

# Lecture 3: Linear Models II

André Martins, Chrysoula Zerva, Mário Figueiredo



Deep Learning Course, Winter 2024-2025

# Today's Roadmap

- Logistic regression
- Regularization and optimization
- Stochastic gradient descent.

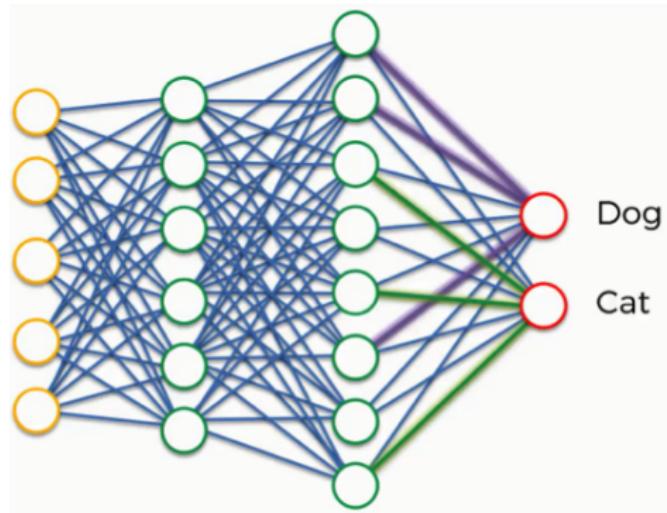
# Why Linear Classifiers?

We know the course title promised “deep”, ...

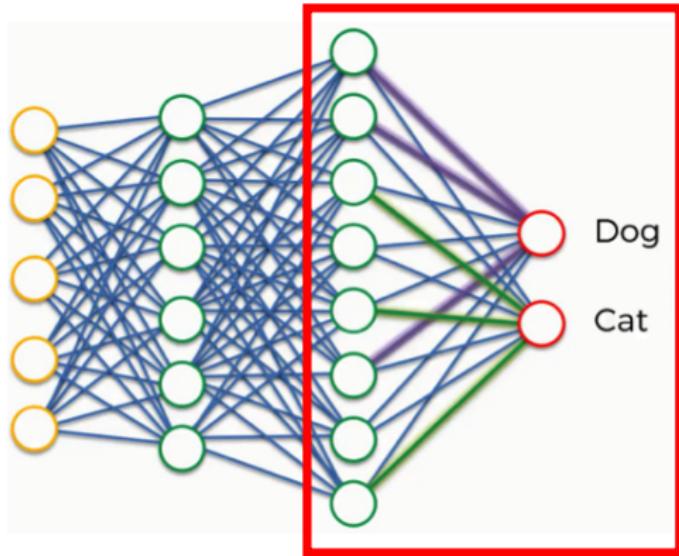
...but (as explained in Lecture 2):

- The underlying machine learning concepts are the same
- The theory (statistics and optimization) are much better understood
- Linear classifiers still widely used (very effective when data is scarce)
- Linear classifiers are **a component of neural networks.**

# Linear Classifiers and Neural Networks

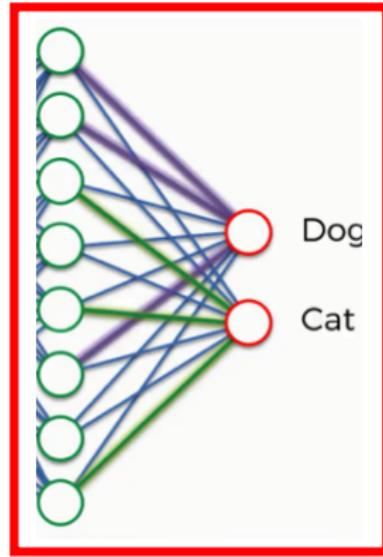


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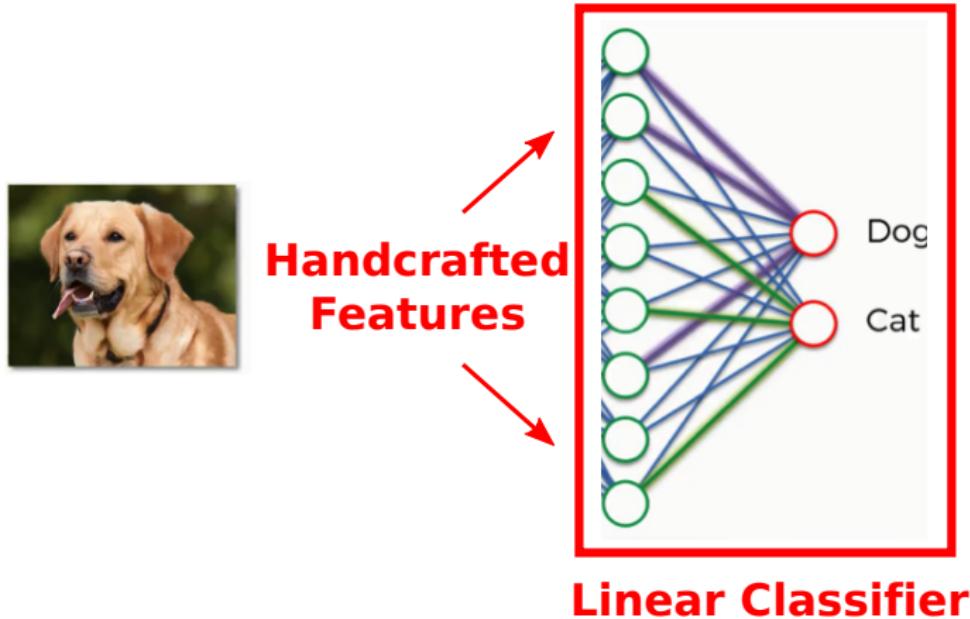
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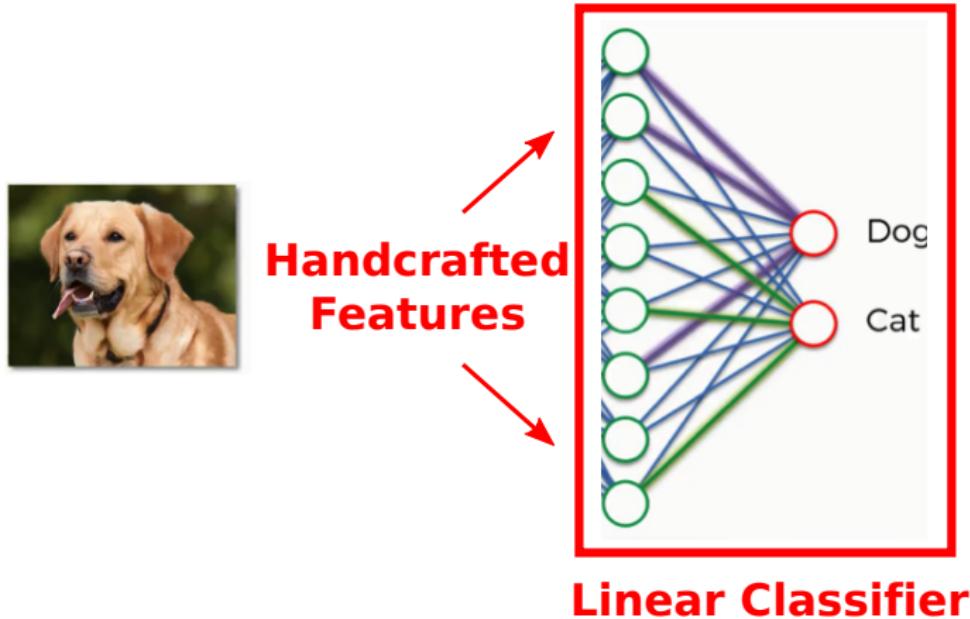


