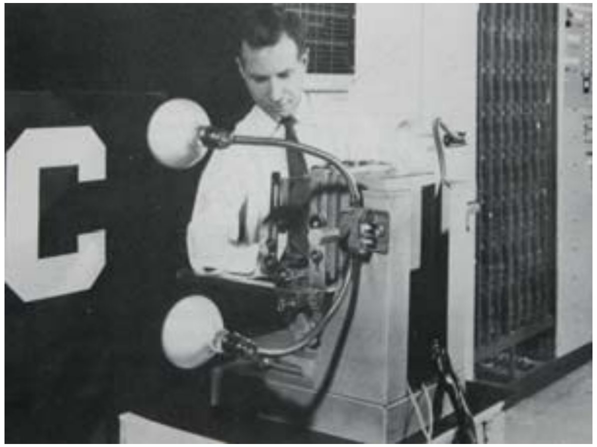
Still works up to a point but no guarantee!

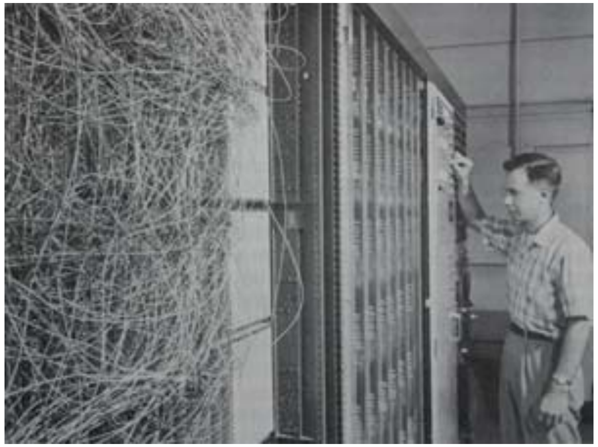
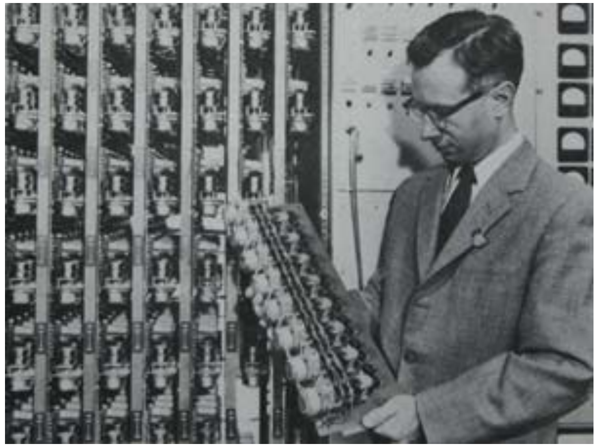
Optional: Ancient History

- The perceptron is a simple algorithm, but imagine coding it on this IBM 704, which Frank Rosenblatt used to implement it in 1957.

- There was much initial enthusiasm. But, it was later realized there were serious limitations, such as the linear separability requirement.

Optional: Dedicated Hardware (1960)



Imagine coding on that!

Optional: Python Implementation (1)

```
def perceptronRand(xs,ys,nIt=200,randP=True):
    N, D = xs.shape                # Get data shape.
    w = np.zeros(D)                # Init weights.
    for it in range(nIt):          # Train.
        allCorrect = True          # Generate indices.
        inds = np.random.permutation(N) if randP else np.arange(N)
        for i in inds:
            x = xs[i]              # Pick one sample.
            y = 2*(np.inner(x,w) > 0)-1  # Predict the label.
            if y != ys[i]:         # Misclassified.
                w += ys[i] * x     # Update weights.
                w /= np.linalg.norm(w)   # Normalize length.
                allCorrect = False # Something has changed.
        print('It {}: {}'.format(it + 1,linearAccuracy(xs, ys, w)))
        if allCorrect:
            break                  # Finish training.
    return w

def linearAccuracy(xs,ys,ws):
    return(sum(ys   == (2 * (xs @ ws >0)) - 1) * 100/len(ys))
```

Call to numpy. Mostly coded in C or Fortran.

Optional: Python Implementation (2)

```
def perceptronRand(xs,ys,nIt=200,randP=True):
    N, D = xs.shape                    # Get data shape.
    w = np.zeros(D)                    # Init weights.
    bestW = None
    bestA = 0.0
    for it in range(nIt):              # Train.
        allCorrect = True              # Generate indices.
        inds = np.random.permutation(N) if randP else np.arange(N)
        for i in inds:
            x = xs[i]                  # Pick one sample.
            y = 2*(np.inner(x,w) > 0)-1  # Predict the label.
            if y != ys[i]:             # Misclassified.
                w += ys[i] * x         # Update weights.
                w /= np.linalg.norm(w)  # Normalize length.
                allCorrect = False     # Something has changed.
                acc  = linearAccuracy(xs, ys, w)
                if(acc>bestA):
                    bestW = w
                    bestA = acc
        print('It {}: {}'.format(it + 1,bestA))
        if allCorrect:
            break                      # Finish training.
    return bestW
```

Record best solution.

Optional: JAVA Implementation

```
import org.nd4j.linalg.api.ndarray.INDArray;
import org.nd4j.linalg.factory.Nd4j;
import java.lang.Float;

class Perceptron {
    public Perceptron() {}

    public static INDArray perceptronRand(INDArray xs, INDArray ys, int nIt, boolean randP){
        long[] shape = xs.shape();                                  // Get data shape
        long N       = shape[0];
        long D       = shape[1];

        INDArray w   = Nd4j.zeros(D,1); // Init weights

        for (int it = 0; it < nIt; it++){
            boolean allCorrect = true;
            INDArray inds = Nd4j.arange(0,D);                       // Generate samples indices.

            if (randP)
                Nd4j.shuffle(inds);

            for (int i = 0; i < N; i++){
                INDArray x = xs.getRow(i);                          // Pick one sample.
                INDArray y = (x.mmul(w).gt(0)).mul(2).sub(1) ;      // Predict the label.
                if (y.data().asFloat()[0] != ys.getRow(i).data().asFloat()[0]){ // Misclassified.

                    w = x.mul(ys.getRow(i)).add(w.transpose());     // Update weights.
                    w = w.div(w.norm2().add(1e-3)).transpose();     // Unit normal length.

                    allCorrect = false;
                }
            }
            System.out.println("It " + it + ": " + linearAccuracy(xs, ys, w));
            if (allCorrect){
                break;
            }
        }
        return w;
    }

    public static String linearAccuracy(INDArray xs,INDArray ys,INDArray w){
            INDArray y = (xs.mmul(w).gt(0)).mul(2).sub(1);
            return Nd4j.sum((y.eq(ys))).div(4).toString();
    }

public class Main{
    public static void main (String[] args){

        INDArray xs      = Nd4j.create(new float[][]{{1,0},{0,1},{1,1},{0,0}});
        INDArray ys      = Nd4j.create(new float[][]{{1},{1},{1},{-1}});
        int nIt          = 200;
        boolean randP    = true;
        INDArray weights = Perceptron.perceptronRand(xs, ys, nIt, randP);
    }
}
```

More verbose!

