Neural networks

COMS 4771 Fall 2025

Feature maps revisited

Justification for simple statistical models (e.g., logistic regression):

- They are reasonable with a judicious choice of features or feature map
- In linear models, best prediction of Y given $X = x$ is based entirely on

$$w^{\mathsf{T}} \varphi(x)$$

  where φ is the feature map

Weierstrass approximation theorem: For any continuous function $f \colon \mathbb{R}^d \to \mathbb{R}$, any bounded region $B \subset \mathbb{R}^d$, and any $\varepsilon > 0$, there exists a polynomial $g \colon \mathbb{R}^d \to \mathbb{R}$ such that

$$\max_{x \in B} \quad |f(x) - g(x)| \leq \varepsilon$$

- Polynomials give good approximations uniformly over an interval (Cf. Taylor's theorem: only guarantees local approximations)
- Universal justification of polynomial expansion + linear functions
- Caveat: Degree of g may be large (e.g., growing with d and $1/\varepsilon$)
  - Somewhat ameliorated by kernel methods

Kernel machine: function learned by kernel method

$$g(x) = \sum_{i=1}^{n} \alpha_i \; \mathrm{k}(x, x^{(i)})$$

where $\mathrm{k}(\cdot, \cdot)$ is the kernel function, and $x^{(1)}, \ldots, x^{(n)}$ are from training data

Stone-Weierstrass approximation theorem: For any continuous function $f \colon \mathbb{R}^d \to \mathbb{R}$, any bounded region $B \subset \mathbb{R}^d$, and any $\varepsilon > 0$, there exists a function $g \colon \mathbb{R}^d \to \mathbb{R}$ of the form

$$g(x) = \sum_{i=1}^{p} \alpha_i \; \exp(x^\mathsf{T} w^{(i)})$$

such that

$$\max_{x \in B} \quad |f(x) - g(x)| \leq \varepsilon$$

- Can replace "$\exp$" with other "activation functions"
- Caveat: p may be large
- Another interpretation: linear function $\alpha^\mathsf{T} \varphi(x)$ with feature map

  $$\varphi(x) = (\exp(x^\mathsf{T} w^{(1)}), \ldots, \exp(x^\mathsf{T} w^{(p)}))$$

  Except the $w^{(i)}$'s may need to depend on f
- This kind of function is called a (two-layer) neural network

Kernel machine

$$g(x) = \sum_{i=1}^{n} \alpha_i \; \mathrm{k}(x, x^{(i)})$$

- Only α_i's are learned using data

(Two-layer) neural network

$$g(x) = \sum_{i=1}^{p} \alpha_i \; \exp(x^\top w^{(i)})$$

- Both α_i's and $w^{(i)}$'s are learned
- Can use $p > n$

Neural networks as straight-line programs

Very abbreviated history:

- McCulloch and Pitts (early 1940s):
  Neural networks as computational model for brain
- Arnold and Kolmogorov (late 1950s):
  Solved Hilbert's 13th problem (about polynomial roots) using neural networks
- **Modern use of neural networks with Linnainmaa's autodiff (early 1970s) started with Werbos (early 1980s)**
- Many other researchers have since discovered other approximation-theoretic properties and practical uses of neural networks (e.g., Cybenko, Rumelhart and Hinton, LeCun)

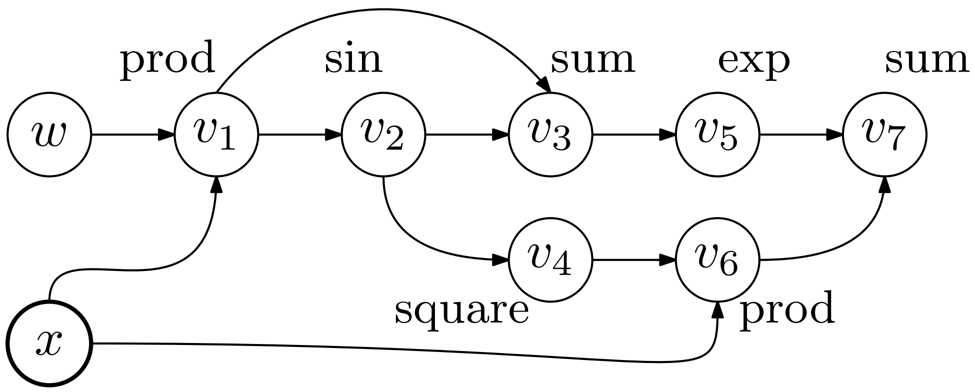
Today, for machine learning purposes: a neural network is (almost) any function f such that $f(x)$ can be computed by a straight-line program

Straight-line program: each line declares a new variable as a function of inputs (e.g., x), numerical parameters (e.g., w), or previously defined variables

Example:

$$f(x) = \exp(xw + \sin(xw)) + \sin^2(xw)x$$

$$\begin{aligned}
v_1 &:= \mathrm{prod}(x, w) \\
v_2 &:= \sin(v_1) \\
v_3 &:= \mathrm{sum}(v_1, v_2) \\
v_4 &:= \mathrm{square}(v_2) \\
v_5 &:= \exp(v_3) \\
v_6 &:= \mathrm{prod}(v_4, x) \\
v_7 &:= \mathrm{sum}(v_5, v_6)
\end{aligned}$$



Computation directed acyclic graph (DAG) $G = (V, E)$

Example (allowing slightly more advanced functions):

$$f(x) = \alpha_0 + \sum_{i=1}^{p} \alpha_i \operatorname{logistic}(x^\top w^{(i)} + b^{(i)})$$

$$\begin{aligned}
v_1 &:= \operatorname{logistic}(x^\top w^{(1)} + b^{(1)}) \\
v_2 &:= \operatorname{logistic}(x^\top w^{(2)} + b^{(2)}) \\
&\;\vdots \\
v_p &:= \operatorname{logistic}(x^\top w^{(p)} + b^{(p)}) \\
\hat{y} &:= \alpha_0 + \alpha_1 \cdot v_1 + \alpha_2 \cdot v_2 + \cdots + \alpha_p \cdot v_p
\end{aligned}$$

- $v_1, \ldots, v_p$ called hidden units (antiquated terminology)
- A single-line using modern numerical software (e.g., pytorch):

