Lecture 3: Linear Models II

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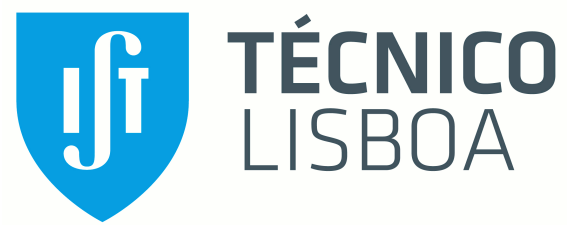


Deep Learning Course, Winter 2023-2024

Today's Roadmap

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

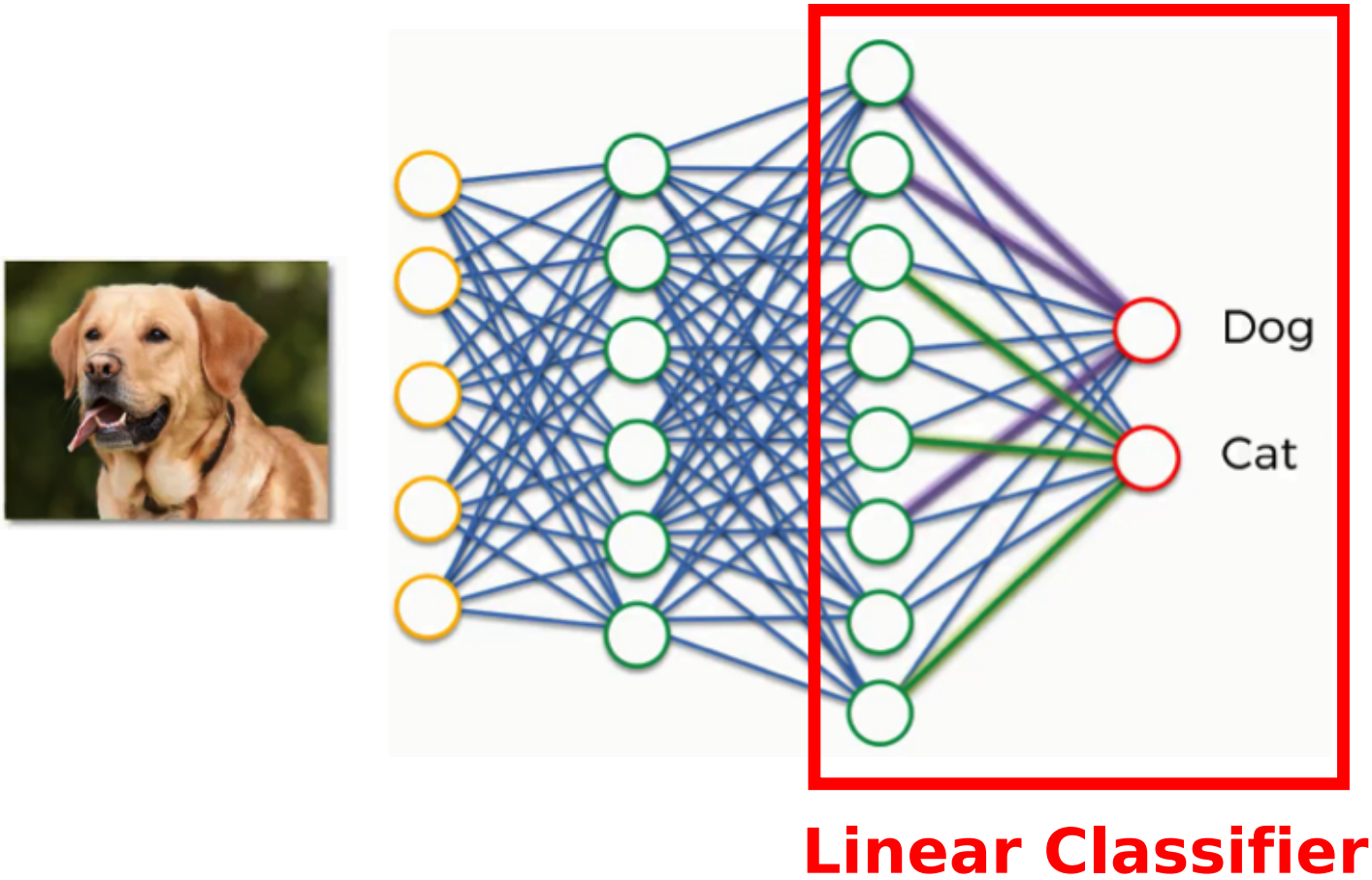
Why Linear Classifiers?

We know the course title promised "deep", ...

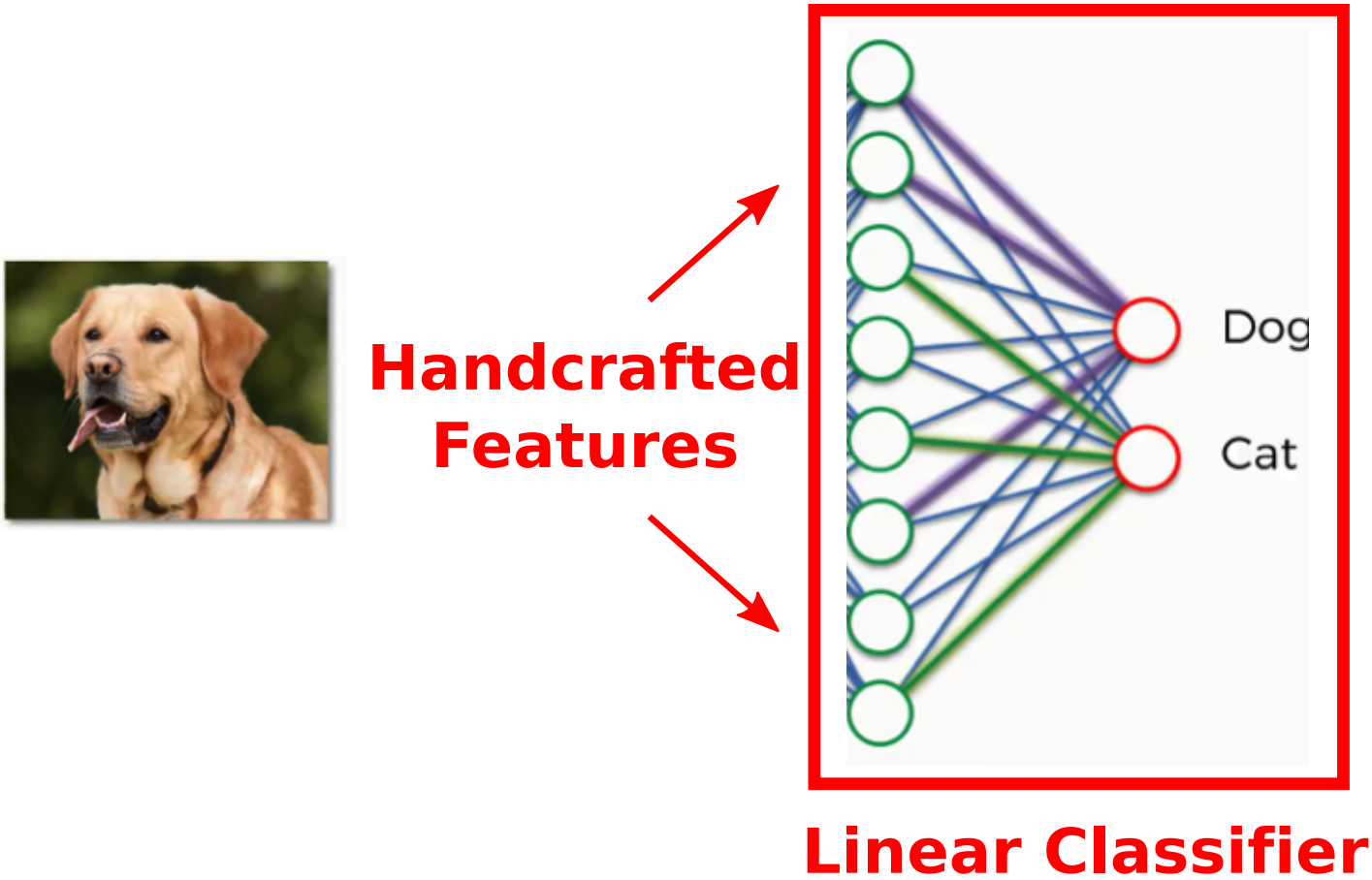
...but (as explained in Lecture 2):