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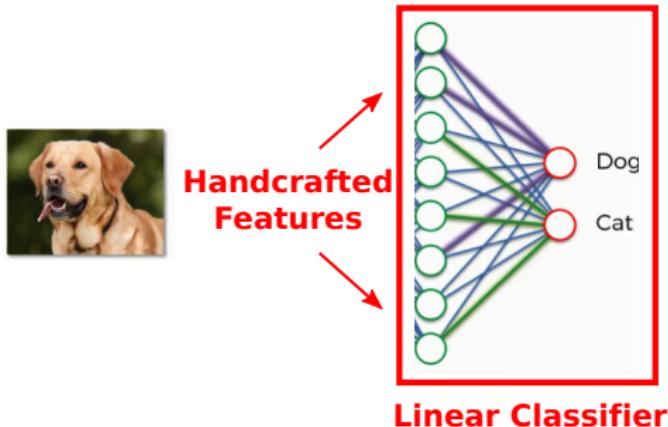


# Linear Classifiers and Neural Networks



...in fact, these may also be **learned features**, from all the previous layers of some **deep neural network**.

## Reminder: Linear Classifier

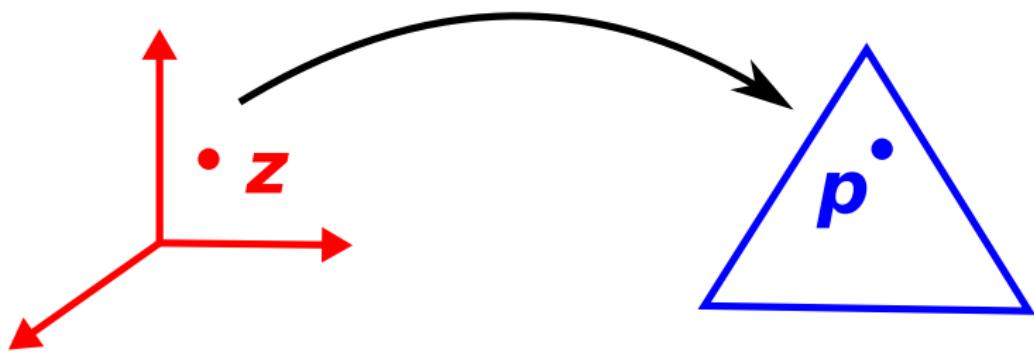


$$\hat{y} = \arg \max_y ((\mathbf{W}\phi(x))_y), \quad \mathbf{W} = \begin{bmatrix} w_1^T \\ \vdots \\ w_{|\mathcal{Y}|}^T \end{bmatrix}$$

As before, assume  $\phi_0(x) = 1$ , absorbing the bias terms.

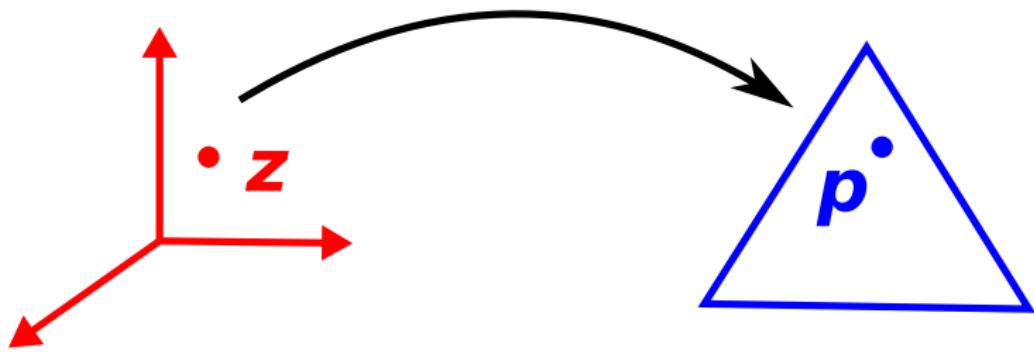
## Key Problem

Mapping from a vector of scores  $\mathbb{R}^{|Y|}$  to a probability distribution over  $Y$ ?



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We will see an important mapping: softmax (next).

# Outline

- ① Logistic Regression
- ② Regularization
- ③ Non-Linear Classifiers

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The decision boundaries are still hyperplanes w.r.t.  $\phi(x)$ .

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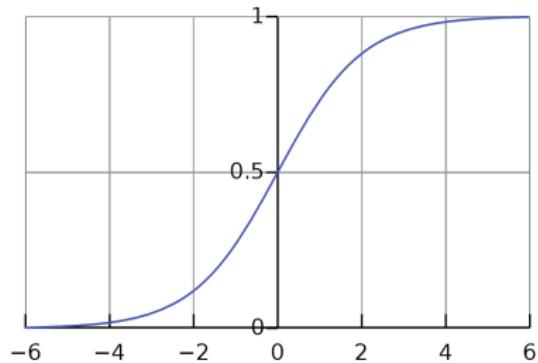
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This is called a **sigmoid transformation**.