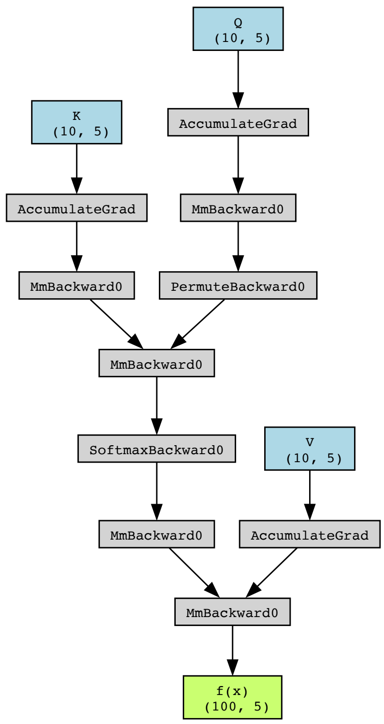
$$\hat{y} := \alpha_0 + \alpha^\top \operatorname{logistic}(Wx + b)$$

Parameters: $W \in \mathbb{R}^{p \times d}$, $b, \alpha \in \mathbb{R}^p$, $\alpha_0 \in \mathbb{R}$
$\operatorname{logistic}\colon \mathbb{R} \to \mathbb{R}$ is applied component-wise

Example (in pytorch):

```python
K = torch.randn(d, p, requires_grad=True)
Q = torch.randn(d, p, requires_grad=True)
V = torch.randn(d, p, requires_grad=True)

def f(x):
  k = x @ K
  q = x @ Q
  a = torch.softmax(k @ q.T, dim=1)
  return a @ x @ V
```



In practice, neural network "architectures" (i.e., program "templates") are built by using/composing component modules

Simplest module is fully-connected layer:

$$h \mapsto \sigma(Wh + b)$$

Affine transformation followed by non-linear transformation

Some examples of non-linear transformations σ:

- Rectified linear unit: $\mathrm{relu}(t) = [t]_+ = \max\{0, t\}$
- Hyperbolic tangent: $\tanh(t) = 2\,\mathrm{logistic}(t) - 1$
- Softmax: $\mathrm{softmax}\colon \mathbb{R}^k \to \mathbb{R}^k$, where $\mathrm{softmax}(u)_i = \frac{\exp(u_i)}{\sum_{j=1}^k \exp(u_j)}$

Q: How to choose the "architecture"?

A: Primary constraint is that functions should be "differentiable" (explained later)

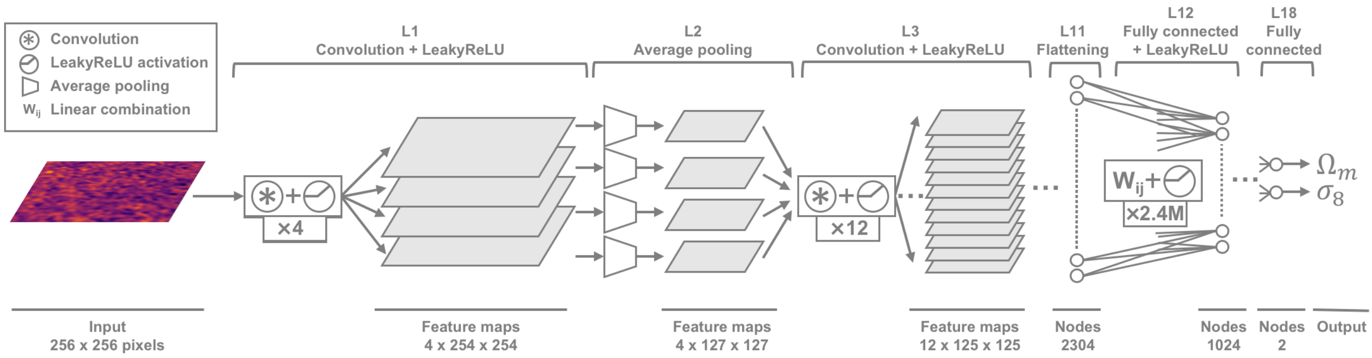
- According to Stone-Weierstrass theorem, two-layer architecture

  $$f(x) = \alpha^{\mathsf{T}} \sigma(Wx)$$

  for $\sigma = \exp$, $\alpha \in \mathbb{R}^p$, $W \in \mathbb{R}^{p \times d}$ is "sufficient" for almost any purpose (provided p is large enough)

- Other architectural designs typically based on application-specific considerations (e.g., convnets), optimization-based empirical observations (e.g., resnets), and/or manual experimentation (e.g., SwiGLU)

- Typical approach: Start from existing architecture that someone already used for a similar problem, and consider small modifications



Problem: How to fit neural network f_θ (with parameters θ) to training data?

- Typical training objective:

$$J(\theta) := \sum_{i=1}^{n} \mathrm{loss}(f_\theta(x^{(i)}), y^{(i)})$$

```
loss = torch.nn.NLLLoss(reduction='sum')
J = loss(f(training_features), training_labels)
```

- Objective function can also be computed using a straight-line program

Amazing fact: Can compute gradient of $J(\theta)$ with respect to θ in (roughly) same amount of time as computing $J(\theta)$ itself (using autodiff, discussed later)

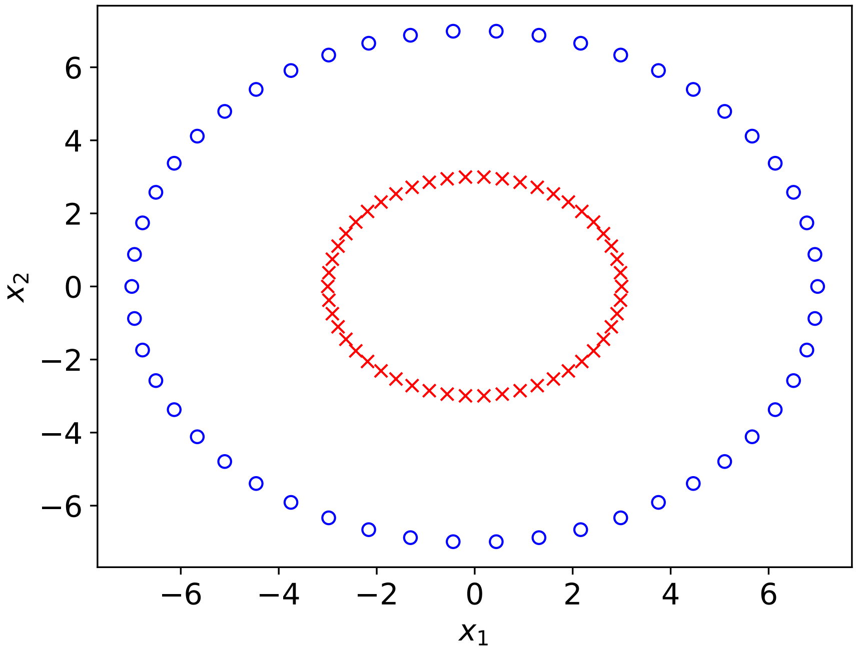
Therefore can use gradient-based methods to (try to) minimize training objective