- 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

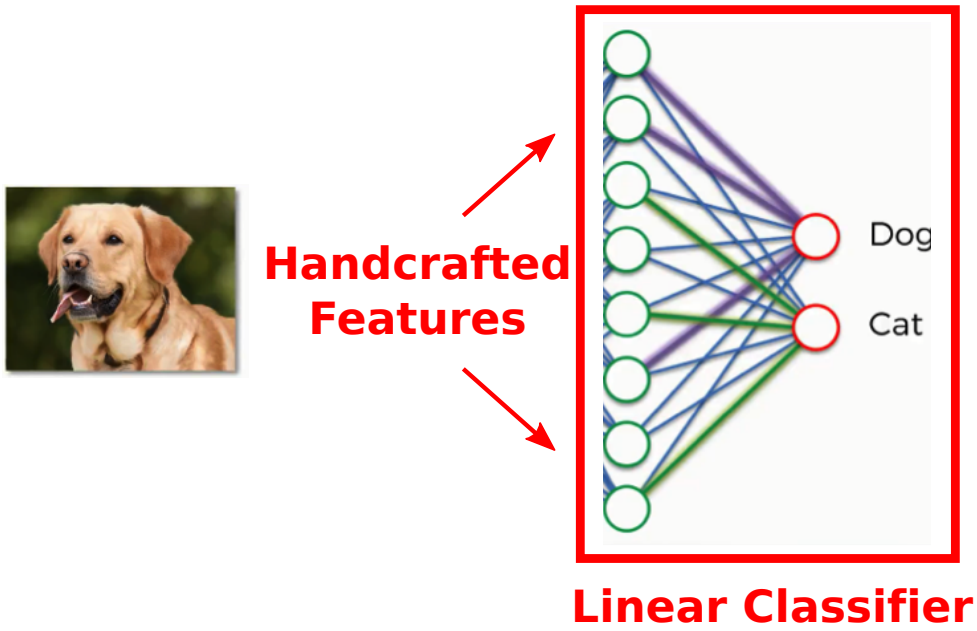


Linear Classifiers and Neural Networks



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

Reminder: Linear Classifier

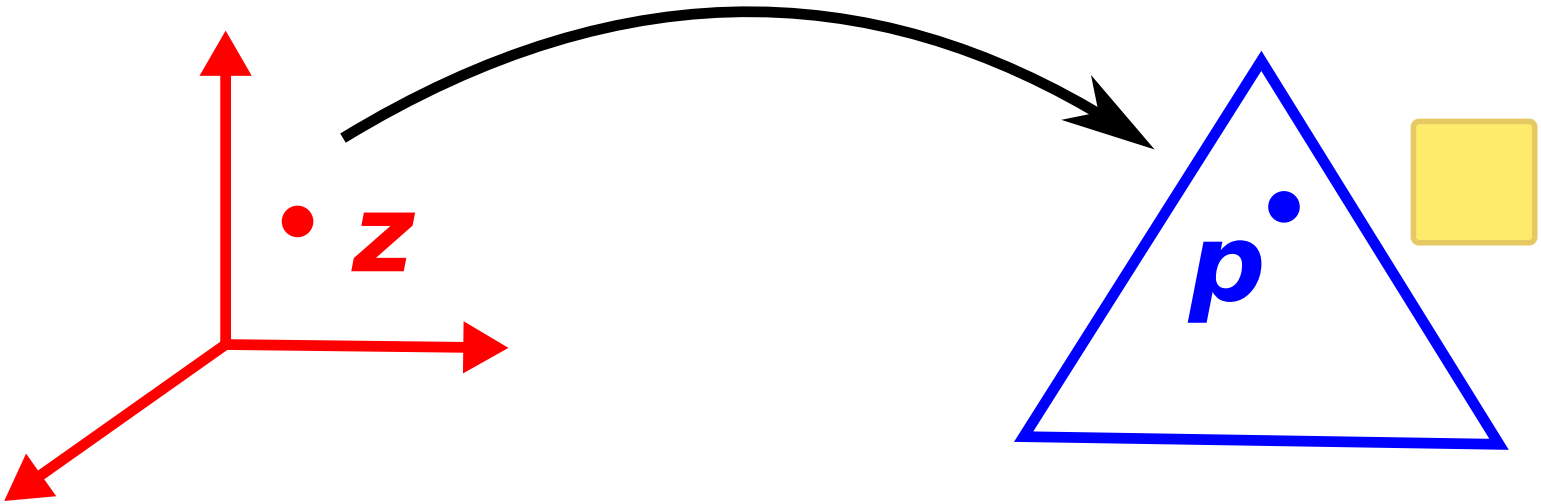


$$\widehat{y} = \arg\max_y \big((\boldsymbol{W}\boldsymbol{\phi}(x))_y \big), \quad \boldsymbol{W} = \begin{bmatrix} w_1^T \\ \vdots \\ w_{|\mathcal{Y}|}^T \end{bmatrix}$$

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

Key Problem

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



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

Outline

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

Logistic Regression

A linear model gives a score for each class y: $w_y^T \phi(x)$,

...from which we may compute a conditional (posterior) probability:

$$P(y|x) = \frac{\exp\left(w_y^T \phi(x)\right)}{Z_x}, \qquad \text{where } Z_x = \sum_{y' \in \mathcal{Y}} \exp\left(w_{y'}^T \phi(x)\right)$$

This is called the softmax transformation

Still a linear classifier, if we choose the most probable class:

$$\begin{aligned} \arg\max_y \; P(y|x) &= \arg\max_y \; \frac{\exp\left(w_y^T \phi(x)\right)}{Z_x} \\ &= \arg\max_y \; \exp\left(w_y^T \phi(x)\right) \\ &= \arg\max_y \; w_y^T \phi(x) \end{aligned}$$

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

Binary Logistic Regression

Binary labels ($\mathcal{Y} = \{\pm 1\}$)

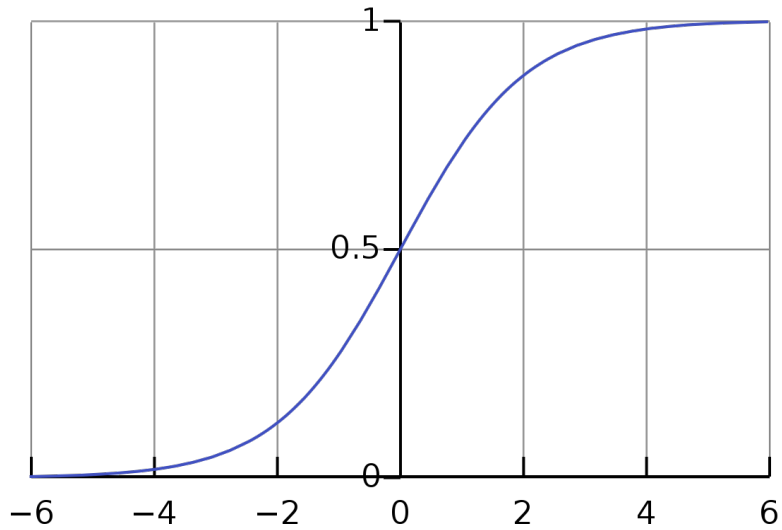
Since adding a constant to all scores does not change the probabilities, we can use score 0 for the -1 class, and $w^T \phi(x)$ for $+1$ class,

$$\begin{aligned} P(y = +1 \mid x) &= \frac{\exp\big(w^T \phi(x)\big)}{1 + \exp\big(w^T \phi(x)\big)} \\ &= \frac{1}{1 + \exp\big(-w^T \phi(x)\big)} \\ &\equiv \sigma\big(w^T \phi(x)\big). \end{aligned}$$

This is called a sigmoid transformation.