# Sigmoid Transformation

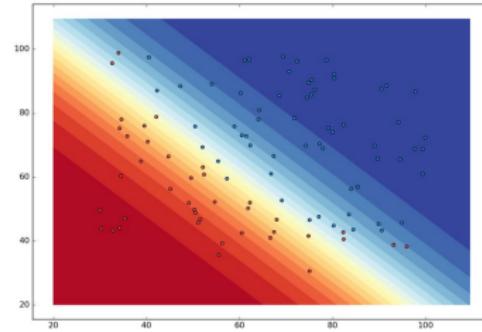
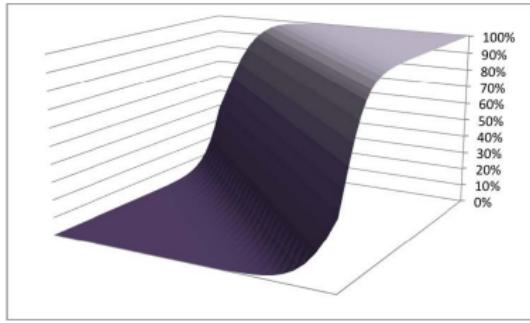
$$\sigma(u) = \frac{e^u}{1 + e^u}$$



- Widely used in neural networks.
- Maps  $\mathbb{R}$  into  $[0, 1]$ .
- The output can be interpreted as a probability.
- Positive, bounded, strictly increasing.

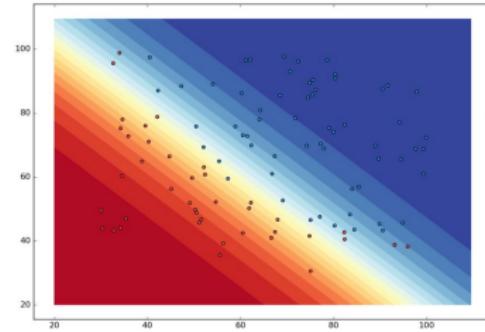
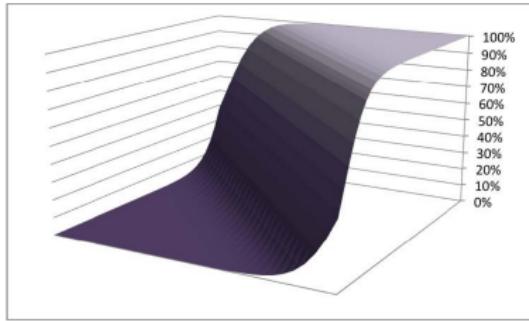
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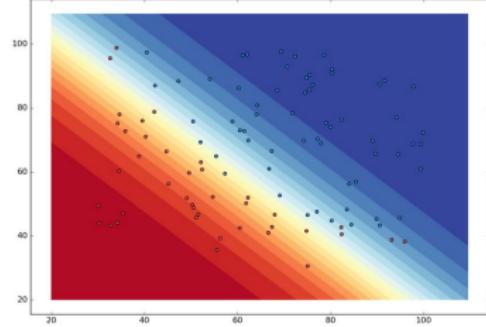
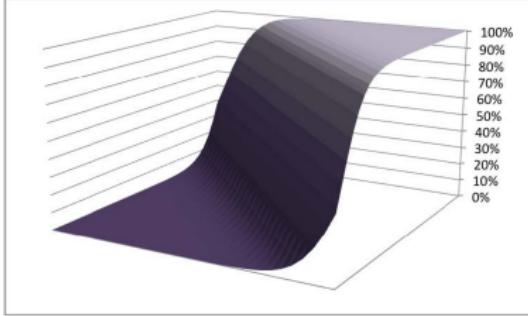
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- Some other threshold,  $P(y = +1 | x) = \tau \Leftrightarrow \mathbf{w}^T \phi(x) = \log(\frac{\tau}{1-\tau})$ ; linear w.r.t.  $\phi(x)$ .

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- Maximize the **conditional log-likelihood** of training data:

$$\begin{aligned}\widehat{\mathbf{W}} &= \arg \max_{\mathbf{W}} \log \left( \prod_{t=1}^N P_{\mathbf{W}}(y_t | x_t) \right) \\ &= \arg \min_{\mathbf{W}} - \sum_{t=1}^N \log P_{\mathbf{W}}(y_t | x_t) \\ &= \arg \min_{\mathbf{W}} \sum_{t=1}^N \left( \underbrace{\log \sum_{y'} \exp(w_{y'}^T \phi(x_t))}_{Z_{x_t}} - w_{y_t}^T \phi(x_t) \right),\end{aligned}$$

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- i.e., choose  $\mathbf{W}$  to maximize the probability of the true labels.

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- This objective function is **strictly convex**.
- Proof left as exercise! (hint, compute the Hessian).
- Therefore, any local minimum is a global minimum.
- No closed-form solution; many numerical methods have been proposed
  - ✓ Gradient methods (gradient descent, conjugate gradient).
  - ✓ Quasi-Newton methods (L-BFGS, ...).

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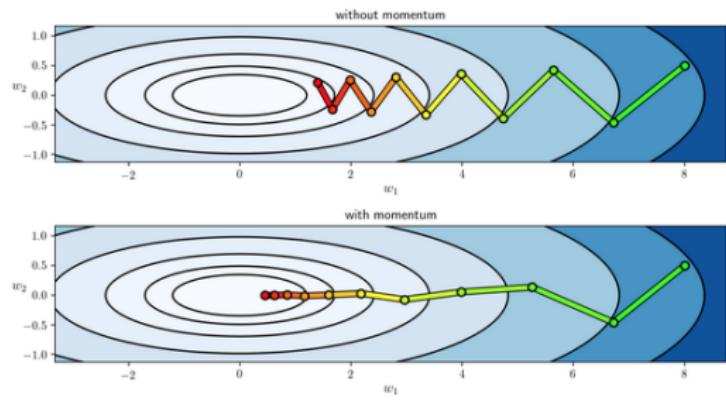
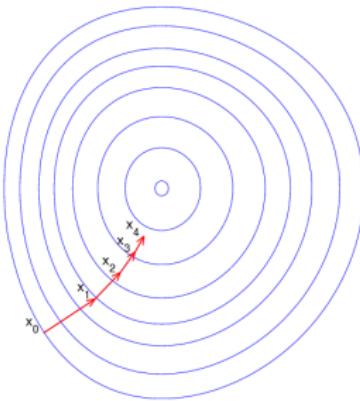
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- Choosing the **step-size**: crucial for convergence and performance.
- GD may work well, or not so well. There are many ways to improve it.