Main challenge: Objective function $J(\theta)$ might not be convex, so use of gradient-based optimization is more complicated (e.g., initialization, step sizes)

- Many tips and tricks (e.g., "Efficient BackProp", LeCun et al, 1998)
- Ultimately need a lot of experimentation

Synthetic example

Data: classes are two concentric circles, 50 examples per class

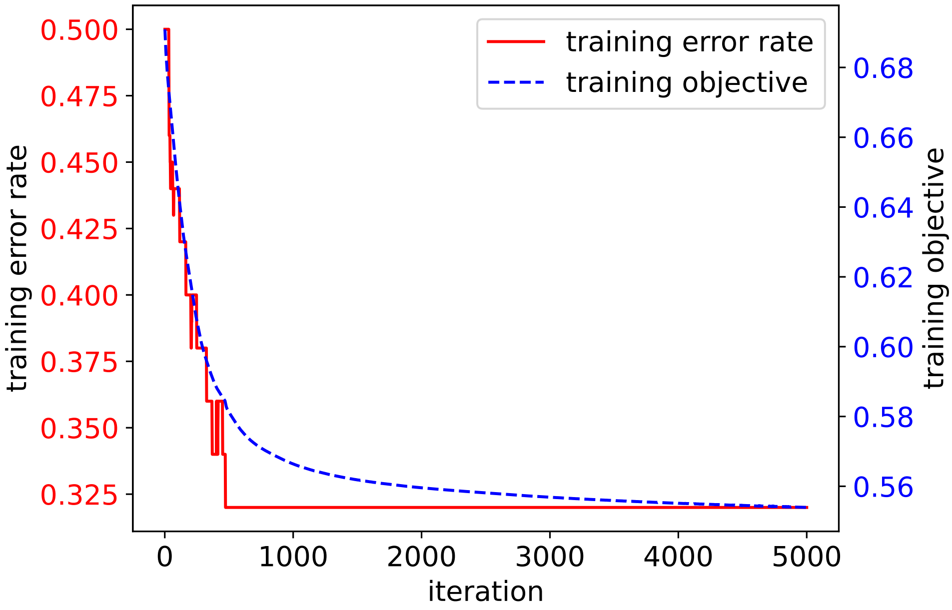


- Feature transformation: standardization
- Neural net: $f(x) = \text{softmax}(A\,\text{relu}(Wx + b) + c)$
  - Parameters: $W \in \mathbb{R}^{p \times 2}$, $b \in \mathbb{R}^p$, $A \in \mathbb{R}^{2 \times p}$, $c \in \mathbb{R}^2$
    (We will vary the "width" p)
  - k-th output is prediction of $\Pr(Y = k \mid X = x)$
- Use gradient descent on average logarithmic loss on training data
  - Random initialization:

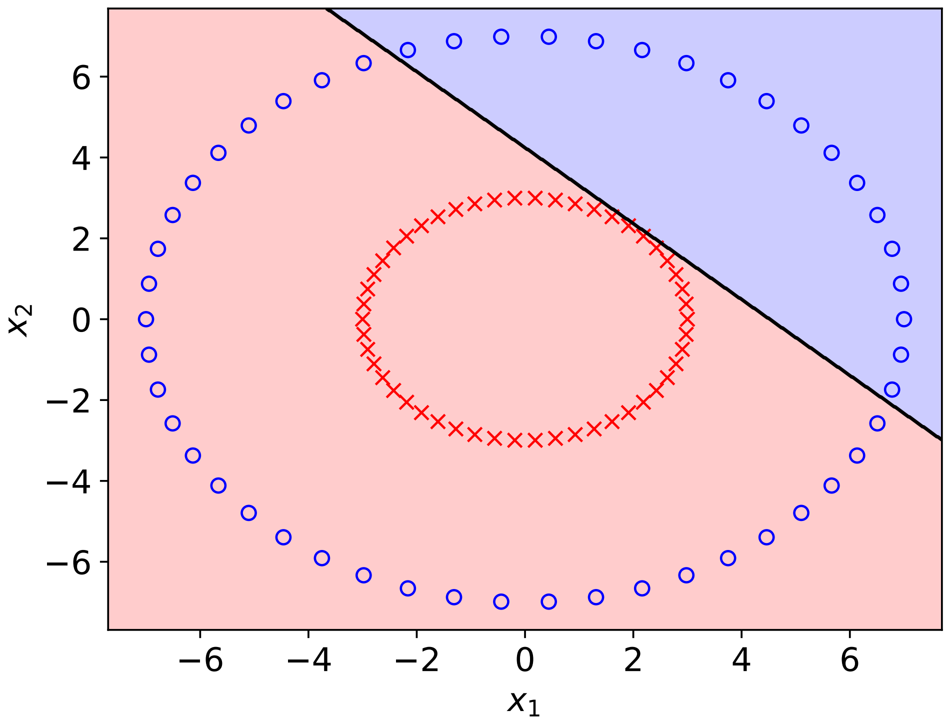
$$W_{i,j}, b_i \overset{\text{i.i.d.}}{\sim} \mathrm{N}(0, \tfrac{1}{3}), \quad A_{i,j}, c_i \overset{\text{i.i.d.}}{\sim} \mathrm{N}(0, \tfrac{2}{p+1})$$