EPFL

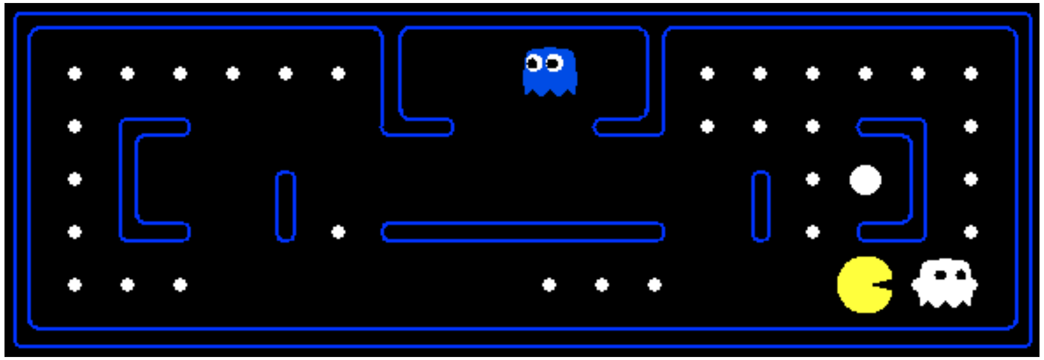
NumPy/SciPy

The time-critical loops are usually **implemented in C, C++ or Fortran**. Parts of SciPy are thin layers of code on top of the scientific routines that are freely available at http://www.netlib.org/. Netlib is a huge repository of incredibly valuable and robust scientific algorithms written in C and Fortran.

One of the design goals of NumPy was to make it buildable without a Fortran compiler, and if you don't have LAPACK available NumPy will use its own implementation. SciPy requires a Fortran compiler to be built, and **heavily depends on wrapped Fortran code**.

https://www.scipy.org/scipylib/faq.html

Optional: Pacman Apprenticeship



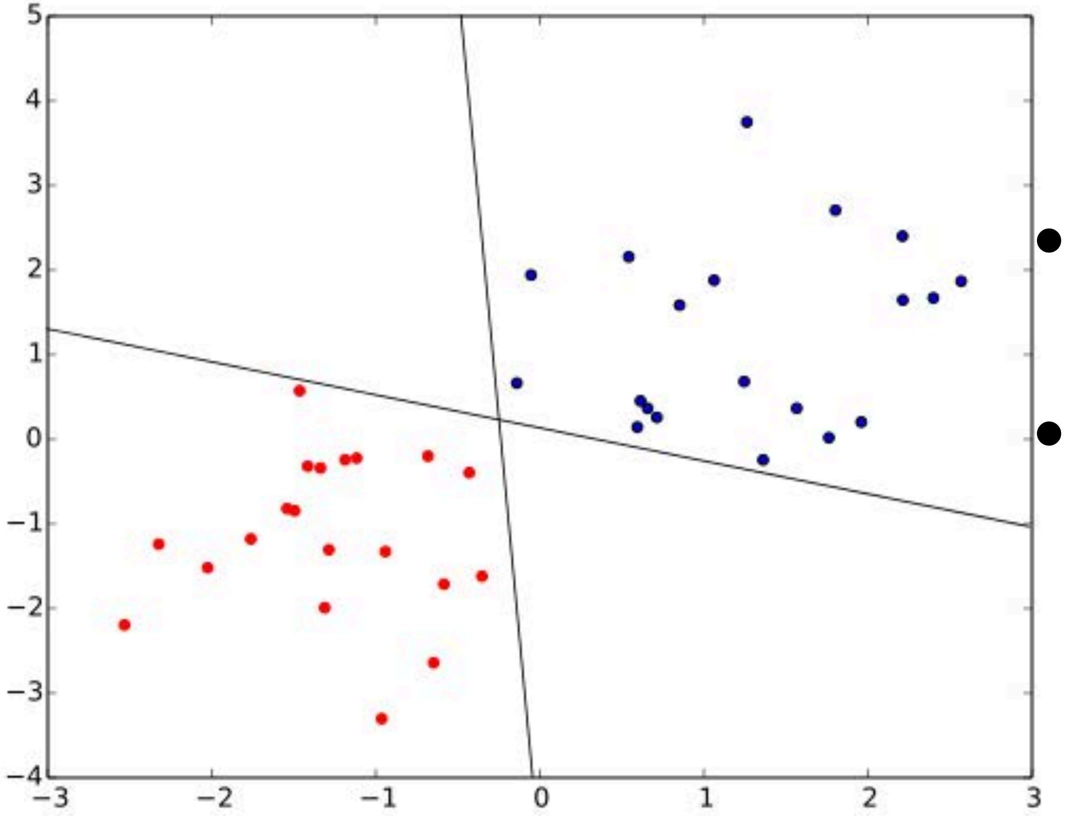
- Examples are state s.
- Correct actions are those taken by experts.
- Feature vectors defined over pairs ϕ(a,s).
- Score of a pair taken to be **w** · ϕ(a,s).
- Adjust **w** so that

$$\forall a, \mathbf{w} \cdot \phi(a^*, s) \geq \mathbf{w} \cdot \phi(a, s)$$

when a* is the correct action for state s.