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- $L(\mathbf{W})$  convex  $\Rightarrow$  gradient descent will reach the global optimum  $\mathbf{W}$ , with appropriate choice of step-size  $\eta_k$ .

## Stochastic Gradient Descent

Monte Carlo approximation of the gradient (more frequent updates, convenient with large datasets):

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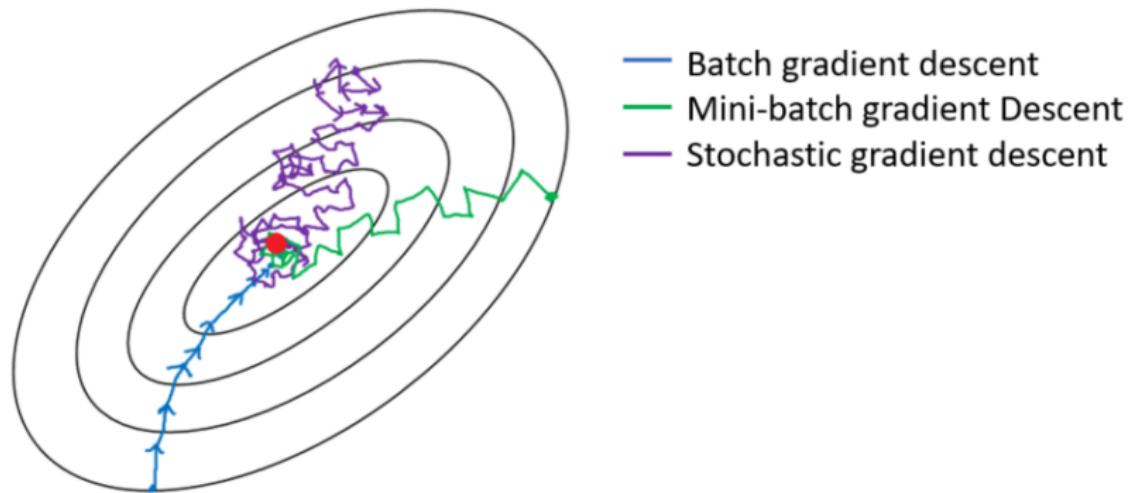
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- Variant between GD and SGD: mini-batch (pick  $B$ , rather than 1 pair)
- All guaranteed to find the optimal  $\mathbf{W}$  (for suitable step sizes)

# Stochastic vs Batch Gradient Descent



## Computing the Gradient

- We need to compute  $\nabla_{\mathbf{W}} L(\mathbf{W}; (x_t, y_t))$ , where

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- One-hot vector representation of class  $y$ :

$$\mathbf{e}_y = [0, \dots, 0, 1, 0, \dots, 0]^T, \quad \text{1 in } y\text{-th position}$$

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$$\begin{aligned}\nabla L(\mathbf{W}; (x, y)) &= \nabla \left( \log \sum_{y'} \exp(\mathbf{w}_{y'}^T \phi(x)) - \mathbf{w}_y^T \phi(x) \right) \\ &= \nabla \log \sum_{y'} \exp(\mathbf{w}_{y'}^T \phi(x)) - \nabla \mathbf{w}_y^T \phi(x) \\ &= \frac{1}{\sum_{y'} \exp(\mathbf{w}_{y'}^T \phi(x))} \sum_{y'} \nabla \exp(\mathbf{w}_{y'}^T \phi(x)) - \mathbf{e}_y \phi(x)^T \\ &= \frac{1}{Z_x} \sum_{y'} \exp(\mathbf{w}_{y'}^T \phi(x)) \nabla \mathbf{w}_{y'}^T \phi(x) - \mathbf{e}_y \phi(x)^T \\ &= \sum_{y'} \frac{\exp(\mathbf{w}_{y'}^T \phi(x))}{Z_x} \mathbf{e}_{y'} \phi(x)^T - \mathbf{e}_y \phi(x)^T \\ &= \sum_{y'} P_{\mathbf{W}}(y' | x) \mathbf{e}_{y'} \phi(x)^T - \mathbf{e}_y \phi(x)^T \\ &= \left( \begin{bmatrix} P_{\mathbf{W}}(1 | x) \\ \vdots \\ P_{\mathbf{W}}(|\mathcal{Y}| | x) \end{bmatrix} - \mathbf{e}_y \right) \phi(x)^T.\end{aligned}$$

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- Run gradient descent, or another gradient-based algorithm, using

$$\nabla L(\mathbf{W}; (x, y)) = \sum_{y'} P_{\mathbf{W}}(y'|x) e_{y'} \phi(x)^{\top} - e_y \phi(x)^{\top}$$

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$$\mathbf{W}^{(k+1)} = \mathbf{W}^{(k)} + \eta_k \left( \mathbf{e}_y \phi(x)^\top - \sum_{y'} P_w(y'|x) \mathbf{e}_{y'} \phi(x)^\top \right)$$

- The **perceptron** is also **discriminative**, but non-probabilistic classifier
  - ✓ perceptron's updates look like

$$\mathbf{W}^{(k+1)} = \mathbf{W}^{(k)} + \mathbf{e}_y \phi(x)^\top - \mathbf{e}_{\hat{y}} \phi(x)^\top$$

- SGD updates for logistic regression and the perceptron look similar!