  - Step size: $\eta_t = 0.1$

Results: $p = 2$



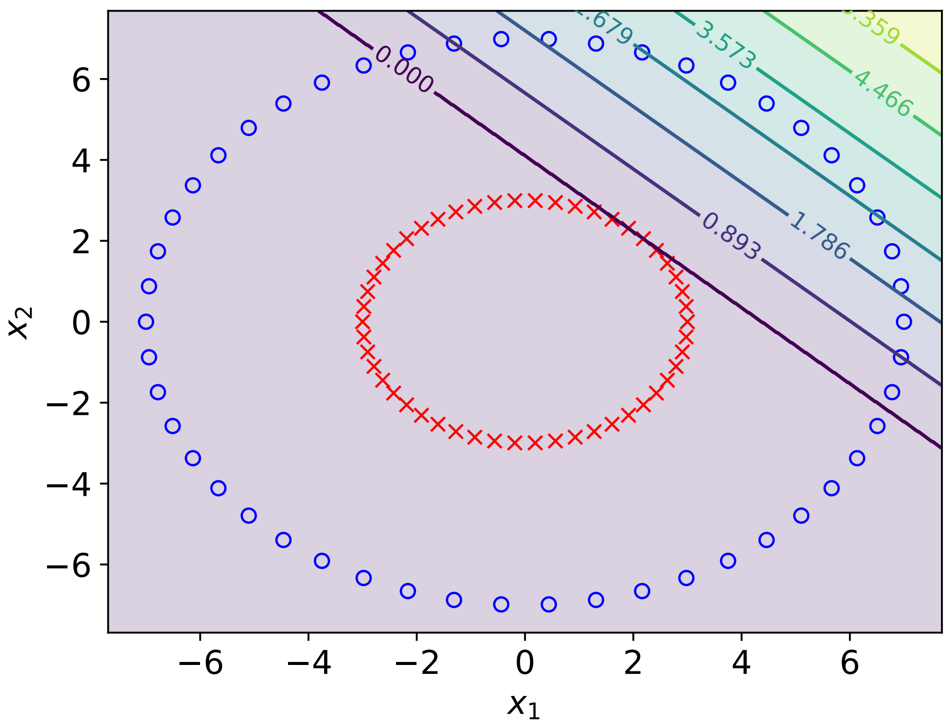
Results: $p = 2$



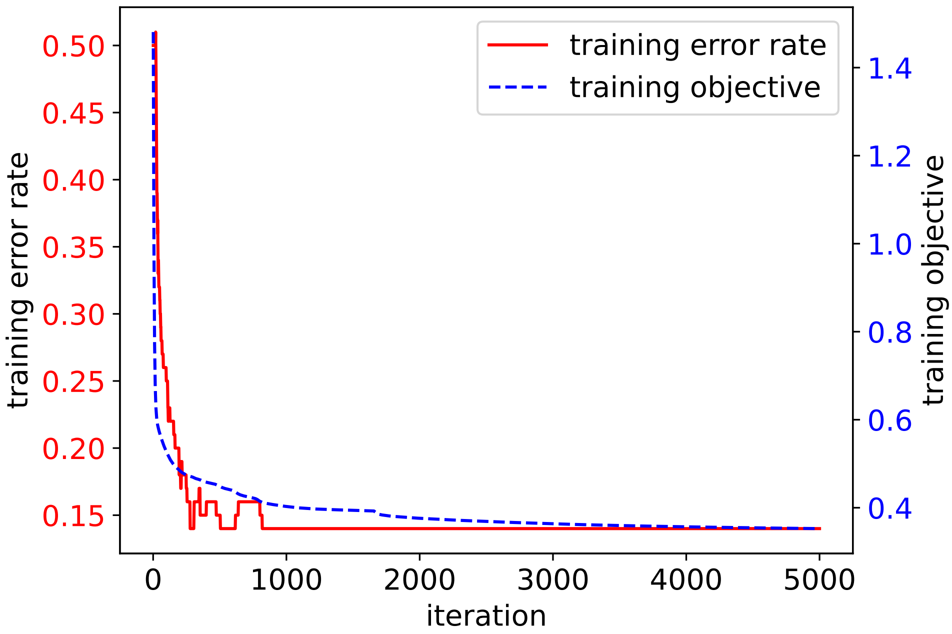
Results: $p = 2$

- Behaves like a linear classifier
- First component of $\mathrm{relu}(Wx + b)$ is constant (0) over training data
- Only second component of $\mathrm{relu}(Wx + b)$ varies over training data

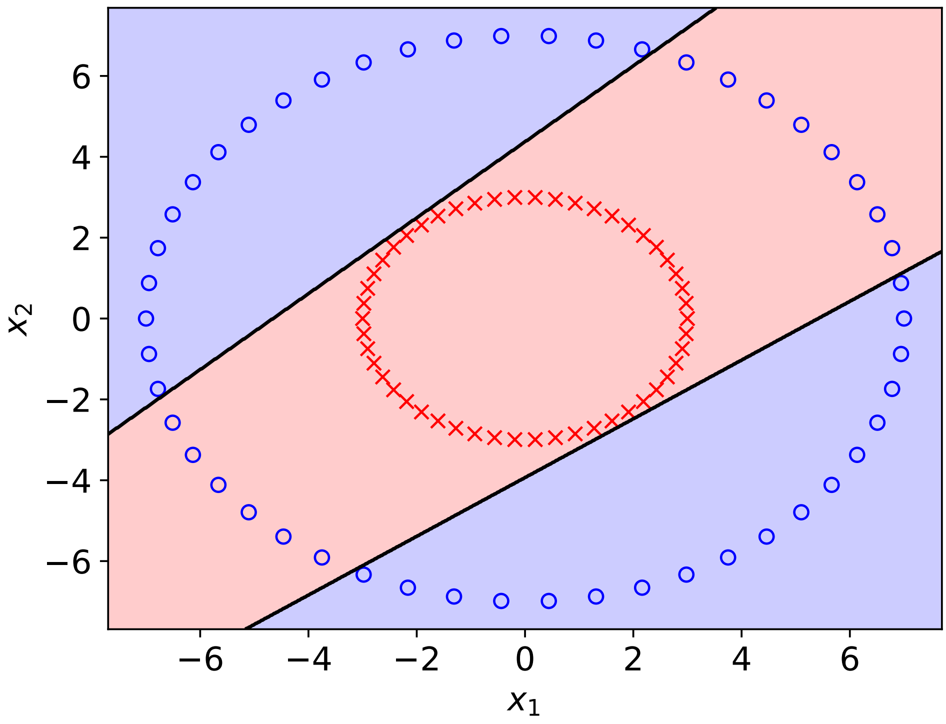
Results: $p = 2$ — second component of $\mathrm{relu}(Wx + b)$