Sigmoid Transformation

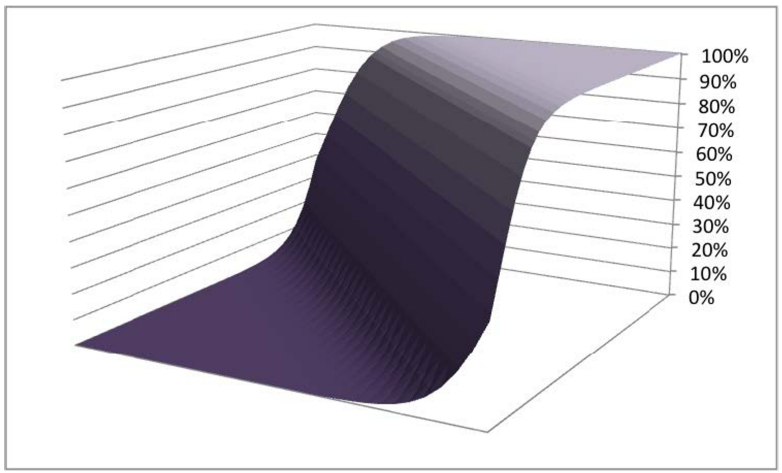
$$\sigma(u) = \frac{e^u}{1 + e^u}$$

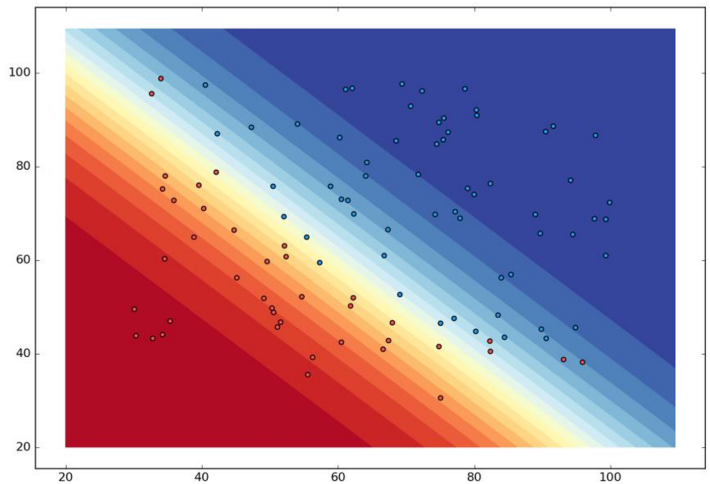


- Widely used in neural networks.
- Maps $\mathbb{R}$ into $[0, 1]$.
- The output can be interpreted as a probability.
- Positive, bounded, strictly increasing.

Binary Logistic Regression

- In two dimensions, i.e., $\boldsymbol{w}$, $\boldsymbol{\phi}(x) \in \mathbb{R}^2$





- MAP boundary, $P(y = +1 \mid x) = 1/2 \Leftrightarrow \boldsymbol{w}^T \boldsymbol{\phi}(x) = 0$, is linear w.r.t. $\boldsymbol{\phi}(x)$.
- Some other threshold, $P(y = +1 \mid x) = \tau \Leftrightarrow \boldsymbol{w}^T \boldsymbol{\phi}(x) = \log(\frac{\tau}{1-\tau})$; linear w.r.t. $\boldsymbol{\phi}(x)$.

Multinomial Logistic Regression

$$P_{\boldsymbol{W}}(y \mid x) = \frac{\exp\left(w_y^T \phi(x)\right)}{Z_x}$$

- How to learn weights $\boldsymbol{W}$?
- Maximize the conditional log-likelihood of training data:

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

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

Logistic Regression

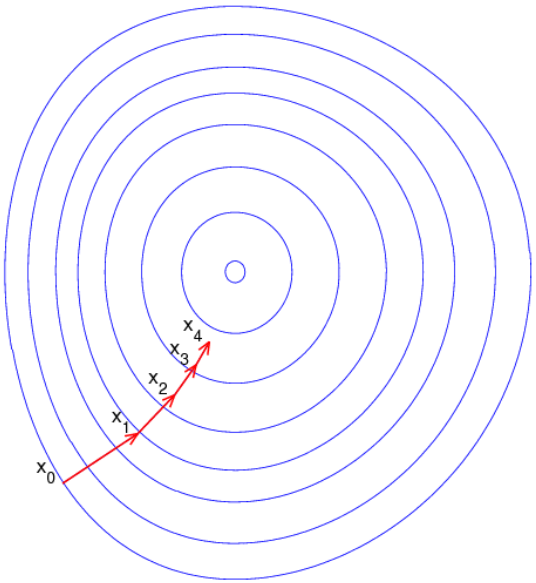
- This objective function is strictly convex.
- Proof left as exercise! (hint, compute the Hessian).
- Therefore, any local minimum is a global minimum.
- No closed-form solution; many numerical methods have been proposed
  - ✓ Gradient methods (gradient descent, conjugate gradient).
  - ✓ Quasi-Newton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

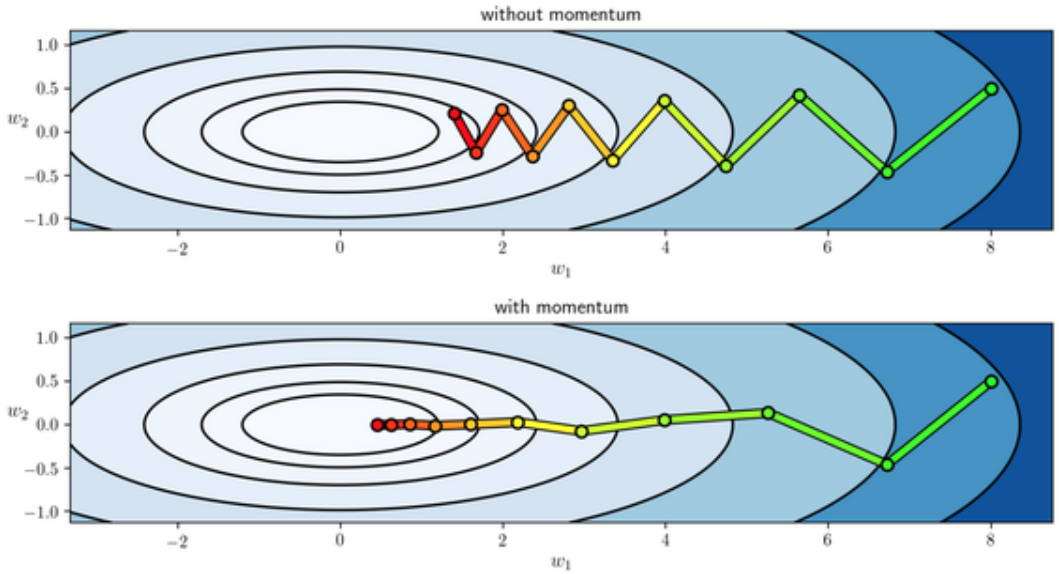
Recap: Gradient Descent

- Goal: minimize $f : \mathbb{R}^d \to \mathbb{R}$, for differentiable f
- Take small steps in the negative gradient direction until a stopping criterion is met:

$$x^{(t+1)} \leftarrow x^{(t)} - \eta_t \nabla f(x^{(t)})$$

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





Gradient Descent

- Loss function in logistic regression is

$$L(\boldsymbol{W};(x,y)) = \log \sum_{y'} \exp\left(w_{y'}^T \phi(x)\right) - w_y^T \phi(x).$$

- We want to find: $\arg\min_{\boldsymbol{W}} \sum_{t=1}^{N} L(\boldsymbol{W};(x_t,y_t))$
  - ✓ Set $\boldsymbol{W}^{(0)} = 0$
  - ✓ Iterate until convergence (for suitable stepsize η_k):

$$\begin{aligned} \boldsymbol{W}^{(k+1)} &= \boldsymbol{W}^{(k)} - \eta_k \nabla_{\boldsymbol{W}} \left(\sum_{t=1}^{N} L(\boldsymbol{W}^{(k)};(x_t,y_t)) \right) \\ &= \boldsymbol{W}^{(k)} - \eta_k \sum_{t=1}^{N} \nabla_{\boldsymbol{W}} L(\boldsymbol{W}^{(k)};(x_t,y_t)) \end{aligned}$$