## Other Options: Maximizing Margin

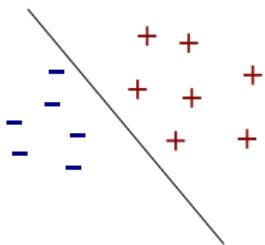
- For a training set  $\mathcal{D} = \{(x_t, y_t), t = 1, \dots, N\}$
- Margin achieved by a weight matrix  $\mathbf{W}$ : smallest  $\gamma$  such that, for every training instance  $(x_t, y_t) \in \mathcal{D}$ ,

$$w_{y_t}^T \phi(x_t) \geq w_{y'}^T \phi(x_t) + \gamma, \quad \text{for any } y' \neq y_t$$

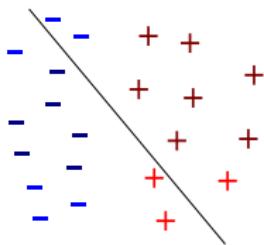
- i.e., score of the correct label is at least  $\gamma$  higher than that of any other label.

# Margin

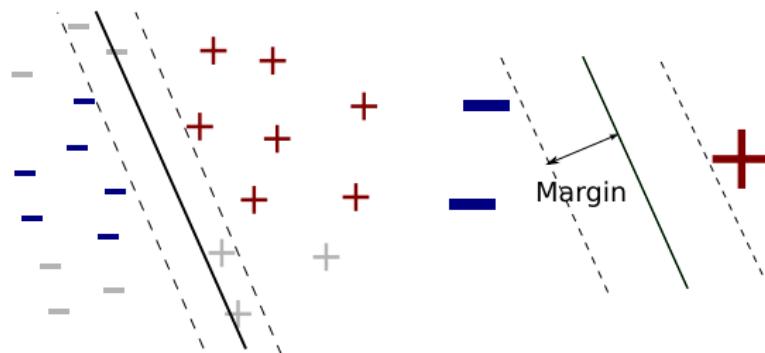
Training



Testing



Denote the value of the margin by  $\gamma$



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  - ✓ However, the perceptron **does not** pick  $\mathbf{W}$  to maximize the margin!
  - ✓ **Support vector machines** (SVM) do exactly this (not covered)

# Summary

## What we saw:

- Linear Classifiers
  - ✓ Logistic regression
  - ✓ Perceptron
  - ✓ Support vector machines (not covered)

## Next:

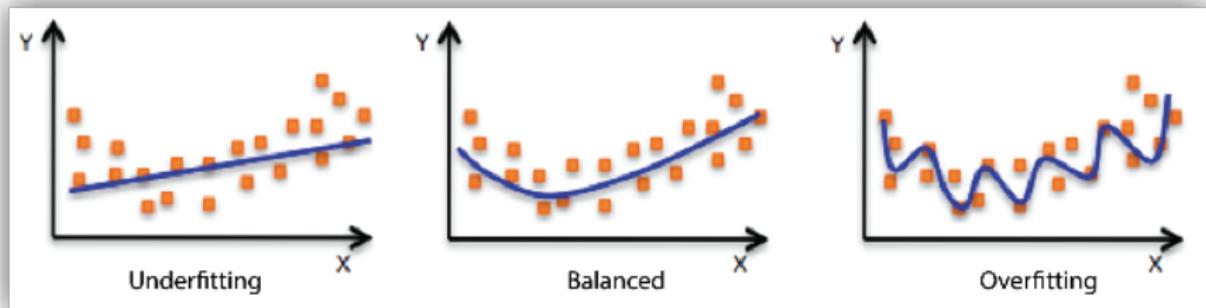
- Regularization
- Softmax
- Non-linear classifiers

# Outline

- ① Logistic Regression
- ② Regularization
- ③ Non-Linear Classifiers

# Overfitting

If the model is too complex (too many parameters) and the data is scarce, we run the risk of **overfitting**:



# Regularization

In practice, we **regularize** to prevent overfitting

$$\arg \min_{\mathbf{W}} \sum_{t=1}^N L(\mathbf{W}; (x_t, y_t)) + \lambda \Omega(\mathbf{W}),$$

$\Omega(\mathbf{W})$  is the regularization function, and  $\lambda$  controls its weight.

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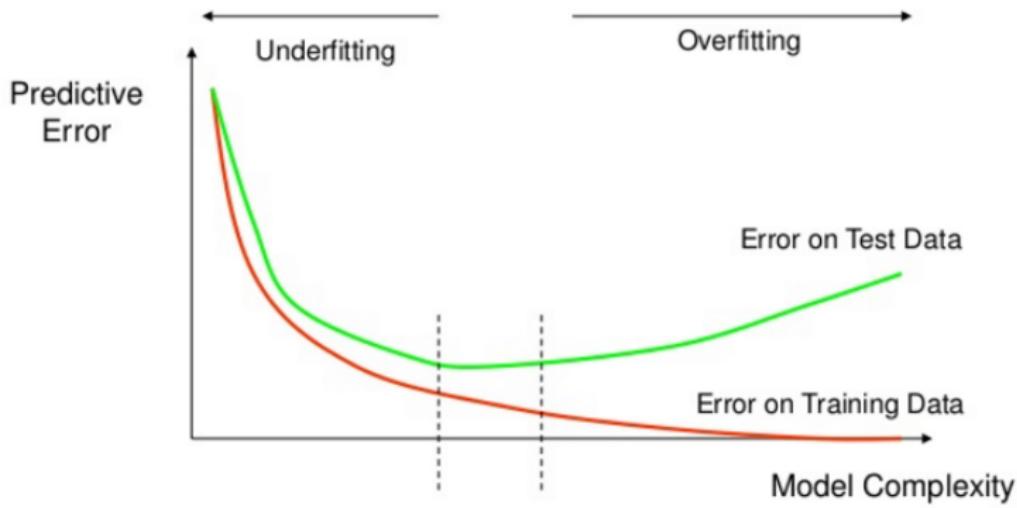
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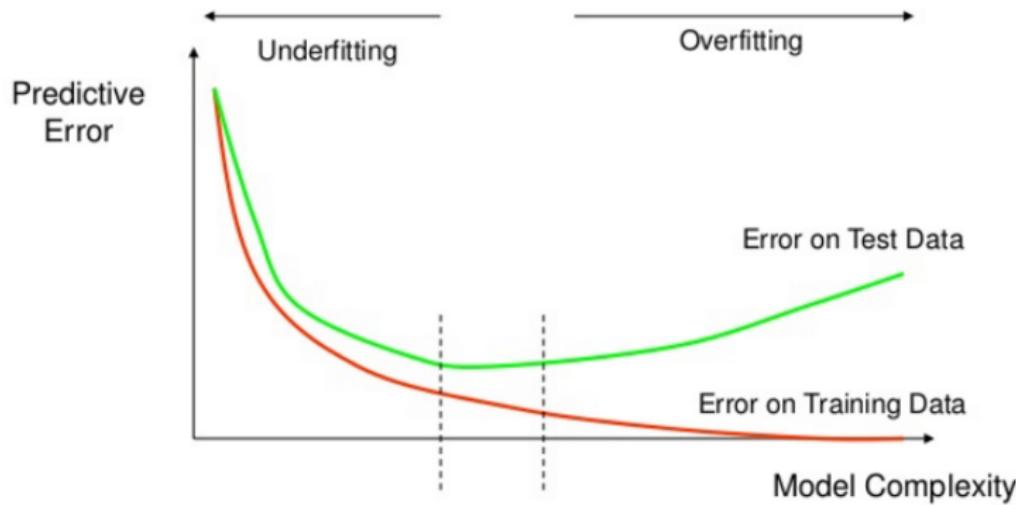
- $\ell_1$  regularization promotes **smaller** and **sparse** weights!