http://ai.berkeley.edu/project_overview.html

The Problem with the Perceptron

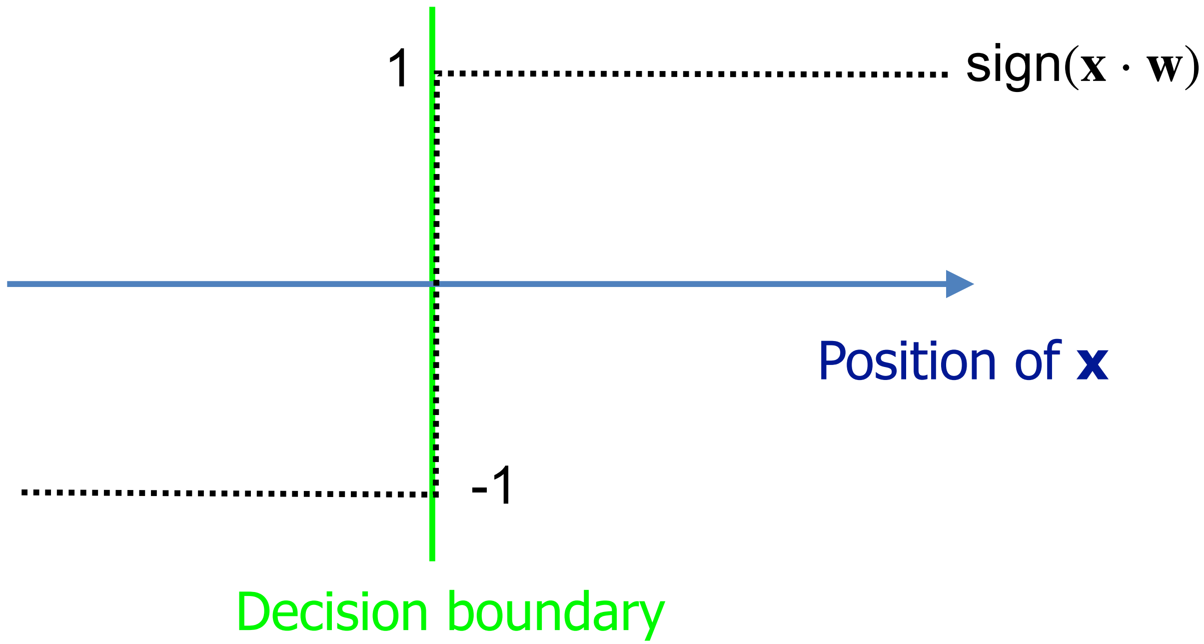


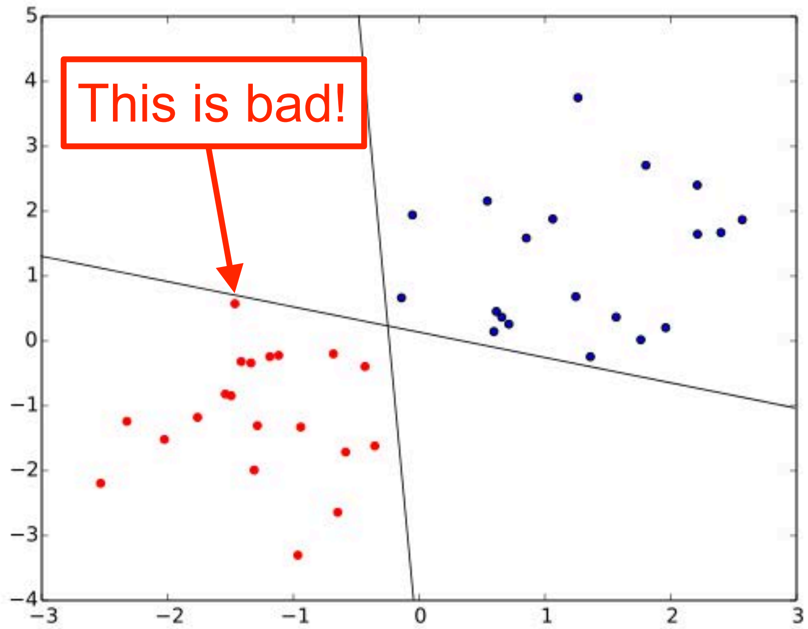
- Two different solutions among infinitely many.
- The perceptron has no way to favor one over the other.

The culprit

$$E(\tilde{\mathbf{w}}) = -\sum_{n=1}^{N} \operatorname{sign}(\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}}_n) t_n$$

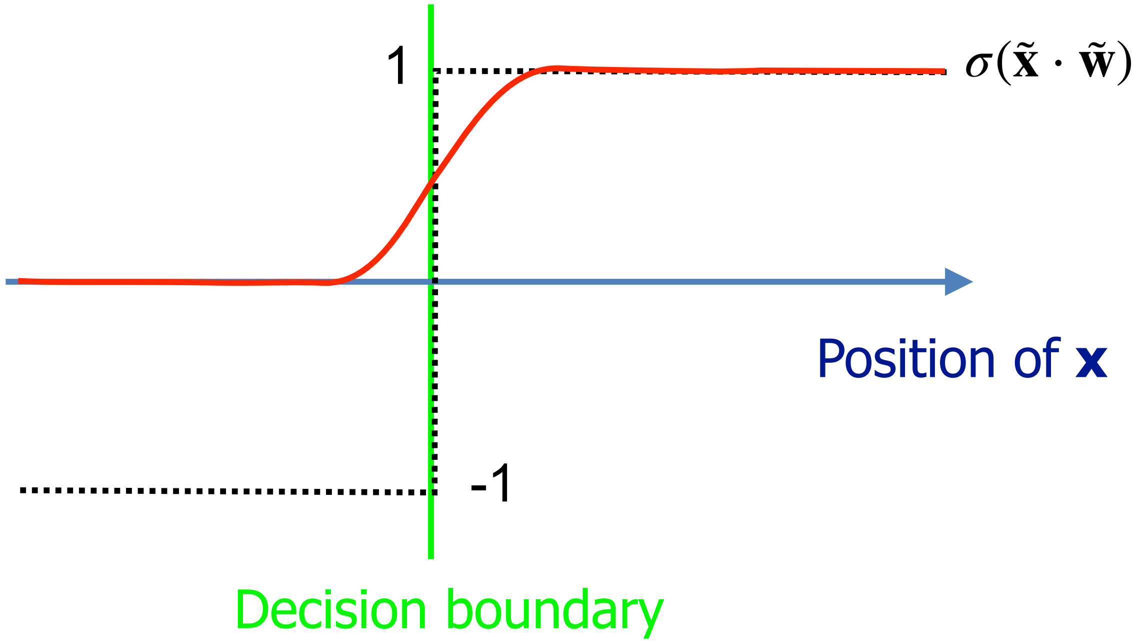
The Problem with the Perceptron





- There is no difference between close and far from the decision boundary.
- We want the positive and negative examples to be as far as possible from it.

From Perceptron to Logistic Regression



Replace the step function (black) by a smoother one (red).