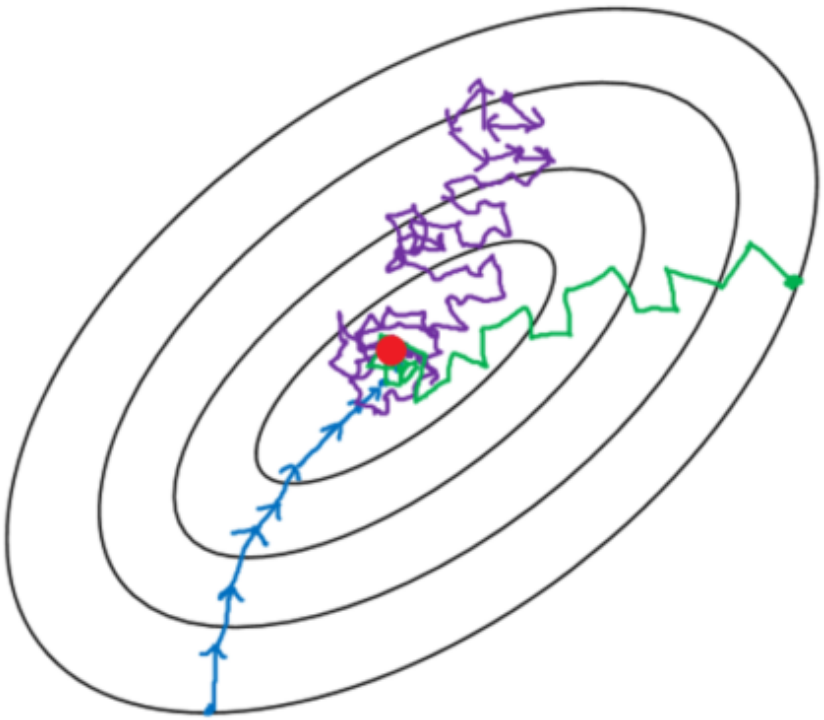
- $L(\boldsymbol{W})$ convex $\Rightarrow$ gradient descent will reach the global optimum $\boldsymbol{W}$, with appropriate choice of step-size η_k.

Stochastic Gradient Descent

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

- Set $\boldsymbol{W}^{(0)} = 0$
- Iterate until convergence:
  - Pick (x_t, y_t) randomly.
  - Update $\boldsymbol{W}^{(k+1)} = \boldsymbol{W}^{(0)} - \eta_k \nabla_{\boldsymbol{W}} L(\boldsymbol{W}^{(k)}; (x_t, y_t))$
- *i.e.* approximate the gradient with a noisy, unbiased, version based on a single sample
- Variant between GD and SGD: mini-batch (pick B, rather than 1 pair)
- All guaranteed to find the optimal $\boldsymbol{W}$ (for suitable step sizes)

Stochastic vs Batch Gradient Descent



Batch gradient descent
Mini-batch gradient Descent
Stochastic gradient descent

Computing the Gradient

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

$$L(\boldsymbol{W}; (x, y)) = \log \sum_{y'} \exp\left(w_{y'}^T \phi(x)\right) - w_y^T \phi(x)$$

- Some reminders (we next omit the subscript $\boldsymbol{W}$ for simplicity)
  1. $\nabla \log F(\boldsymbol{W}) = \dfrac{\nabla F(\boldsymbol{W})}{F(\boldsymbol{W})}$
  2. $\nabla \exp F(\boldsymbol{W}) = \exp(F(\boldsymbol{W}))\nabla F(\boldsymbol{W})$

- We denote by

$$e_y = [0, \ldots, 0, 1, 0, \ldots, 0]^T, \quad \text{1 in } y\text{-th position}$$

the one-hot vector representation of class y.

Computing the Gradient

$$
\begin{aligned}
\nabla L(\boldsymbol{W};(x,y)) &= \nabla\left(\log\sum_{y'}\exp(w_{y'}^T\phi(x)) - w_y^T\phi(x)\right) \\
&= \nabla\log\sum_{y'}\exp(w_{y'}^T\phi(x)) - \nabla w_y^T\phi(x) \\
&= \frac{1}{\sum_{y'}\exp(w_{y'}^T\phi(x))}\sum_{y'}\nabla\exp(w_{y'}^T\phi(x)) - e_y\phi(x)^T \\
&= \frac{1}{Z_x}\sum_{y'}\exp(w_{y'}^T\phi(x))\nabla w_{y'}^T\phi(x) - e_y\phi(x)^T \\
&= \sum_{y'}\frac{\exp(w_{y'}^T\phi(x))}{Z_x}e_{y'}\phi(x)^T - e_y\phi(x)^T \\
&= \sum_{y'}P_{\boldsymbol{W}}(y'|x)e_{y'}\phi(x)^T - e_y\phi(x)^T \\
&= \left(\begin{bmatrix} P_{\boldsymbol{W}}(1|x) \\ \vdots \\ P_{\boldsymbol{W}}(|\mathcal{Y}|\,|\,x)\end{bmatrix} - e_y\right)\phi(x)^T.
\end{aligned}
$$

Logistic Regression Summary

- Define conditional probability

$$P_{\boldsymbol{W}}(y|x) = \frac{\exp\left(w_y^T \phi(x)\right)}{Z_x}$$

- Set weights to maximize conditional log-likelihood of training data:

$$\boldsymbol{W} = \arg\max_{\boldsymbol{W}} \sum_t \log P_{\boldsymbol{W}}(y_t|x_t) = \arg\min_{\boldsymbol{W}} \sum_t L(\boldsymbol{W}; (x_t, y_t))$$

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

$$\nabla L(\boldsymbol{W}; (x, y)) = \sum_{y'} P_{\boldsymbol{W}}(y'|x) \boldsymbol{e}_{y'} \phi(x)^\top - \boldsymbol{e}_y \phi(x)^\top$$

The Story So Far

The Story So Far

- Logistic regression is discriminative: maximizes conditional likelihood
  - ✓ also called log-linear model and max-entropy classifier
  - ✓ no closed-form solution
  - ✓ stochastic gradient updates look like

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

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

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

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

Other Options: Maximizing Margin

- For a training set $\mathcal{D} = \{(x_t, y_t),\ t = 1, ..., N\}$

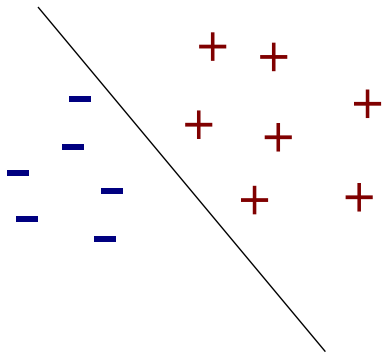
- Margin achieved by a weight matrix $\boldsymbol{W}$: smallest γ such that, for every training instance $(x_t, y_t) \in \mathcal{D}$,

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

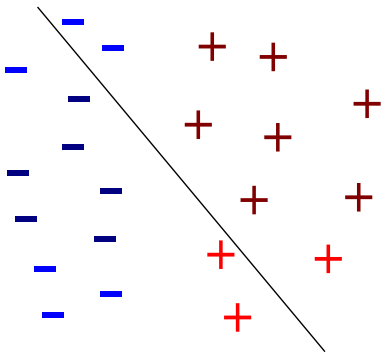
- i.e., score of the correct label is at least γ higher than that of any other label.