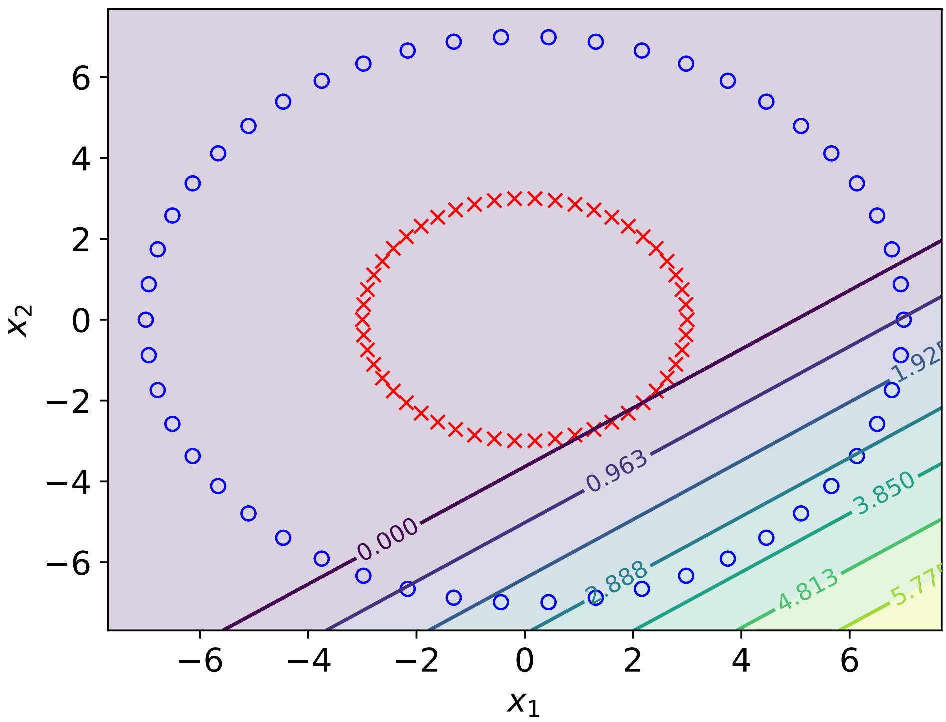
Results: $p = 2$ (different initialization)



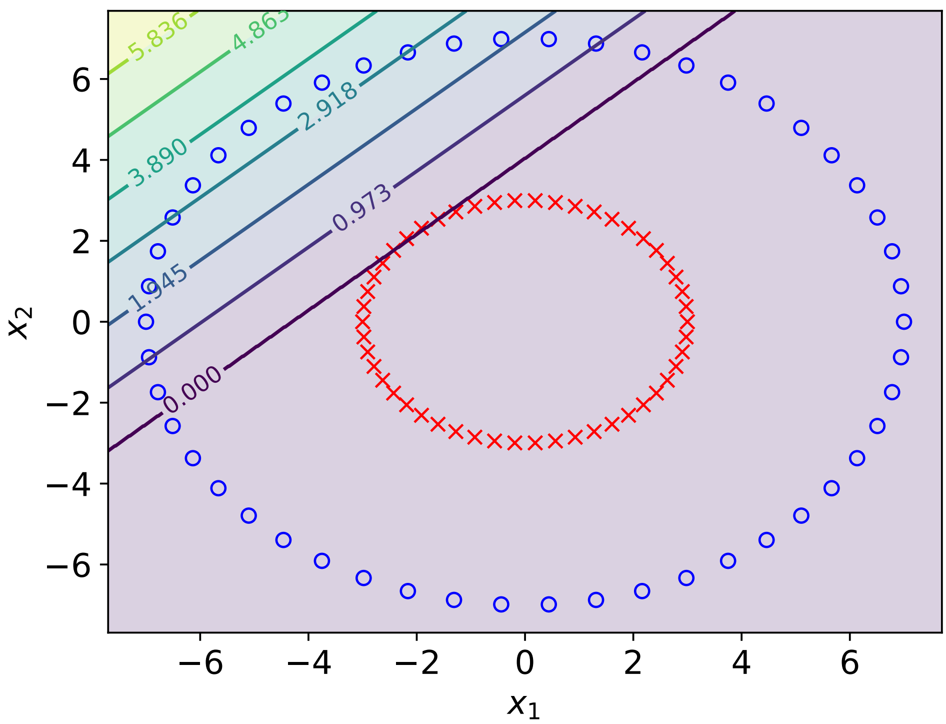
Results: $p = 2$ (different initialization)



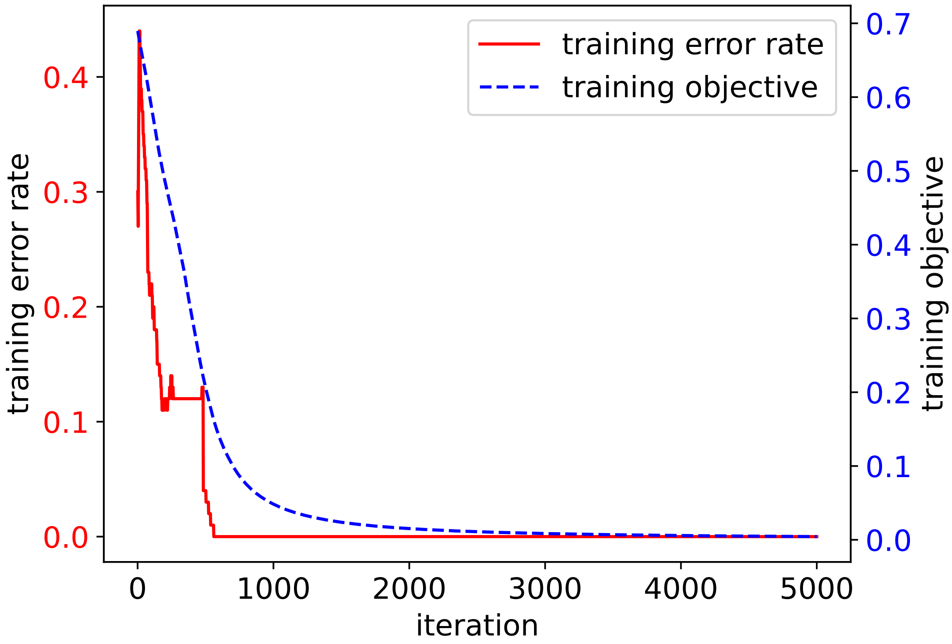
Results: $p = 2$ (different initialization) — first component of $\mathrm{relu}(Wx + b)$