- Replace the step function by a smooth function σ.
- The prediction becomes $y(\mathbf{x}; \widetilde{\mathbf{w}}) = \sigma(\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}})$.
- Given the training set $\{(\mathbf{x}_n, t_n)_{1 \leq n \leq N}\}$ where $t_n \in \{0, 1\}$, minimize the cross-entropy

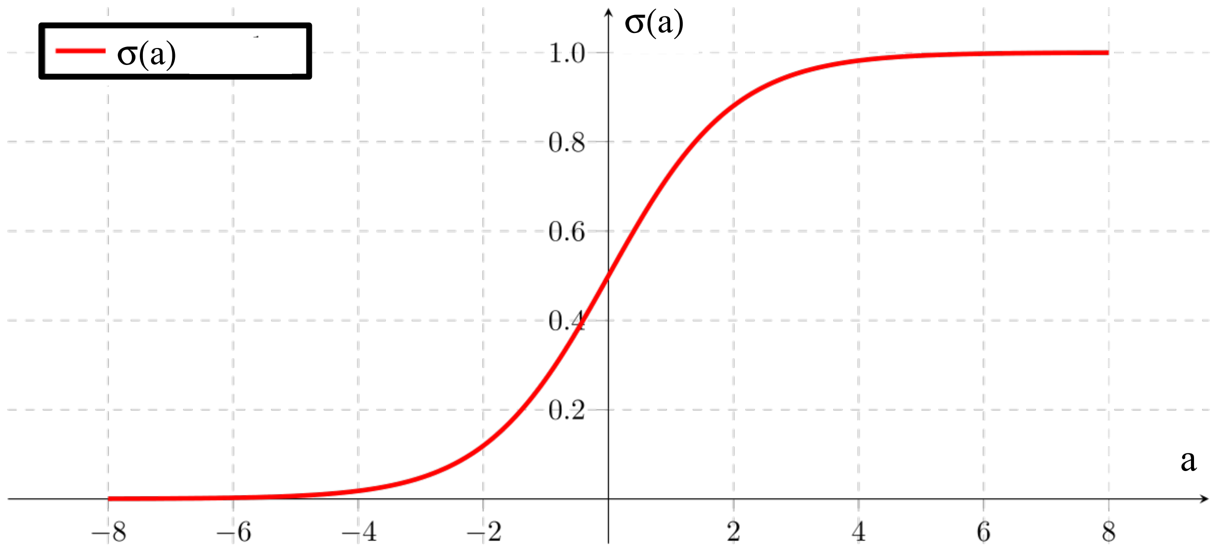
$$E(\widetilde{\mathbf{w}}) = -\sum_n \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\}$$

$$y_n = y(\mathbf{x}_n; \widetilde{\mathbf{w}})$$

This is a convex function of w!

with respect to $\widetilde{\mathbf{w}}$.

Sigmoid Function



$$\sigma(a) = \frac{1}{1 + \exp(-a)}$$

$$\frac{\partial \sigma}{\partial a} = \sigma(1 - \sigma)$$

- It is infinitely differentiable.
- Its derivatives are easy to compute.
- It is asymptotically equal to zero or one.

—> Can be understood as a smoothed step function.

Cross Entropy

$$E(\tilde{\mathbf{w}}) = -\sum_n \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\}$$

$$\nabla E(\tilde{\mathbf{w}}) = \sum_n (y_n - t_n)\tilde{\mathbf{x}}_n$$

$$y_n = \sigma(\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}}_n)$$

- $-(t_n \ln y_n + (1 - t_n)\ln(1 - y_n))$ is close to 0 if $t_n = 1$ and y_n is close to 1 or if $t_n = 0$ and y_n is close to zero. Minimizing E(**w**) encourages that.
- $-(t_n \ln y_n + (1 - t_n)\ln(1 - y_n))$ is larger if $t_n = 1$ and $y_n < 0.5$ or $t_n = 0$ and $y_n > 0.5$. Minimizing E(**w**) discourages that.
- E(**w**) is a convex function whose gradient is easy to compute.

—> The global optimum can be found very effectively.

Probabilistic Interpretation

$$y(\mathbf{x}; \tilde{\mathbf{w}}) = \sigma(\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}})$$
$$= \frac{1}{1 + \exp(-\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}})}$$

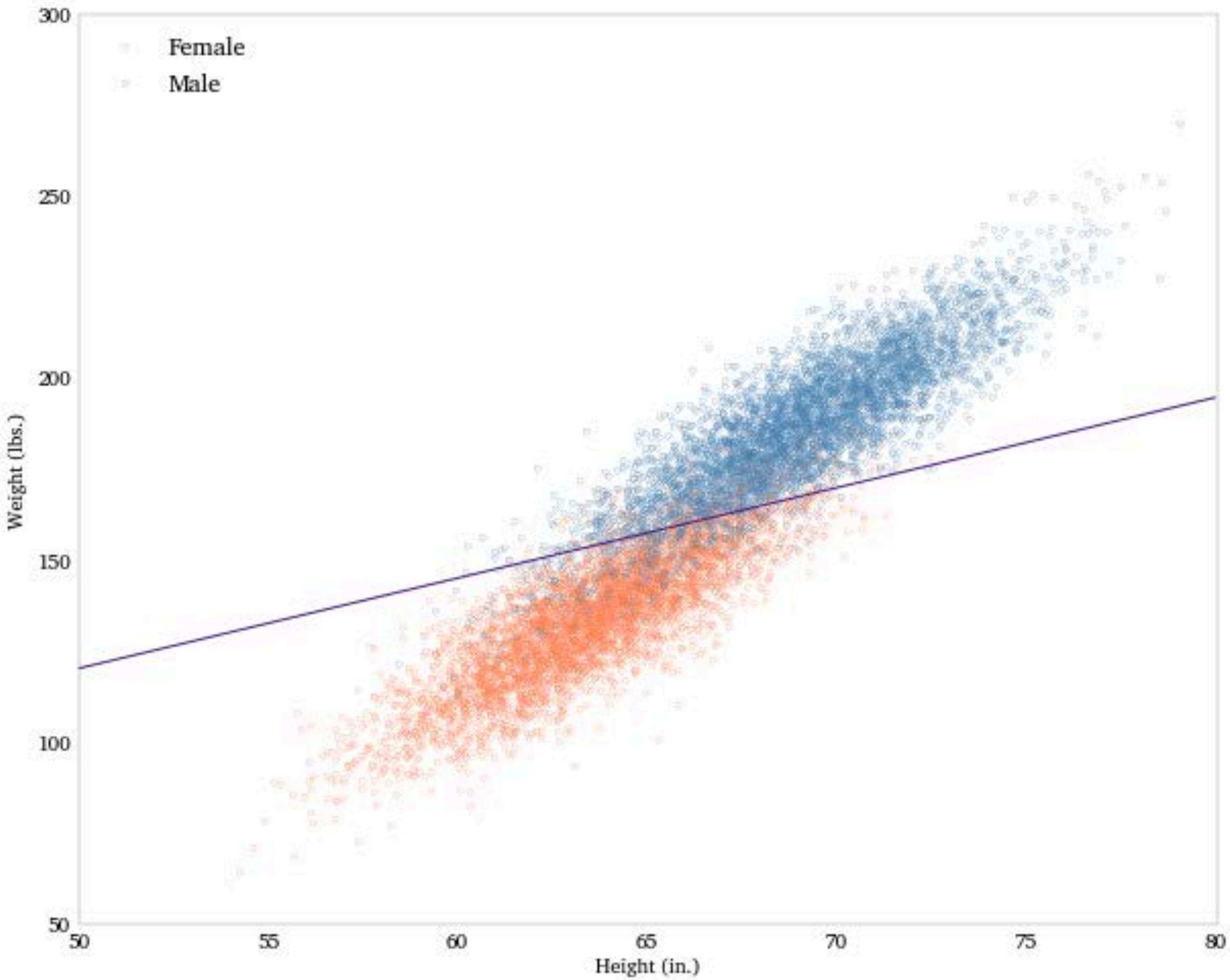
- $0 \leq y(\mathbf{x}; \mathbf{w}) \leq 1$
- $y(\mathbf{x}; \mathbf{w}) = 0.5$ if $\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}} = 0$, i.e. $\mathbf{x}$ is on the decision boundary.
- $y(\mathbf{x}; \mathbf{w}) = 0.0$ or 1.0 if $\mathbf{x}$ far from the decision boundary.