Margin

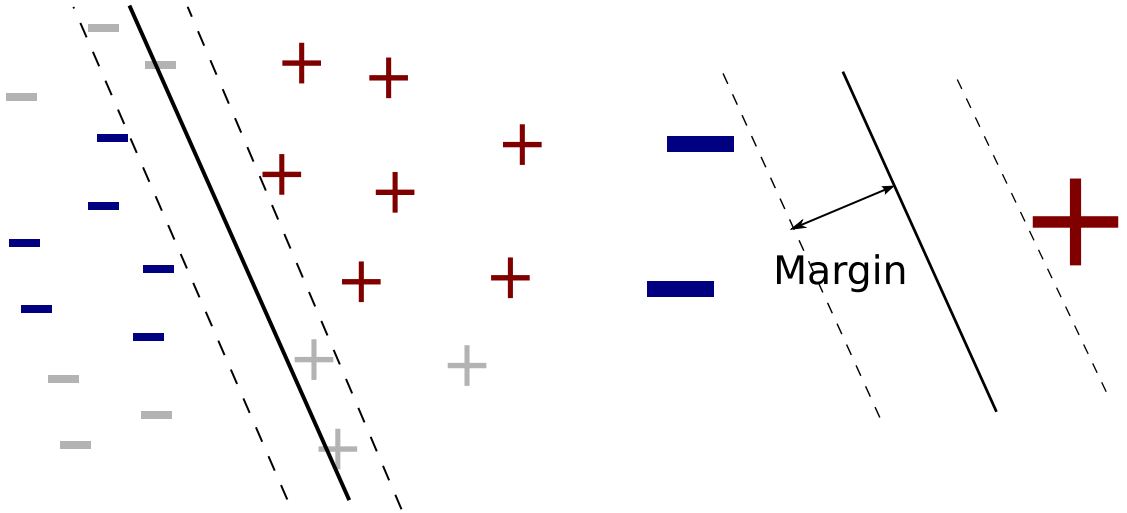
Training



Testing



Denote the value of the margin by γ



Maximizing Margin

- Intuitively maximizing margin makes sense
- More importantly, generalization error to unseen test data is proportional to the inverse of the margin

$$\epsilon \propto \frac{R^2}{\gamma^2 N}$$

- **Perceptron**:
  - ✓ If a training set is separable by some margin, the perceptron will find a $\boldsymbol{W}$ that separates the data
  - ✓ However, the perceptron does not pick $\boldsymbol{W}$ 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:

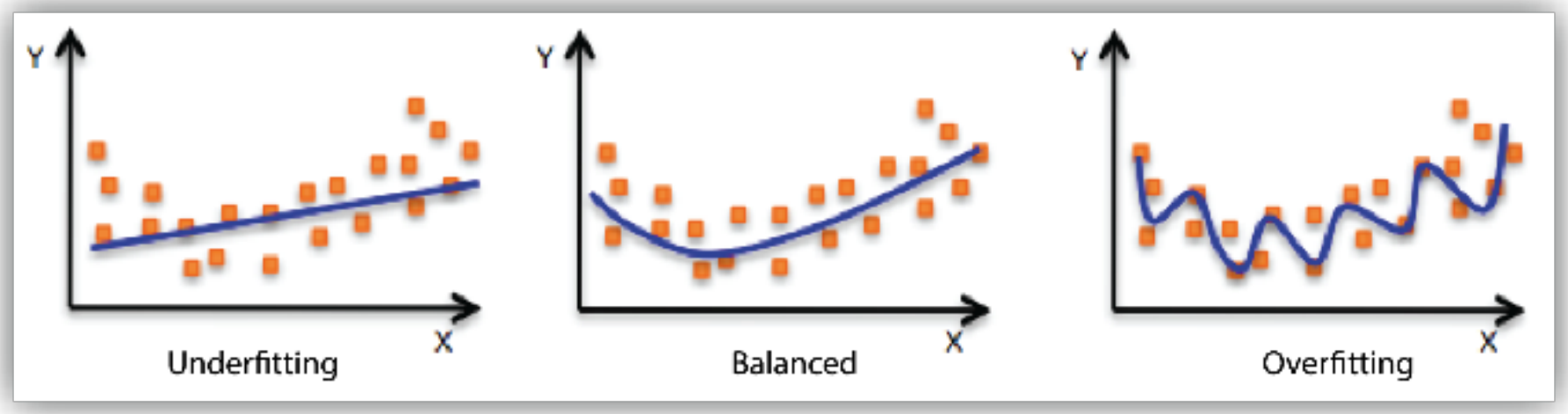
- Regularization
- Softmax
- Non-linear classifiers

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

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

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

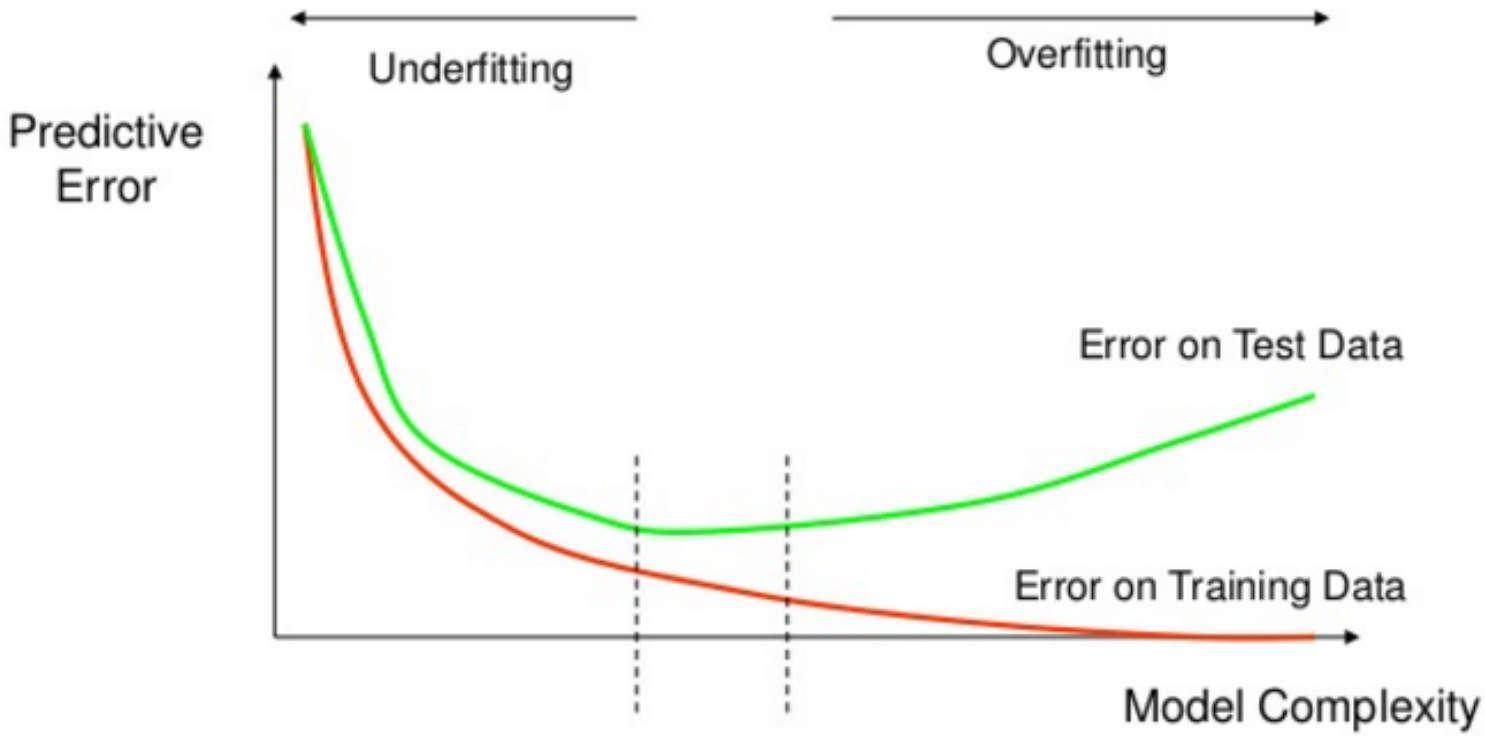
- ℓ_2 regularization promotes smaller weights:

$$\Omega(\boldsymbol{W}) = \sum_y \|w_y\|_2^2 = \sum_y \sum_i w_{y,i}^2.$$

- ℓ_1 regularization promotes smaller and sparse weights!