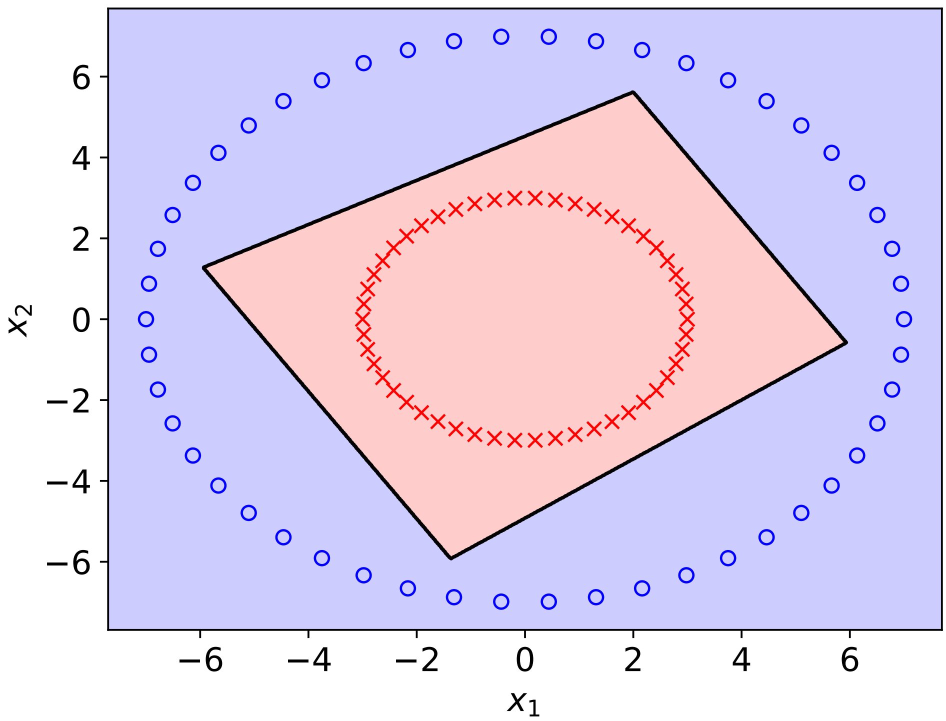
Results: $p = 2$ (different initialization) — second component of $\mathrm{relu}(Wx + b)$