$\Rightarrow y(\mathbf{x}; \tilde{\mathbf{w}})$ can be interpreted as the probability that x belongs to one class or the other.

Logistic regression finds what is called the **maximum likelihood solution** under the assumption that the noise is Gaussian.

Bishop, Chapter 4.3.2.

Example



- The algorithm does the best it can.
- Some samples can be misclassified.

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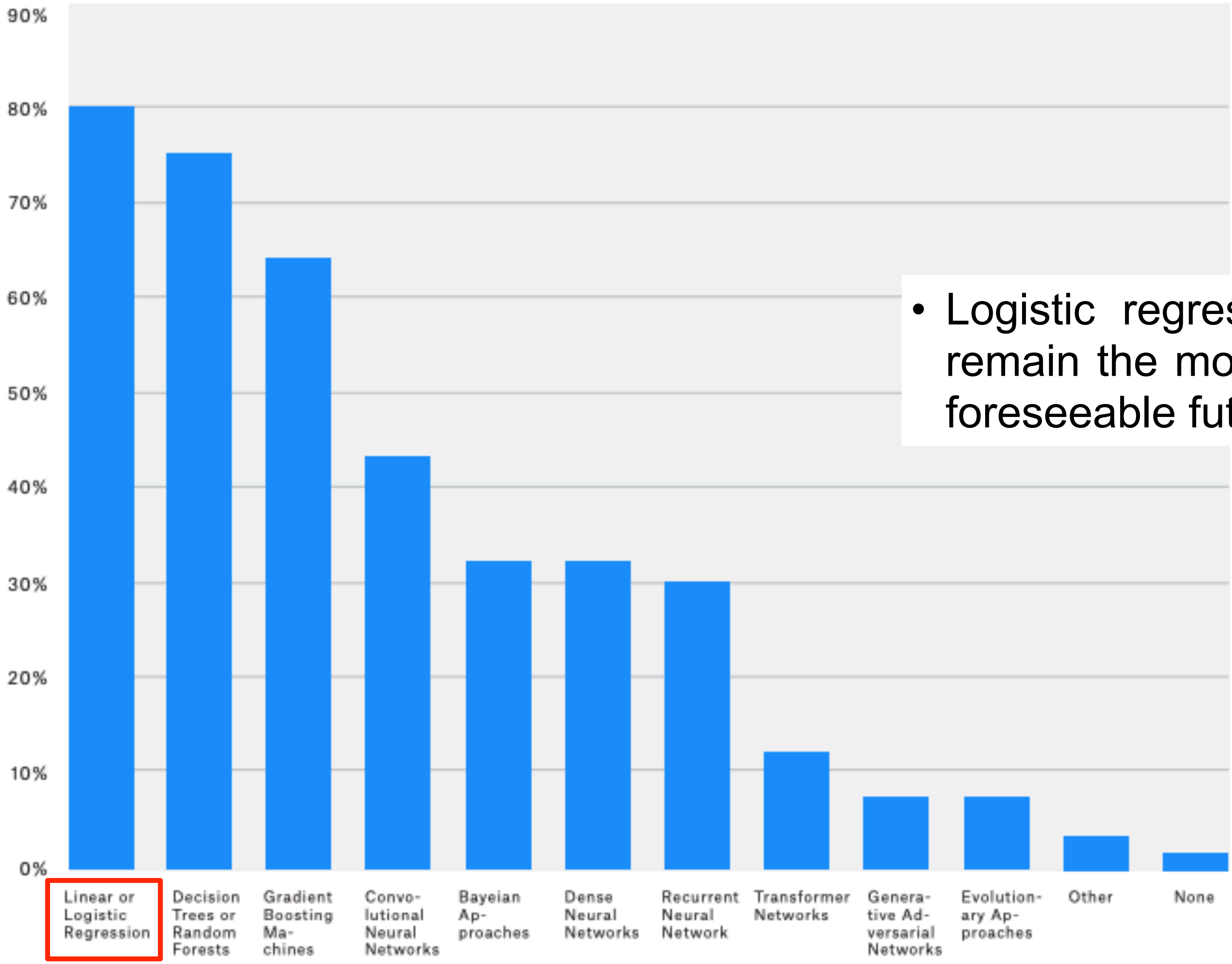
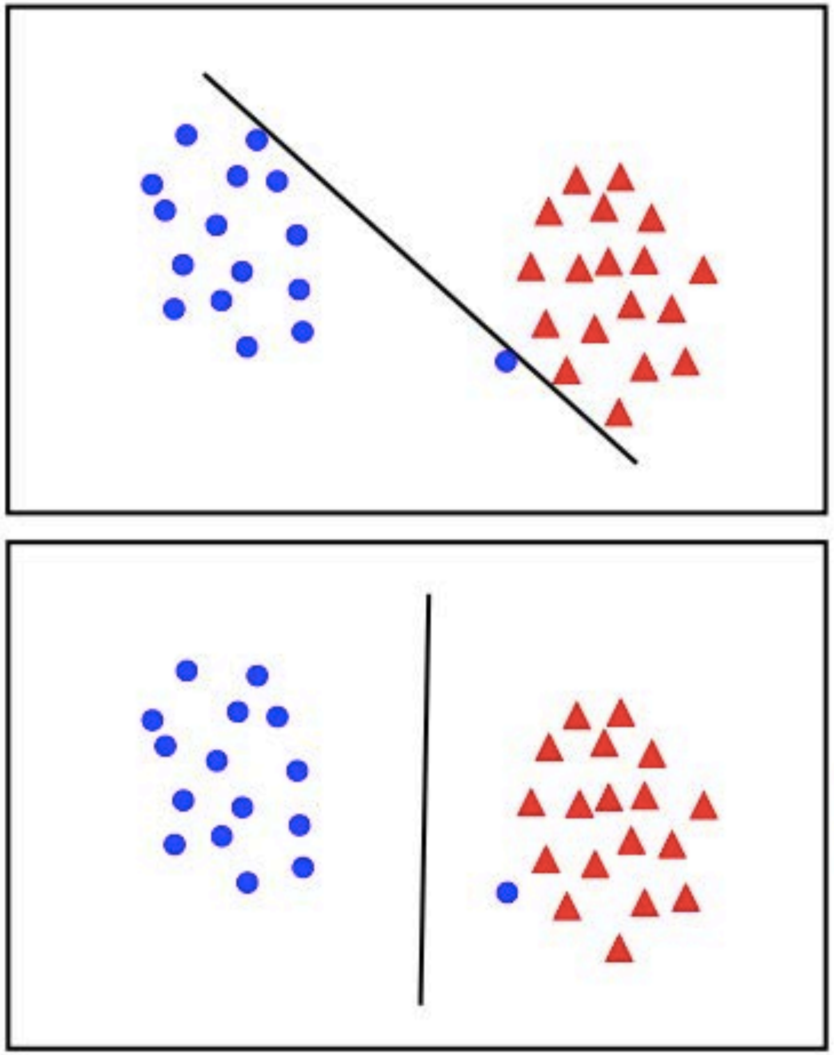
Kaggle Survey (2019)