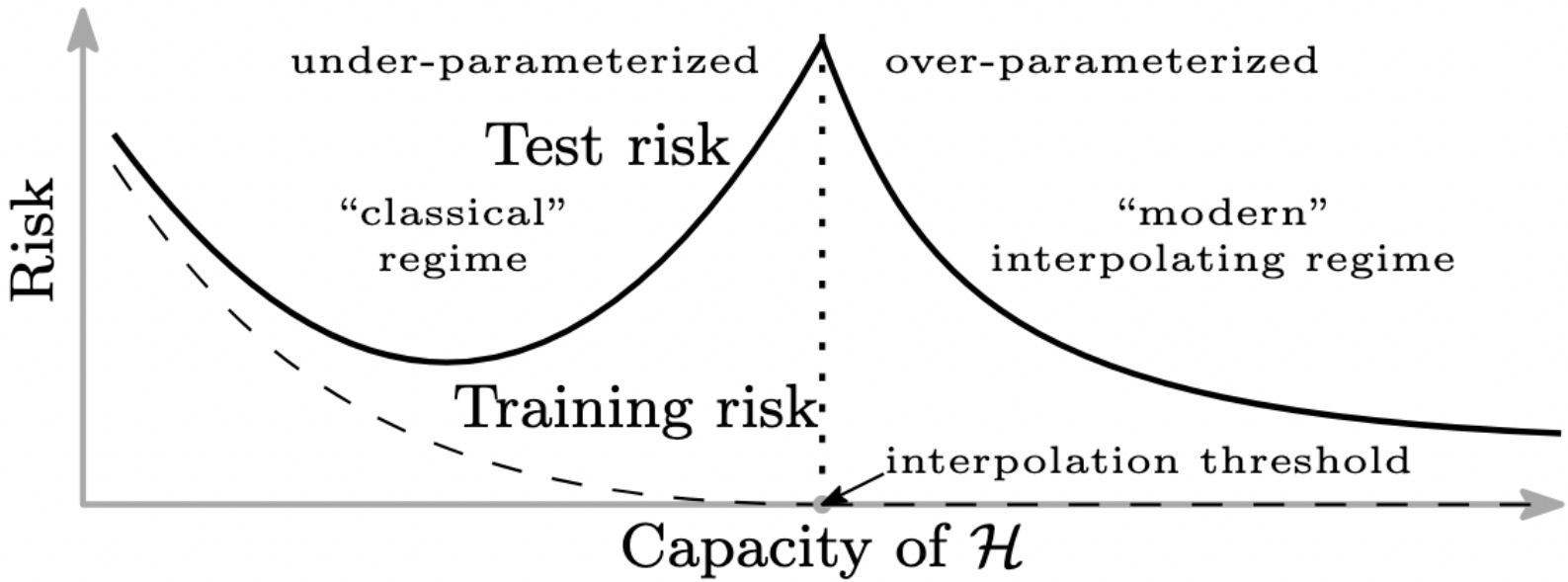
$$\Omega(\boldsymbol{W}) = \sum_y \|w_y\|_1 = \sum_y \sum_i |w_{y,i}|$$

Empirical Risk Minimization: The Classical View



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

Empirical Risk Minimization: Double Descent



Fully understanding double descent is an open research topic.

Logistic Regression with ℓ_2 Regularization

- ℓ_2-regularized (a.k.a. ridge or weight decay) logistic regression

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

- The gradient is now

$$\sum_{t=1}^{N} \nabla L(\boldsymbol{W};(x_t,y_t)) + \frac{\lambda}{2}\nabla\|\boldsymbol{W}\|_2^2$$

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

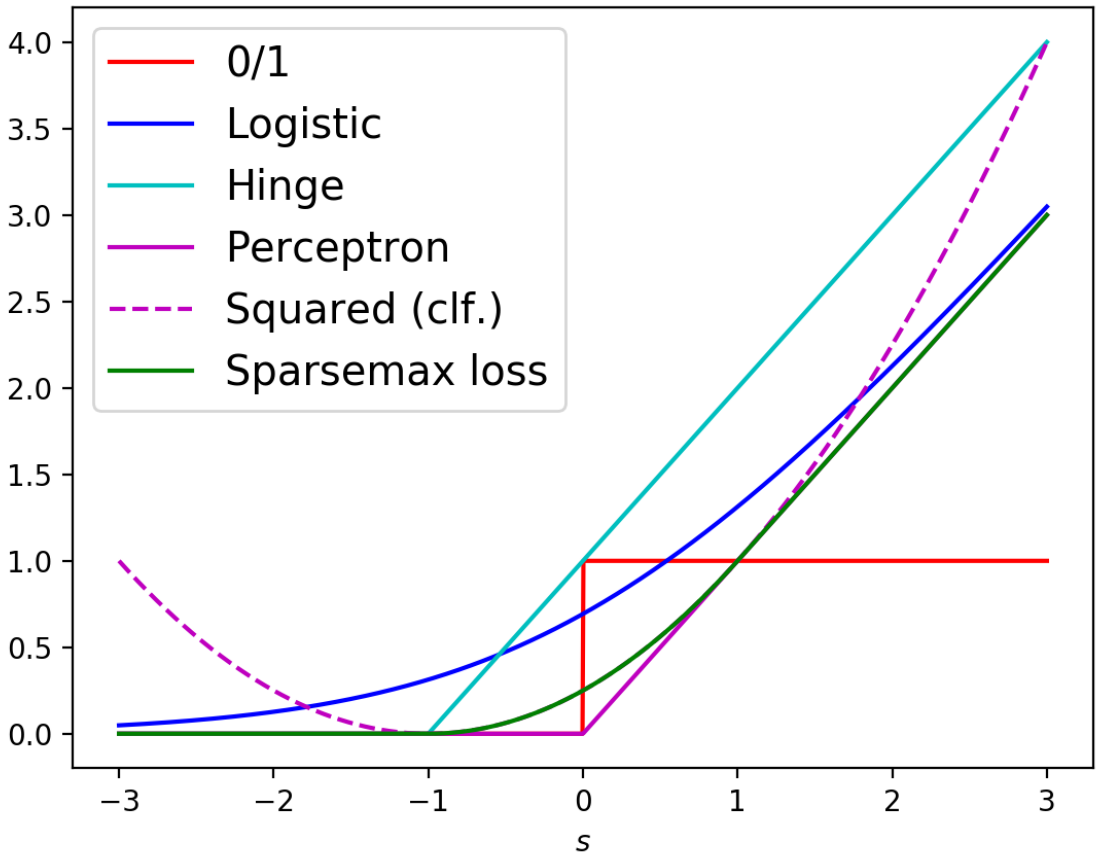
$$\boldsymbol{W}^{(k+1)} = \underbrace{(1-\eta_k\lambda)}_{\substack{\text{weight decay} \\ (1-\eta_k\lambda)<1}} \boldsymbol{W}^{(k)} - \eta_k \sum_{t=1}^{N} \nabla L(\boldsymbol{W};(x_t,y_t))$$

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 lossfor support vector machines (not covered)
  - ✓ Sparsemax loss for multi-class and multi-label classification (not covered)

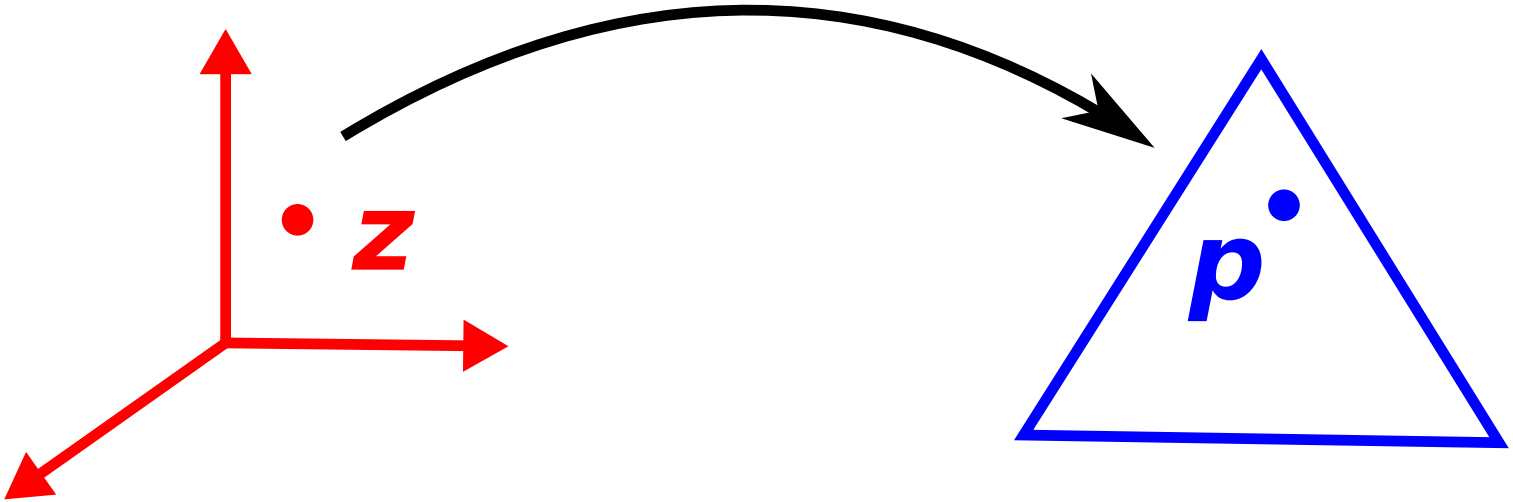
Classification Losses (Binary Case)