$$\Omega(\mathbf{W}) = \sum_y \|\mathbf{w}_y\|_1 = \sum_y \sum_i |w_{y,i}|$$

# Empirical Risk Minimization: The Classical View

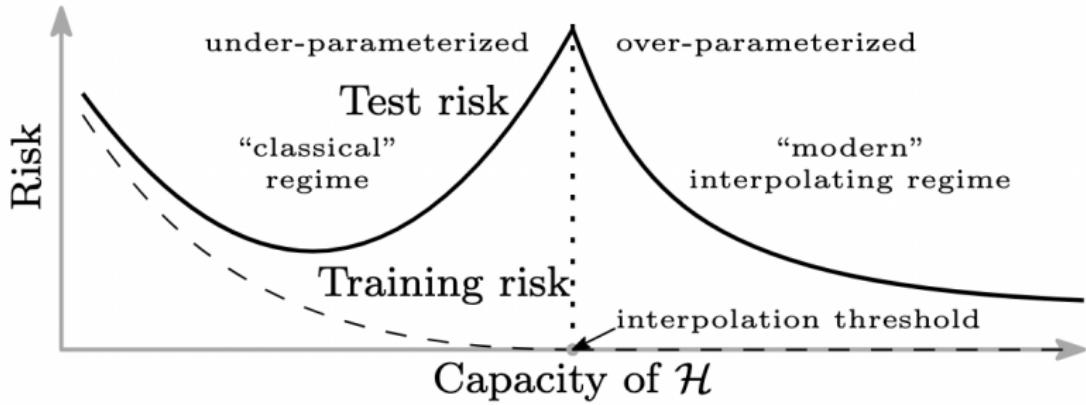


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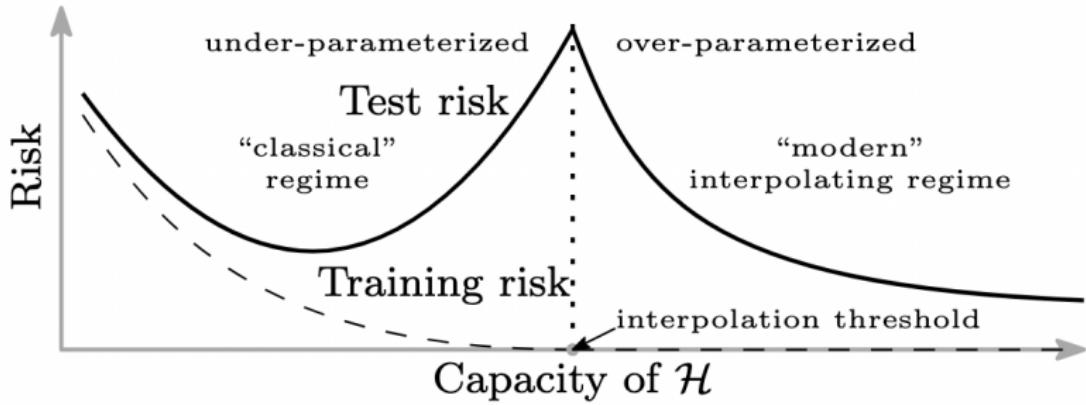


...doesn't explain the excellent performance of deep networks, which are very complex (have many parameters).

# Empirical Risk Minimization: Double Descent



# Empirical Risk Minimization: Double Descent



Fully understanding **double descent** is an open research topic.

## Logistic Regression with $\ell_2$ Regularization

- $\ell_2$ -regularized (a.k.a. ridge or weight decay) logistic regression

$$\min - \sum_{t=1}^N \underbrace{\log \left( \exp(\mathbf{w}_{y_t}^T \phi(x_t)) / Z_x \right)}_{L(\mathbf{w}; (x_t, y_t))} + \frac{\lambda}{2} \|\mathbf{W}\|_F^2$$

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- For gradient descent, we also need  $\nabla \|\mathbf{W}\|_2^2 = 2\mathbf{W}$
- GD step (similarly for SGD) with **weight decay**:

$$\mathbf{W}^{(k+1)} = \underbrace{(1 - \eta_k \lambda)}_{\text{weight decay } (1-\eta_k\lambda)<1} \mathbf{W}^{(k)} - \eta_k \sum_{t=1}^N \nabla L(\mathbf{W}; (x_t, y_t))$$

# Loss Functions

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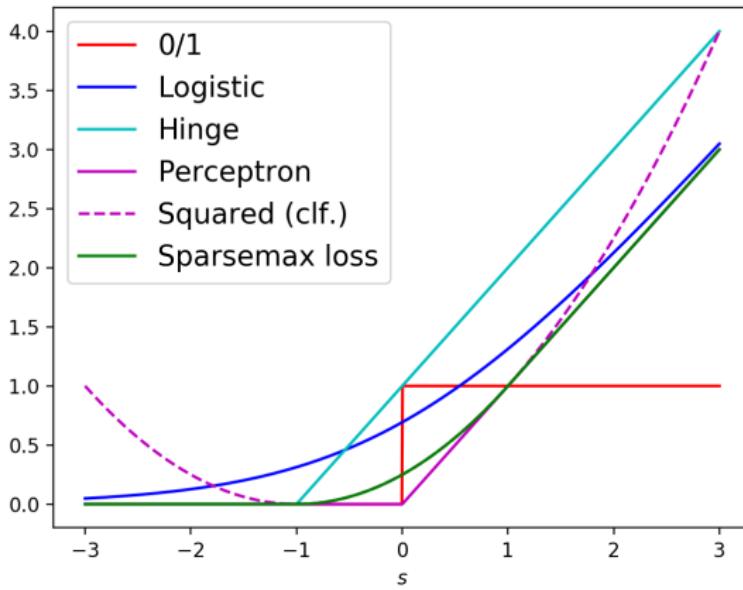
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# Loss Functions