- Logistic regression is and is likely to remain the most used technique for the foreseeable future.

What data science methods do you use at work?

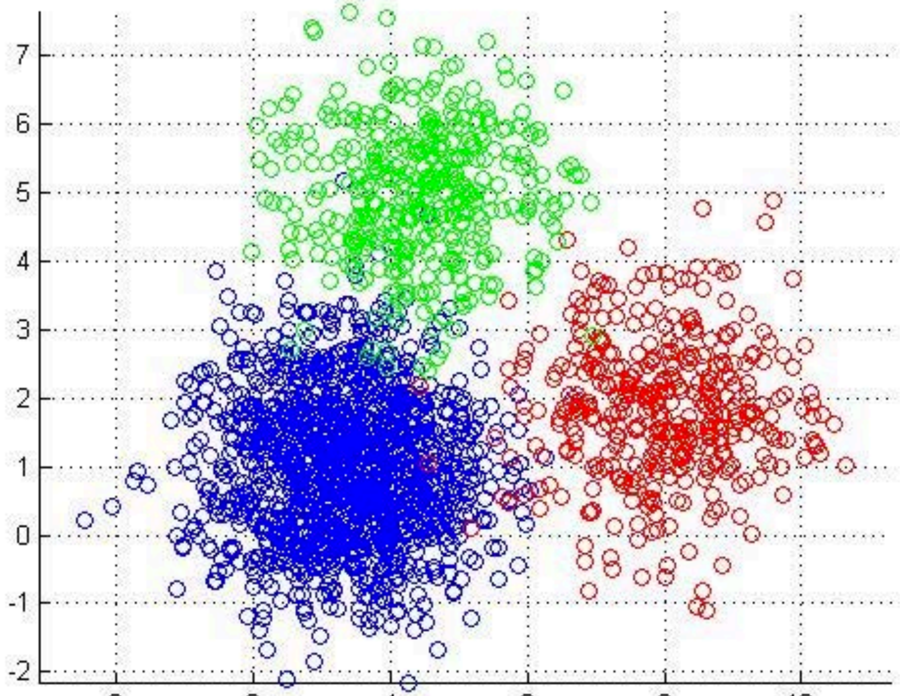
Outliers Can Cause Problems

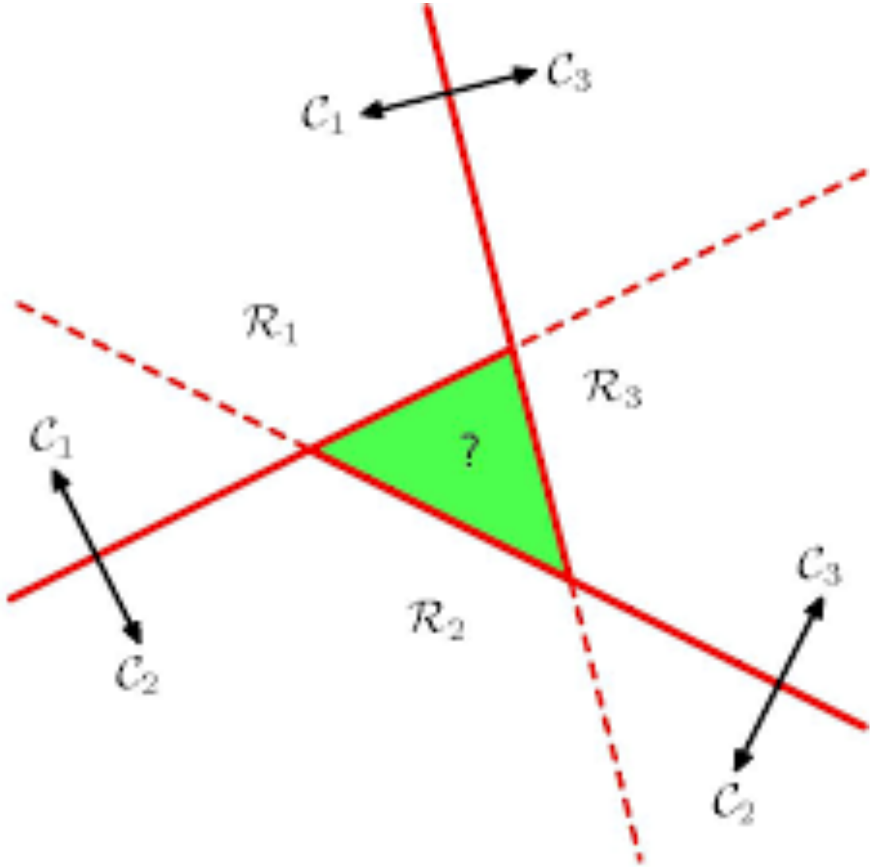


- Logistic regression tries to minimize the error-rate at training time.
- Can result in poor classification rates at test time.

—> We will talk about ways to prevent this in the next lecture.