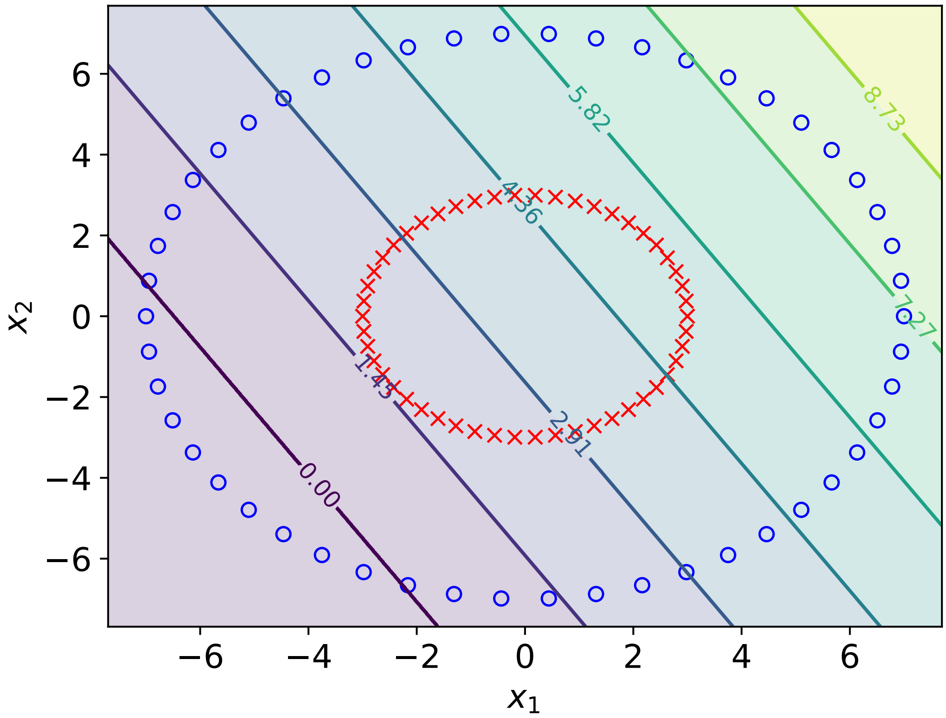
Results: $p = 3$



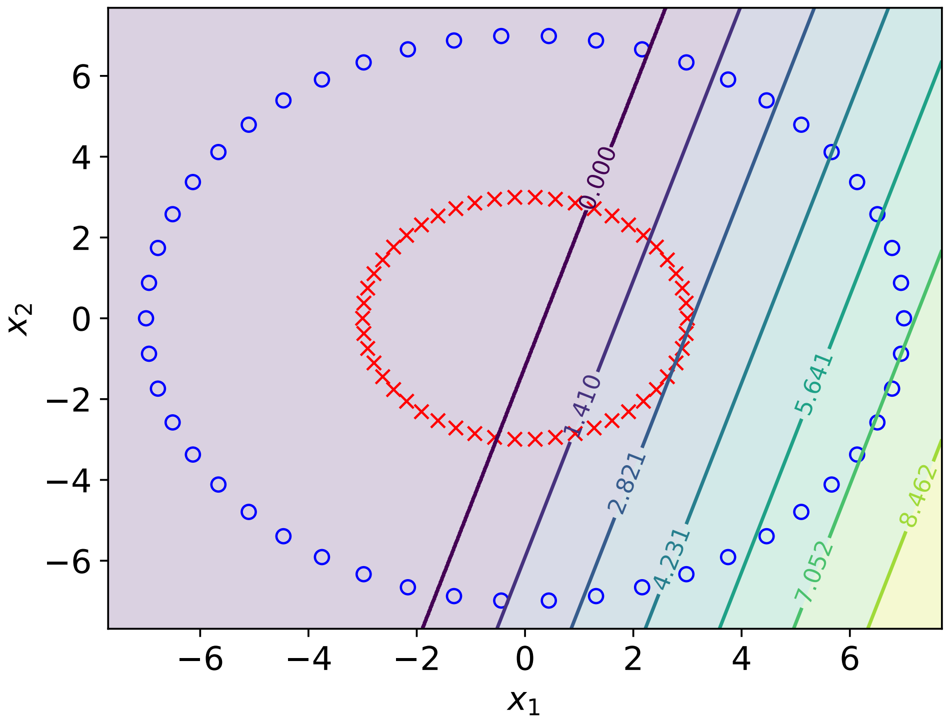
Results: $p = 3$



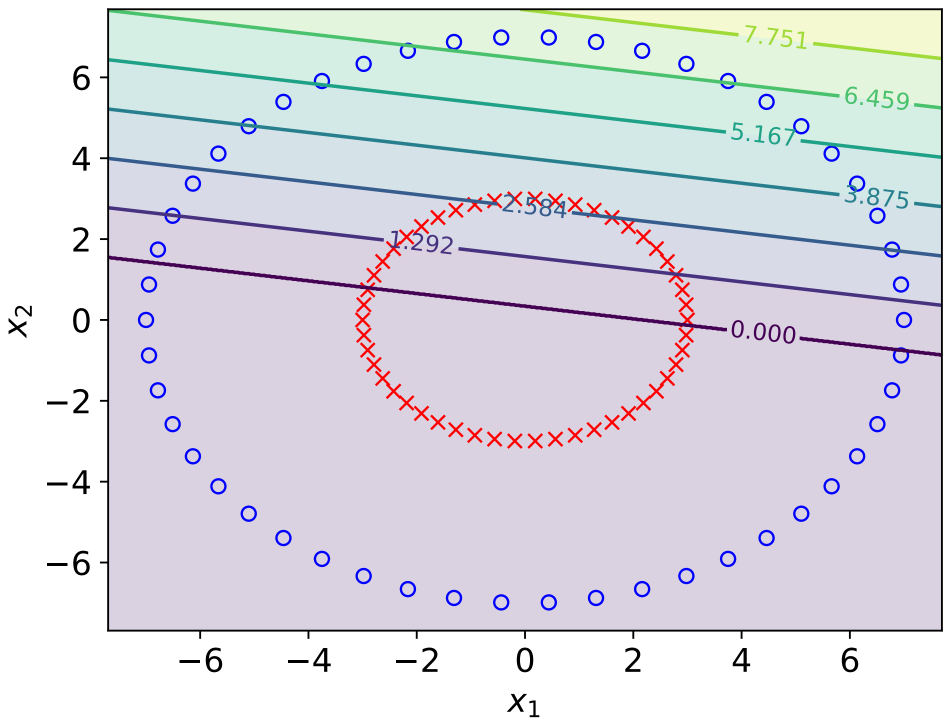
Results: $p = 3$ — first component of $\mathrm{relu}(Wx + b)$



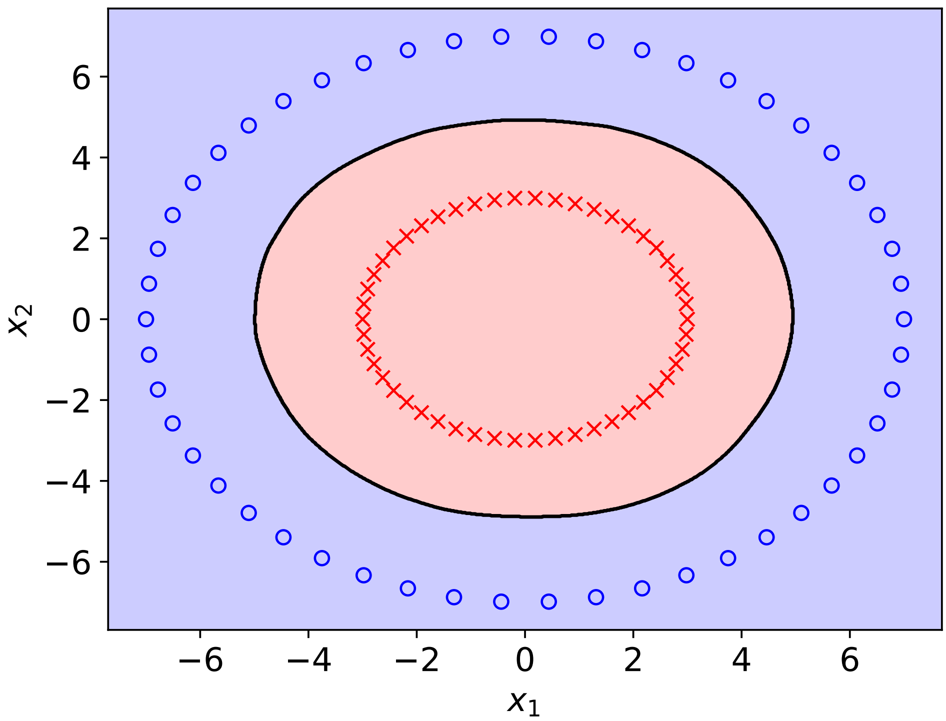
Results: $p = 3$ — second component of $\mathrm{relu}(Wx + b)$