- Should match the metric we want to optimize at test time
- Should be well-behaved (convex, hopefully smooth) for optimization (rules out the 0/1 loss)
- Some examples:
  - ✓ Squared loss for regression
  - ✓ Negative log-likelihood (a.k.a. cross-entropy) for multinomial logistic regression
  - ✓ Hinge loss for support vector machines (not covered)
  - ✓ Sparsemax loss for multi-class and multi-label classification (not covered)

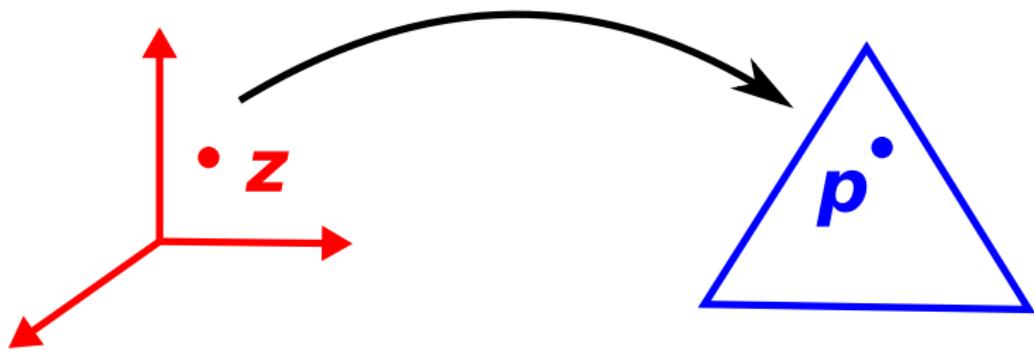
# Classification Losses (Binary Case)

- The horizontal axis shows  $s = -y w^T \phi(x)$ .



## Recap

Mapping a label score vector  $z \in \mathbb{R}^{|\mathcal{Y}|}$  to a probability distribution in  $\mathcal{Y}$ ?



We already saw one example: softmax.

Another example is **sparsemax** (not covered): Martins and Astudillo (2016)

## Recap: Softmax Transformation

The typical transformation for multi-class classification:

$$\text{softmax} : \mathbb{R}^{|\mathcal{Y}|} \rightarrow \Delta_{|\mathcal{Y}|-1}$$

$$\text{softmax}(z) = \left[ \frac{\exp(z_1)}{\sum_c \exp(z_c)}, \dots, \frac{\exp(z_{|\mathcal{Y}|})}{\sum_c \exp(z_c)} \right]^T$$

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- Underlies **multinomial logistic regression**
- Strictly positive, sums to 1
- Resulting distribution has full support:  $\text{softmax}(z) > 0, \forall z$

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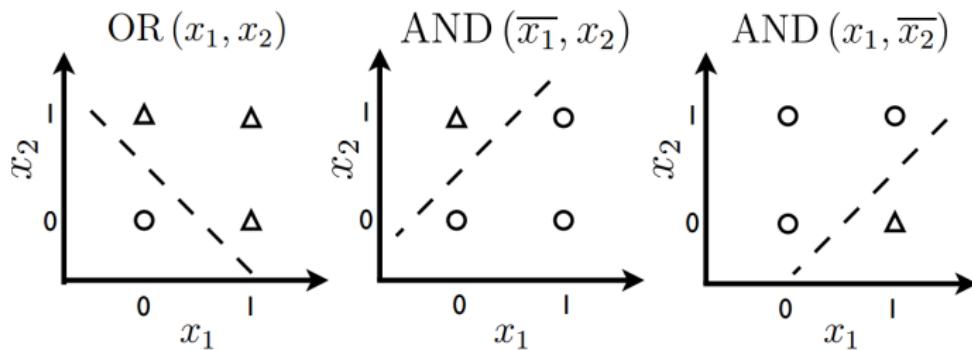
$$\nabla L(\mathbf{W}; (x, y)) = (\text{softmax}(z(x)) - e_y) \phi(x)^T$$

# Outline

- ① Logistic Regression
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- ③ Non-Linear Classifiers

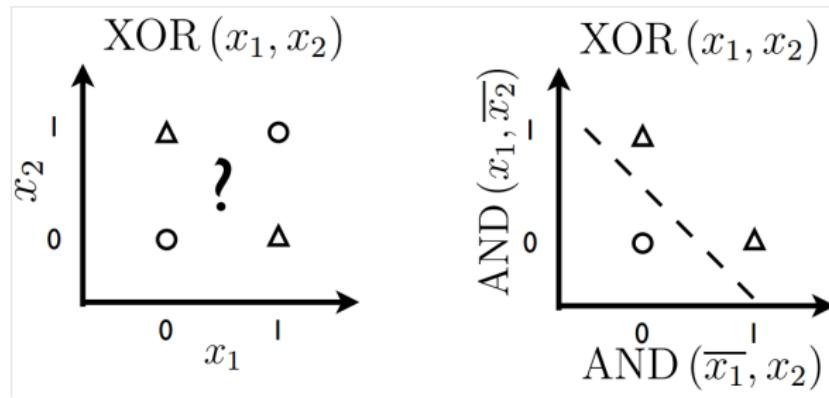
# Recap: What a Linear Classifier Can Do

- It **can** solve linearly separable problems (OR, AND)



## Recap: What a Linear Classifier **Can't** Do

- ... but it **cannot** solve **non-linearly separable** problems such as simple XOR (unless input is transformed into a better representation):



- This was observed by Minsky and Papert (1969) (for the perceptron) and motivated strong criticisms

# Summary: Linear Classifiers

- We have seen
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- All assume the features are well-engineered such that **the data is (nearly) linearly separable**

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**Neural networks** (**next class!**)

- embrace non-convexity and local minima
- instead of engineering features/kernels, engineer the model architecture

# Two Views of Machine Learning

There's two main ways of building machine learning systems:

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Sometimes the two are equivalent!