- 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:

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

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

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

Recap: Multinomial Logistic Regression

- The common choice for a softmax output layer
- The classifier estimates $P(y \mid x; \boldsymbol{W})$
- We minimize the negative log-likelihood:

$$\begin{aligned} L(\boldsymbol{W}; (x, y)) &= -\log P(y \mid x; \boldsymbol{W}) \\ &= -\log \left(\text{softmax}(z(x))\right)_y, \end{aligned}$$

  where $z_c(x) = w_c^T \phi(x)$ is the score of class c for sample x.

- Loss gradient:

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

Outline

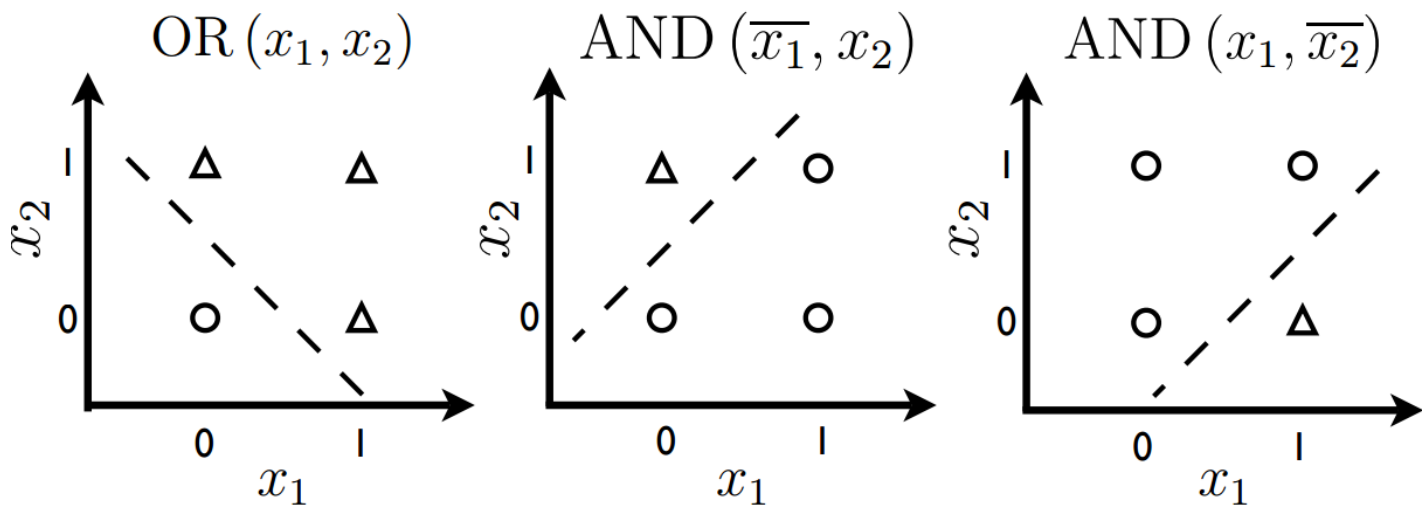
1 Logistic Regression

2 Regularization

3 Non-Linear Classifiers

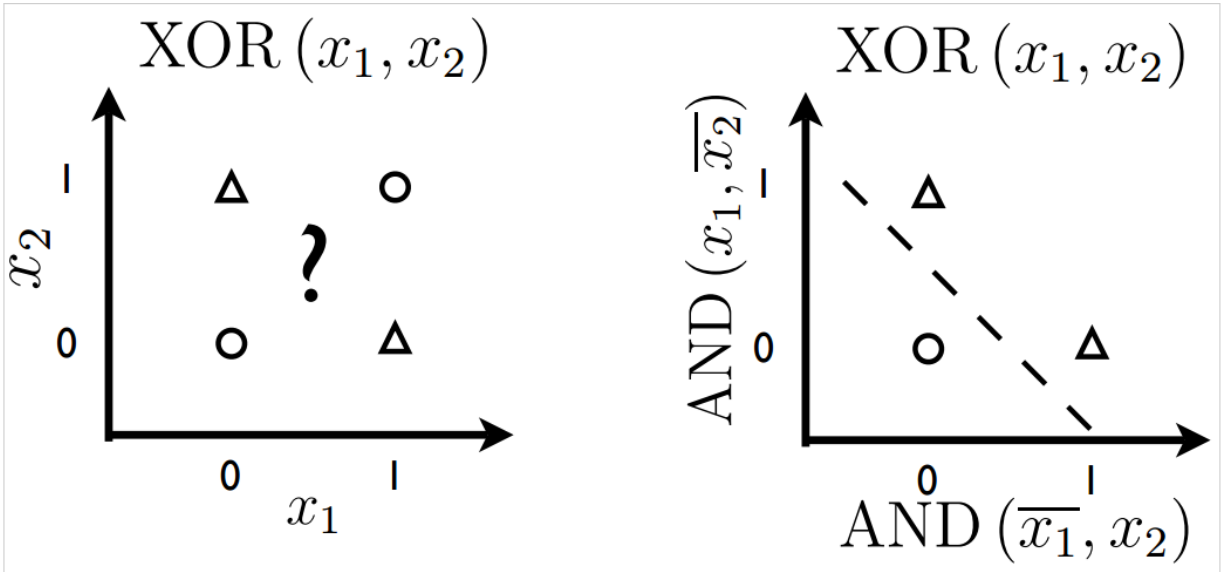
Recap: What a Linear Classifier Can Do

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

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Summary: Linear Classifiers

- We have seen
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  - ✓ Logistic regression
  - ✓ Support vector machines (not covered)
- All lead to convex optimization problems: no issues with local minima.
- All assume the features are well-engineered such that the data is (nearly) linearly separable

What If Data Are Not Linearly Separable?

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Engineer better features (often works!)

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Kernel methods:

- works implicitly in a high-dimensional feature space
- ... but still need to choose/design a good kernel
- model capacity confined to positive-definite kernels

What If Data Are Not Linearly Separable?

Engineer better features (often works!)

Kernel methods:

- works implicitly in a high-dimensional feature space
- ... but still need to choose/design a good kernel
- model capacity confined to positive-definite kernels

Neural networks (next class!)

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

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Sometimes the two are equivalent!

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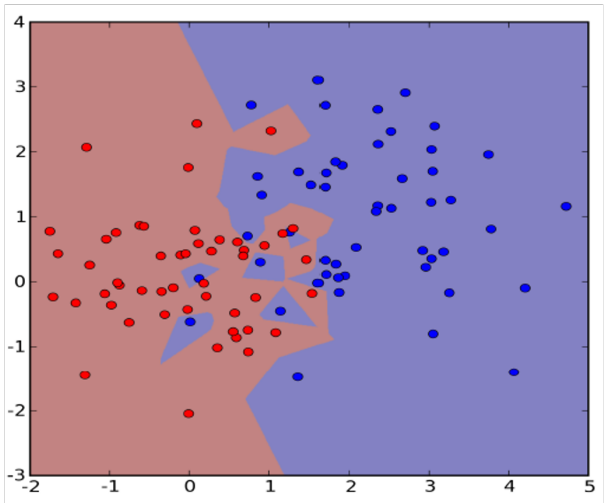
- Specialized data structures can be used to speed up search.