Results: $p = 3$ — third component of $\mathrm{relu}(Wx + b)$



Results: $p = 1000$

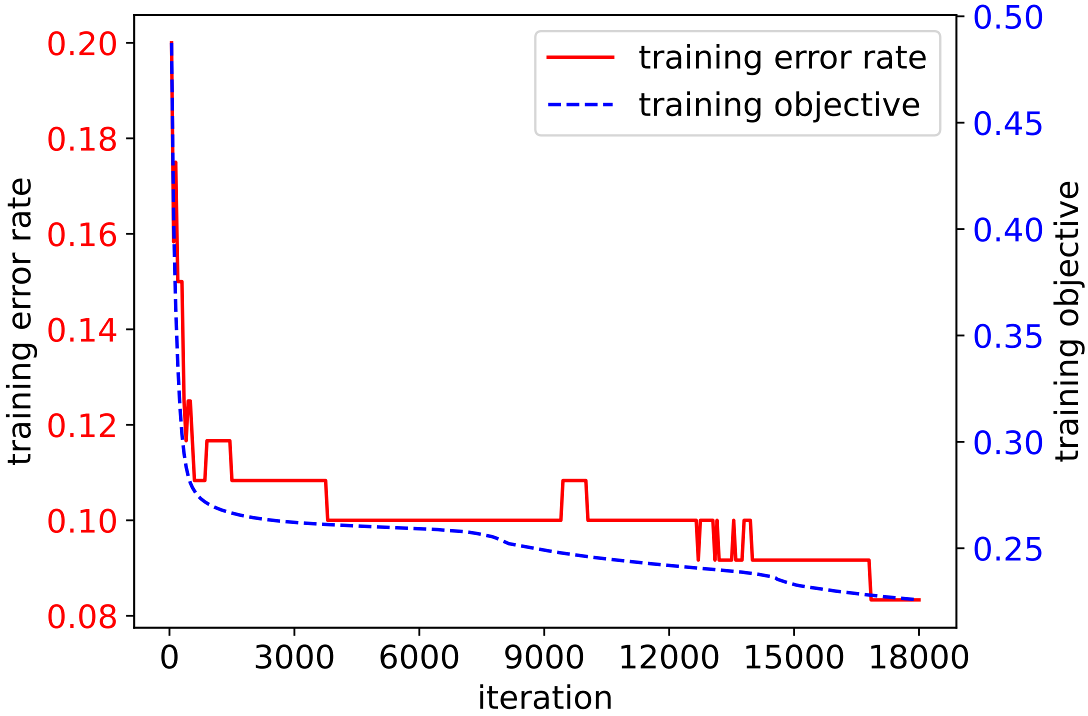


Iris data classifier

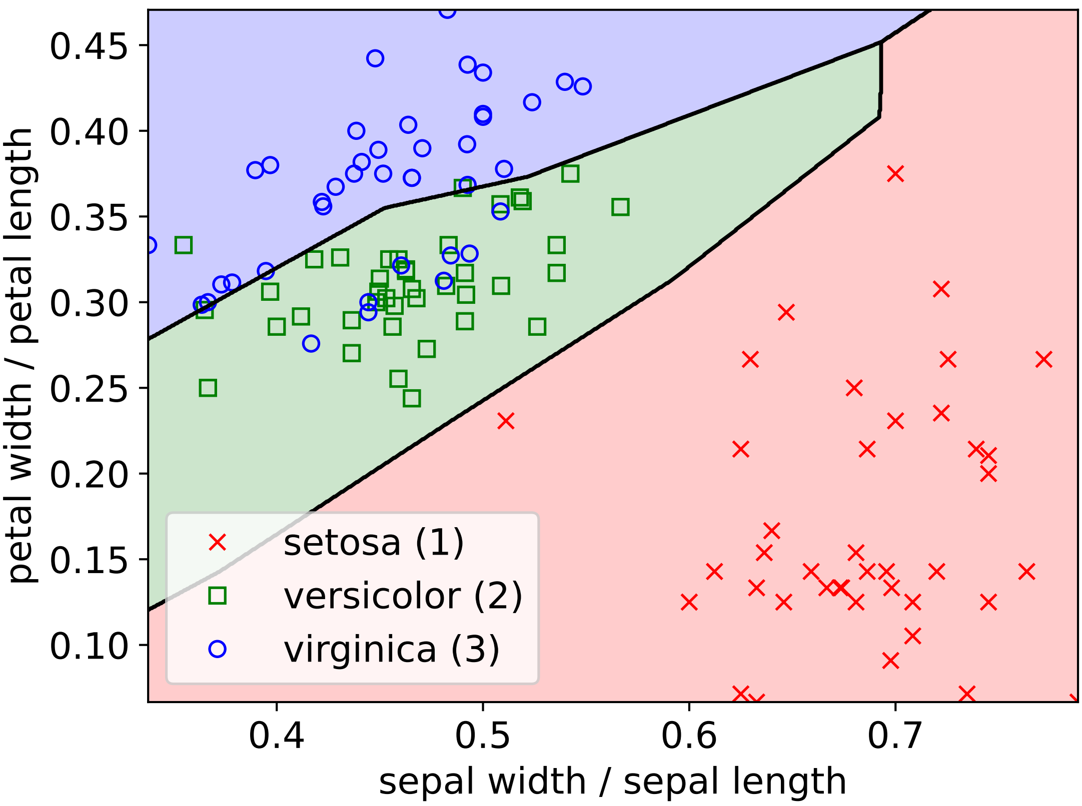
- Features:

$$x_1 = \text{sepal width / sepal length}, \quad x_2 = \text{petal width / petal length}$$

- Neural net: $f(x) = \mathrm{softmax}(A\,\mathrm{relu}(Wx + b) + c)$
  - Parameters: $W \in \mathbb{R}^{10\times 2}$, $b \in \mathbb{R}^{10}$, $A \in \mathbb{R}^{2\times 10}$, $c \in \mathbb{R}^2$
  - k-th output is prediction of $\Pr(Y = k \mid X = x)$
- Feature transformation and training procedure: same as in synthetic example
- Training error rate: 8.33%, test error rate: 10.0%



training error rate
training objective
0.20
0.18
0.16
0.14
0.12
0.10
0.08
0.50
0.45
0.40
0.35
0.30
0.25
0
3000
6000
9000
12000
15000
18000
iteration



setosa (1)
versicolor (2)
virginica (3)
petal width / petal length
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.4
0.5
0.6
0.7
sepal width / sepal length

Deep learning lifestyle

- Since 2006–2012, use of neural networks has exploded in machine learning
- Called "deep learning" due to use of large and "deep" neural networks
  - Use of multiple layers is inspired by some biological systems (e.g., visual system) for processing natural signals
  - Conventional wisdom: very wide but shallow neural network can be replaced by moderately wide but deeper neural network
- Key factors in latest resurgence and success:
  - Graphics processing units (GPUs) to speed-up matrix operations
  - Easy-to-use numerical software with autodiff (e.g., pytorch)
  - Large benchmark datasets (e.g., ImageNet)