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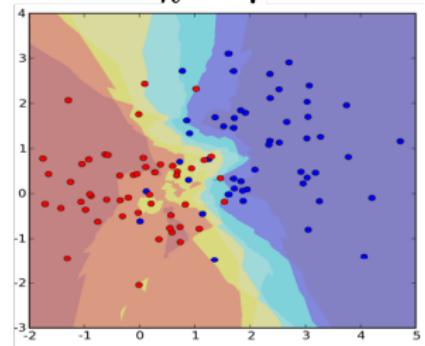
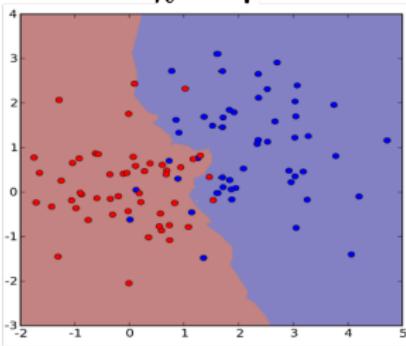
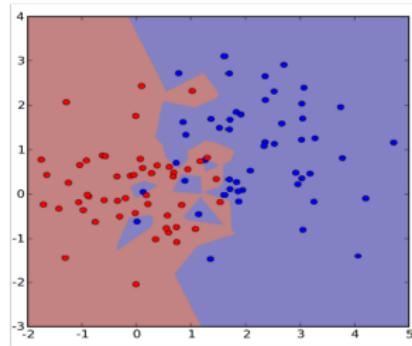
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- Specialized data structures can be used to speed up search.

# Nearest Neighbour(s) Classifiers



class probability estimates

# Kernels

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- **Positive definite:** for all non-zero  $\mathbf{v}$

$$\mathbf{v} \mathbf{K} \mathbf{v}^T \geq 0$$

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- **Mercer's Theorem:** for any kernel  $\kappa : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ , there exists some feature mapping  $\phi : \mathcal{X} \rightarrow \mathcal{H}$ , s.t.:

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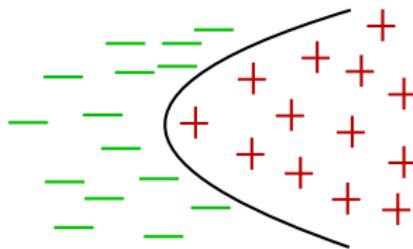
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- Extremely popular idea in the 1990-2000s!

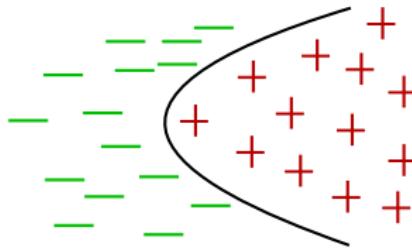
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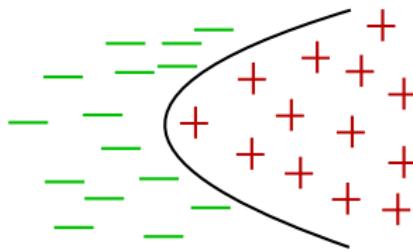
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- Computing a non-linear kernel is often cheaper than calculating the corresponding inner product in the high-dimensional feature space.



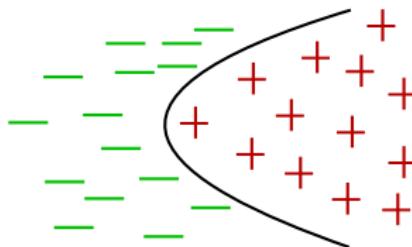
# Kernels = Tractable Non-Linearity

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- Many models can be “kernelized”.

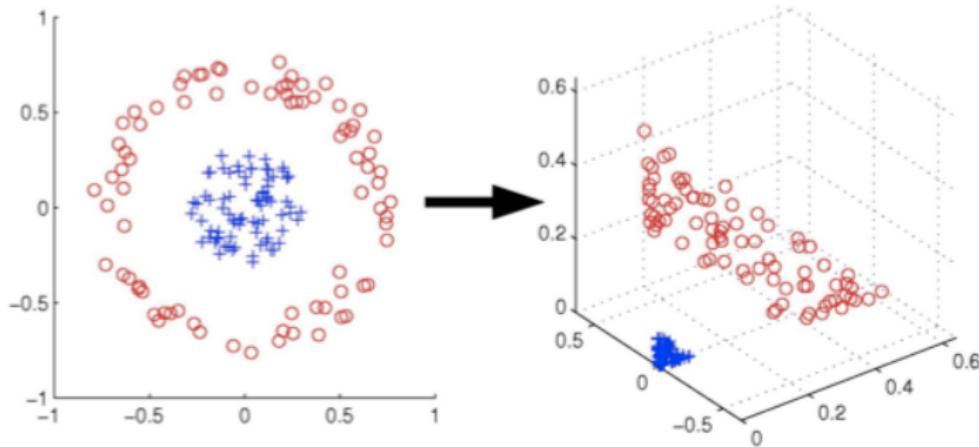


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- Many models can be “kernelized”.
- Drawback: **quadratic** dependency on dataset size



# Linear Classifiers in High Dimension



- Example:  $\phi([x_1, x_2]) = [x_1^2, x_2^2, \sqrt{2} x_1 x_2]$
- Kernel trick; let  $x = [x_1, x_2]$  and  $x' = [x'_1, x'_2]$ :

$$\langle \phi(x), \phi(x') \rangle = \langle [x_1, x_2], [x'_1, x'_2] \rangle^2 = k(x, x')$$

# Popular Kernels

- Polynomial kernel of order  $d$ :

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- Tree kernels (Collins and Duffy, 2002)

# Conclusions

- Linear classifiers are a broad class including well-known methods such as **perceptrons**, **logistic regression**, support vector machines.
- They all involve manipulating weights and features.
- They either lead to closed-form solutions or **convex** optimization problems (**no local minima**)
- Stochastic gradient descent algorithms are useful if training datasets are large.
- However, they require manual specification of feature representations

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