Nearest Neighbour(s) Classifiers



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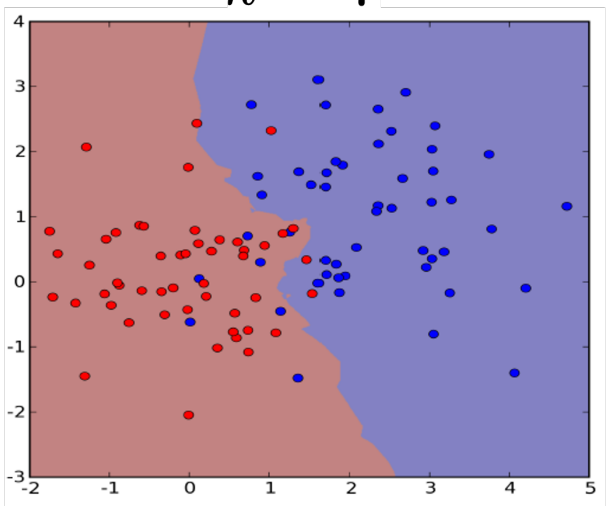

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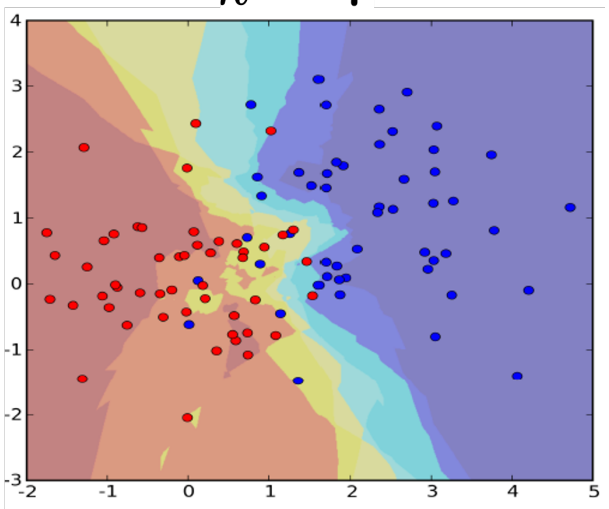

class probability estimates

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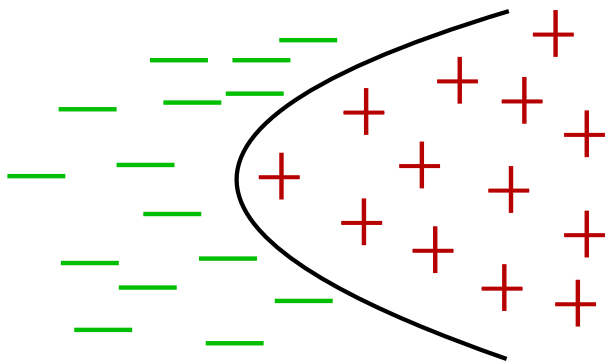
- Extremely popular idea in the 1990-2000s!

Kernels = Tractable Non-Linearity

- A linear classifier in a higher dimensional feature space is a non-linear classifier in the original space



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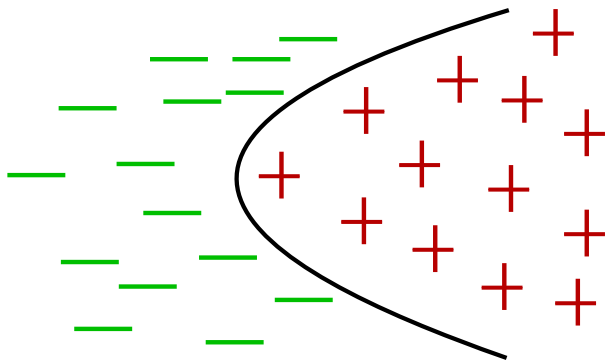

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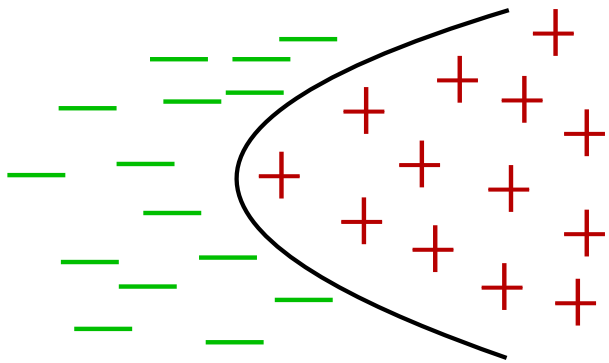

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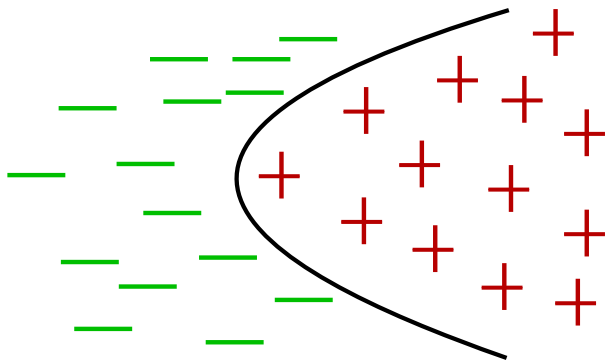
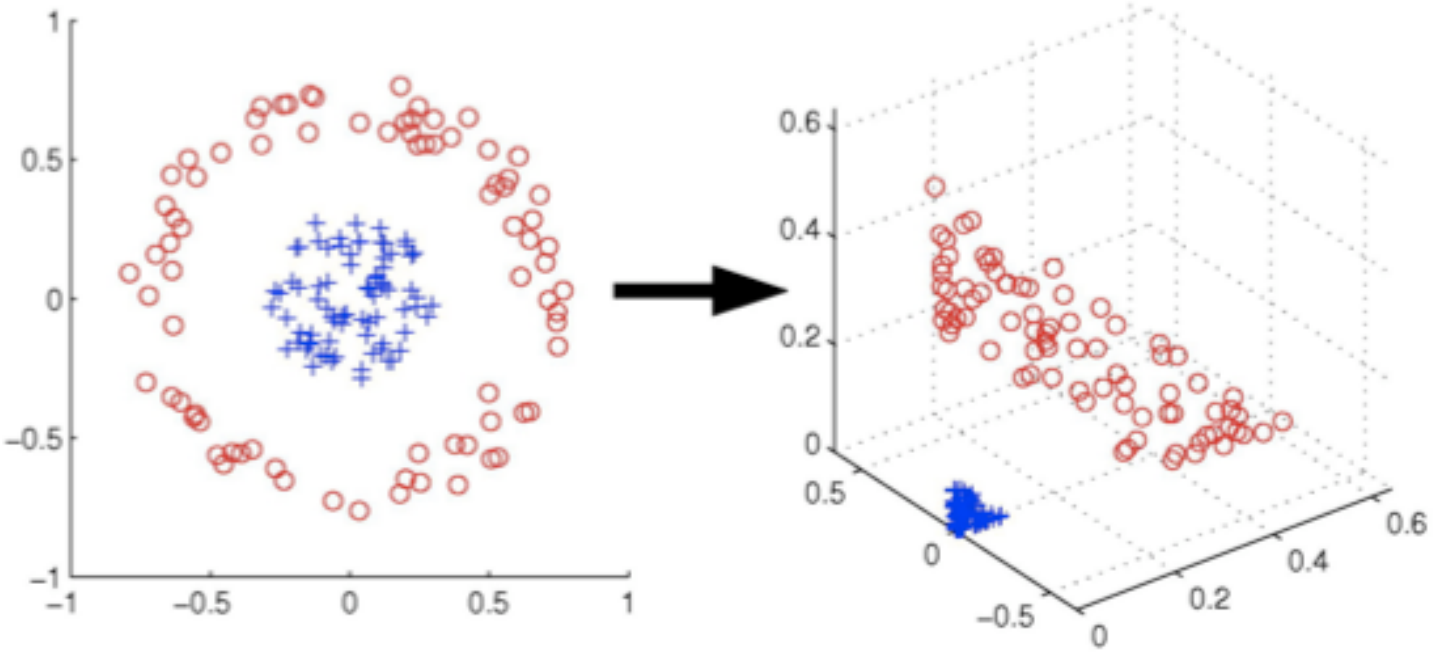
- Many models can be "kernelized".
- Drawback: quadratic dependency on dataset size



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 $x' = [x_1', x_2']$;

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

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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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