From Binary to Multi-Class

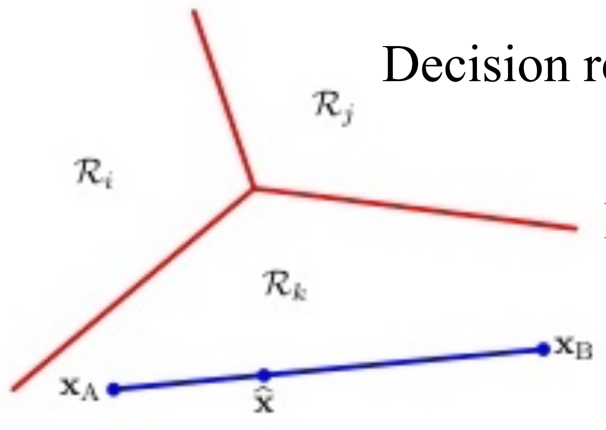




- k classes.
- Simply using k (k-1)/2 binary classifiers results in ambiguities.

Bishop, Chapter 4.1.2

Linear Discriminant



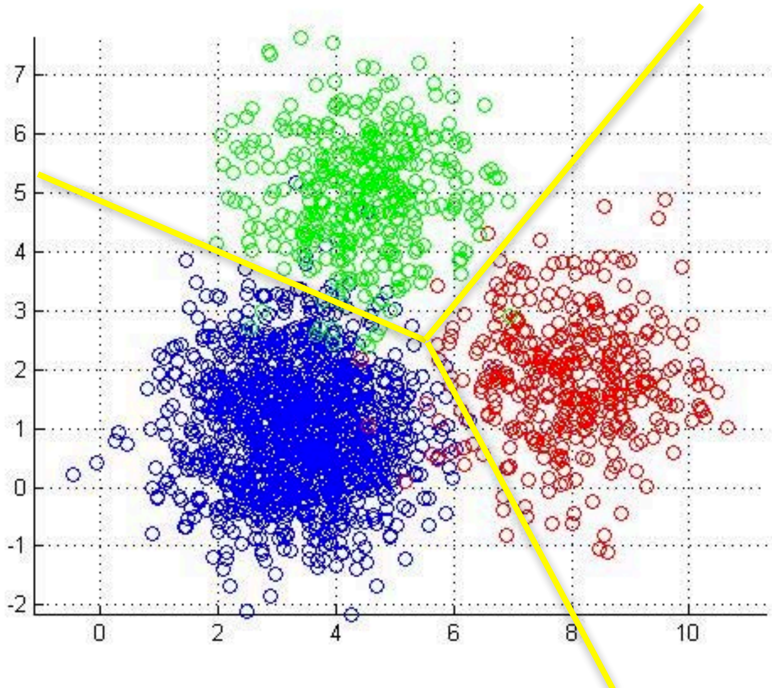
Given K linear classifiers of the form $y_k(\mathbf{x}) = \tilde{\mathbf{w}}_k \cdot \tilde{\mathbf{x}}$:

- Decision boundaries $y_k(\mathbf{x}) = y_l(\mathbf{x}) \Leftrightarrow (\tilde{\mathbf{w}}_\mathbf{k} - \tilde{\mathbf{w}}_\mathbf{l}) \cdot \tilde{\mathbf{x}} = 0.$
- These boundaries define decision regions.
- Decision regions are convex:

$$(\tilde{\mathbf{w}}_k - \tilde{\mathbf{w}}_l) \cdot \tilde{\mathbf{x}}_A > 0$$
$$(\tilde{\mathbf{w}}_k - \tilde{\mathbf{w}}_l) \cdot \tilde{\mathbf{x}}_B > 0$$
$$\Rightarrow \forall \lambda \in [0,1], \text{ if } \mathbf{x} = \lambda \mathbf{x}_A + (1-\lambda)\mathbf{x}_B, \text{ then}$$
$$(\tilde{\mathbf{w}}_k - \tilde{\mathbf{w}}_l) \cdot \tilde{\mathbf{x}} > 0$$

In other words, if two points are on the same side of a decision boundary so are all point between them.

Multi-Class Linear Classification



- K linear classifiers of the form $y^k(\mathbf{x}) = \tilde{\mathbf{w}}_k \cdot \tilde{\mathbf{x}} = \mathbf{w}_k^T \mathbf{x}$.
- Assign x to class k if $y^k(\mathbf{x}) > y^l(\mathbf{x}) \forall l \neq k$.

$$k = \arg\max_j \tilde{\mathbf{w}}_j^T \tilde{\mathbf{x}}$$

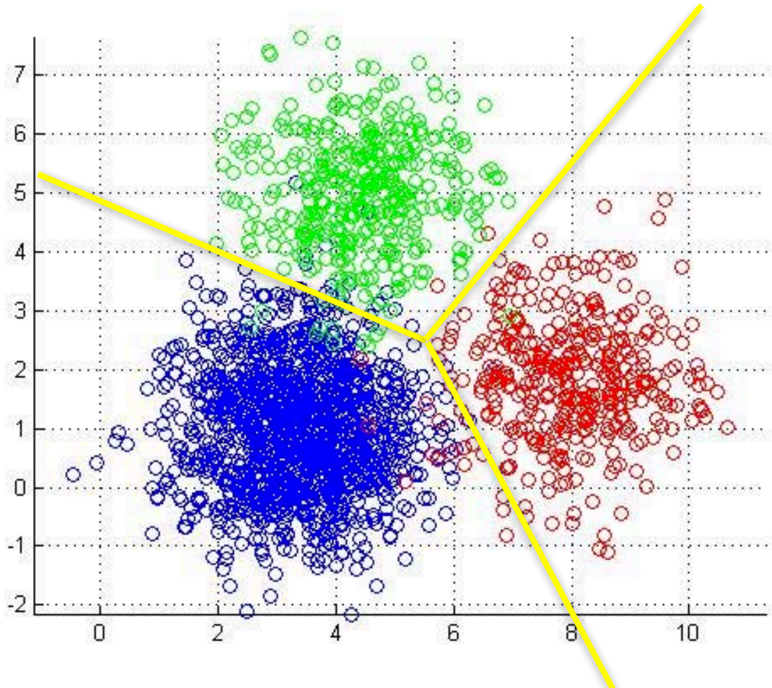
—> This still is a linear classification problem but in a space of dimension K times the dimension of the original one, 6 in this example.

$$\begin{bmatrix} y_1 \\ \vdots \\ y_K \end{bmatrix} = \begin{bmatrix} \tilde{\mathbf{w}}_1^T \\ \vdots \\ \tilde{\mathbf{w}}_K^T \end{bmatrix} \tilde{\mathbf{x}}$$

Vector of dimension K times the dimension of $\tilde{\mathbf{w}}$.

$$k = \arg\max_j y_j$$

Multi-Class Logistic Regression



- K linear classifiers of the form $y^k(\mathbf{x}) = \sigma(\mathbf{w}_k^T \mathbf{x})$.
- Assign x to class k if $y^k(\mathbf{x}) > y^l(\mathbf{x}) \forall l \neq k$.

$$k = \arg\max_j y_k(\mathbf{x})$$

$$\begin{bmatrix} y_1 \\ \vdots \\ y_K \end{bmatrix} = \begin{bmatrix} \tilde{\mathbf{w}}_1^T \\ \vdots \\ \tilde{\mathbf{w}}_K^T \end{bmatrix} \tilde{\mathbf{x}}$$

$$k = \arg\max_j y_j$$

- Because the sigmoid function is monotonic, the formulation is almost unchanged.
- Only the objective function being minimized need to be reformulated.

Multi-Class Cross Entropy

Let the training set be $\{(\mathbf{x}_n, [t_n^1, \ldots, t_n^K])_{1 \leq n \leq N}\}$ where $t_n^k \in \{0,1\}$ is the probability that sample $\mathbf{x}_n$ belongs to class k.

Activation: $$a^k(\mathbf{x}) = \sigma(\mathbf{w}_k^T \mathbf{x})$$

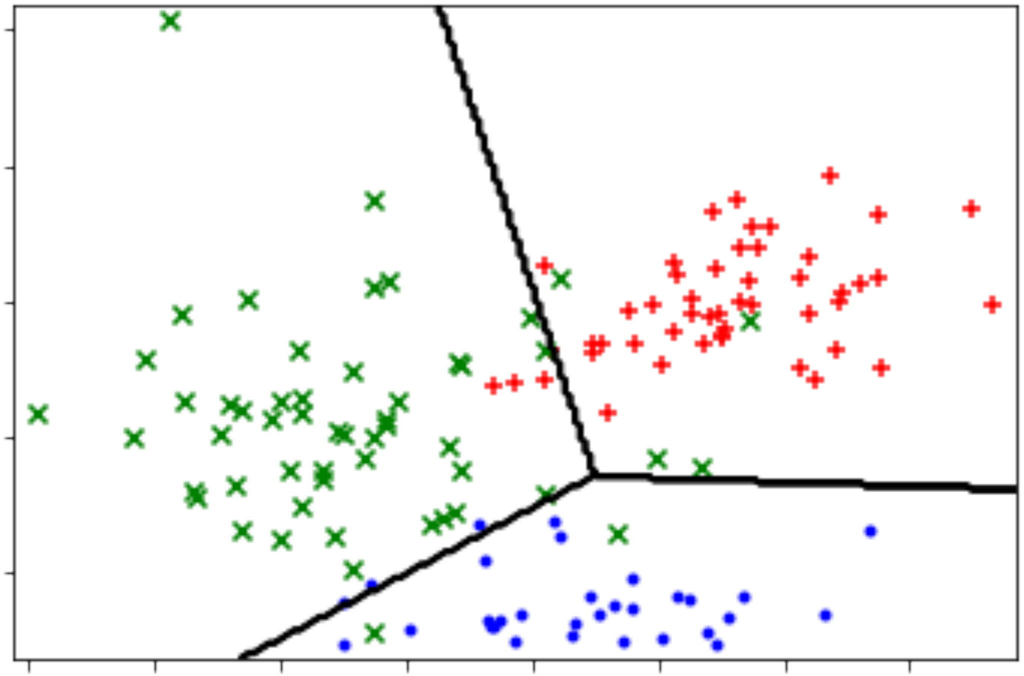
Probability that $\mathbf{x}$ belongs to class k: $$y^k(\mathbf{x}) = \frac{\exp(a^k(\mathbf{x}))}{\sum_j \exp(a^j(\mathbf{x}))}$$

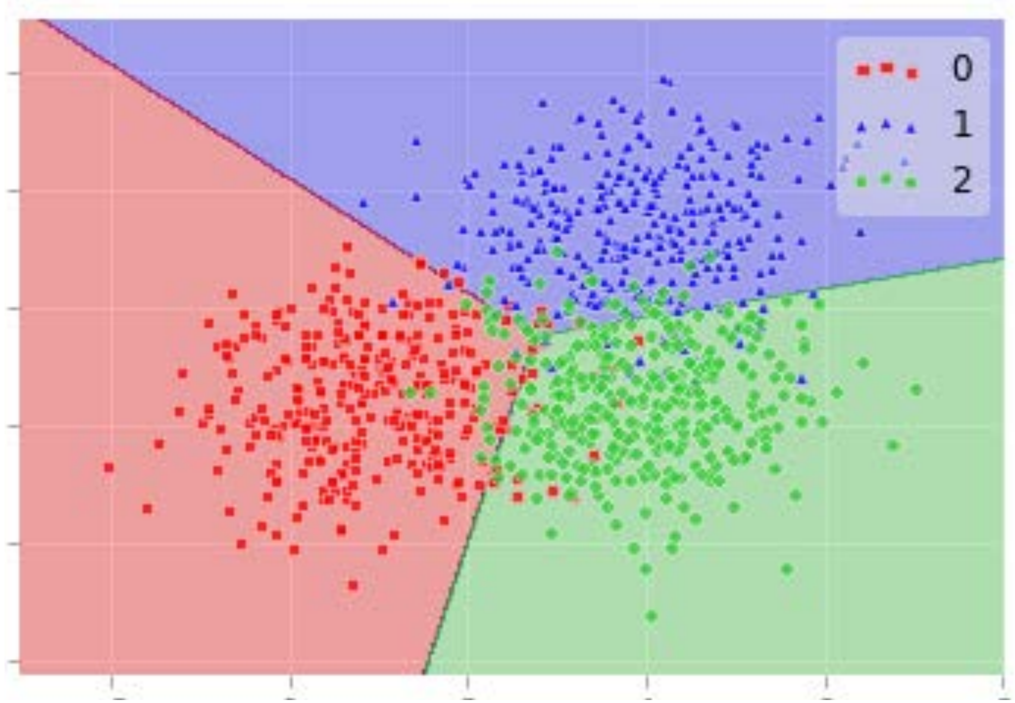
Multi-class entropy: $$E(\tilde{\mathbf{w}}_1, \ldots, \tilde{\mathbf{w}}_K) = -\sum_n \sum_k t_n^k \ln(y^k(\mathbf{x}_n))$$

Gradient of the entropy: $$\nabla E_{\mathbf{w_j}} = \sum_n (y^k(\mathbf{x}_n) - t_n^k)\mathbf{x}_n$$

- This is a natural extension of the binary case.
- The multi-class entropy is still convex and its gradient is easy to compute.

Multi-Class Results





Multiclass logistic regression is a very natural extension of binary logistic regression and has many of the same properties.