Kernel machines
Feature expansions $\varphi: \mathbb{R}^d \rightarrow \mathbb{R}^D$

- In modeling some problems, may not want to assume that target function (e.g., $f(\vec{x}) = \mathbb{E}[Y | \vec{X} = \vec{x}]$) is linear function of $\vec{x}$
- Feature expansions provide a way to “upgrade” linear regression / classification methods to produce non-linear functions / non-hyperplane decision boundaries
- What if you have very little prior knowledge about the target function?
Why polynomials?

**Taylor’s theorem.** For any continuous function $f : \mathbb{R} \to \mathbb{R}$, any $k \in \mathbb{N}$, and any $x_0 \in \mathbb{R}$, if $f$ is "nice" enough, there exists a degree-$k$ polynomial $P : \mathbb{R} \to \mathbb{R}$ such that

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\lim_{x \to x_0} \frac{|f(x) - P(x)|}{|x - x_0|^k} = 0
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- Higher **degree** \( k \) \( \rightarrow \) better approximation (assuming \( f \) is “nice” enough)
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Maybe not so impressive . . .
Weierstrass approximation theorem. For any continuous function $f: \mathbb{R} \to \mathbb{R}$, any bounded interval $[a, b] \subset \mathbb{R}$, and any $\varepsilon > 0$, there exists a polynomial $P: \mathbb{R} \to \mathbb{R}$ such that

$$\max_{x \in [a, b]} |f(x) - P(x)| \leq \varepsilon$$
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**Upshot:** Even with little information about target function, can still hope to get good approximations using polynomials of high-enough degree
Caveat:

▶ In standard IID model, OLS with feature expansion may have bad MSE unless sample size ≫ dimension of feature expansion
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- In standard IID model, OLS with feature expansion may have bad MSE unless sample size \( \gg \) dimension of feature expansion

- Dimension of degree-\( k \) polynomial expansion (in \( \mathbb{R}^d \)): \( \Theta(d^k) \)
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▶ In standard IID model, OLS with feature expansion may have bad MSE unless sample size $\gg$ dimension of feature expansion.

▶ Dimension of degree-$k$ polynomial expansion (in $\mathbb{R}^d$): $\Theta(d^k)$

▶ Saving grace: **inductive bias** (e.g., **data augmentation**, **margins**)
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▶ In standard IID model, OLS with feature expansion may have bad MSE unless sample size $\gg$ dimension of feature expansion

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▶ Saving grace: inductive bias (e.g., data augmentation, margins)

Issue that still remains: **Computation**
Trick to compute dot products quickly (simple case)

Quadratic expansion $\varphi: \mathbb{R}^2 \rightarrow \mathbb{R}^6$: (Don’t mind the $\sqrt{2}$'s)

$$\varphi(x) := (1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, x_2^2, \sqrt{2}x_1x_2)$$

Basic operation needed in feature space: Dot products

$$\varphi(x) \cdot \varphi(z) = 1 + 2x_1z_1 + 2x_2z_2 + x_2^2z_2^2 + 2x_1z_1x_2$$

= $1 + 2(x_1z_1 + x_2z_2) + (x_1z_1 + x_2z_2)^2$

= $(1 + x_1z_1 + x_2z_2)^2$

Some (small) savings! But what about in $\mathbb{R}^d$?
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(6 terms to add)

$$= 1 + 2(x_1z_1 + x_2z_2) + (x_1z_1 + x_2z_2)^2$$
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$$= 1 + 2(x_1z_1 + x_2z_2) + (x_1z_1 + x_2z_2)^2$$

$$= (1 + x_1z_1 + x_2z_2)^2$$

(3 terms to add)
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Some (small) savings! But what about in $\mathbb{R}^d$?
Trick to compute dot products quickly, again

Quadratic expansion $\vec{\varphi}: \mathbb{R}^d \to \mathbb{R}^D$ where $D = 1 + 2d + \binom{d}{2} = \Theta(d^2)$:

$$\vec{\varphi}(\vec{x}) := (1, \sqrt{2}x_1, \ldots, \sqrt{2}x_d, x_1^2, \ldots, x_d^2, \sqrt{2}x_1x_2, \ldots, \sqrt{2}x_{d-1}x_d)$$

- $d$ linear terms
- $d$ square terms
- $\binom{d}{2}$ cross terms
Trick to compute dot products quickly, again

Quadratic expansion $\phi: \mathbb{R}^d \to \mathbb{R}^D$ where $D = 1 + 2d + \binom{d}{2} = \Theta(d^2)$:

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$d$ linear terms $d$ square terms $\binom{d}{2}$ cross terms

Dot products $\phi(x) \cdot \phi(z)$:

$$\phi(x) \cdot \phi(z) = (1 + x \cdot z)^2 \quad \text{(only $d + 1$ terms to add)}$$
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Naïve implementation to compute dot product: $\Theta(d^2)$ time; Using the trick: $\Theta(d)$
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\( \varphi(x) \) consists of:
- \( d \) linear terms
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Degree-\( k \) polynomial expansion \( \varphi: \mathbb{R}^d \to \mathbb{R}^D \) where \( D = \Theta(d^k) \):

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$$\varphi(\bar{x}) := (1, \sqrt{2}x_1, \ldots, \sqrt{2}x_d, x_1^2, \ldots, x_d^2, \sqrt{2}x_1x_2, \ldots, \sqrt{2}x_{d-1}x_d)$$

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But how about dot products between $\varphi(x)$ and weight vector $\vec{w} \in \mathbb{R}^D$?
**Observation:** Many “linear” learning methods yield $\vec{w}$ in the span of the training feature vectors

- OLS, ridge regression, PCR, SVM, PCA
- Gradient descent, SGD (on SSE & SLL objectives) if initialized at zero
- Perceptron, Online Perceptron
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When used with feature expansion $\vec{\varphi}: \mathbb{R}^d \to \mathbb{R}^D$, this means there exist $\alpha_1, \ldots, \alpha_n \in \mathbb{R}$ such that

$$\vec{w} = \sum_{i=1}^{n} \alpha_i \vec{\varphi}(\vec{x}_i)$$

where $(\vec{x}_1, y_1), \ldots, (\vec{x}_n, y_n)$ are the training examples

I.e., there’s an implicit representation of $\vec{w}$ in terms of $\vec{\alpha} := (\alpha_1, \ldots, \alpha_n) \in \mathbb{R}^n$ & training examples
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To compute \( \phi(\mathbf{x}) \cdot \mathbf{w} \), can use

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\phi(\mathbf{x}) \cdot \mathbf{w} = \sum_{i=1}^{n} \alpha_i (\phi(\mathbf{x}) \cdot \phi(\mathbf{x}_i))
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$$\varphi(\vec{x}) \cdot \vec{w} = \sum_{i=1}^{n} \alpha_i \left( \varphi(\vec{x}) \cdot \varphi(\vec{x}_i) \right)$$

But how do you get the $\alpha_i$’s?
Perceptron with feature expansion

Given: Training data \((\vec{x}_1, y_1), \ldots, (\vec{x}_n, y_n) \in \mathbb{R}^d \times \{0, 1\}\)

**Perceptron** with feature map \(\vec{\phi}: \mathbb{R}^d \to \mathbb{R}^D\)

- Initialize \(\vec{w} := \vec{0} \in \mathbb{R}^D\)
- Loop:
  - Pick any example \((\vec{x}_i, y_i)\) that is misclassified by \(\vec{w}\)
  - (If there is no such example, halt and return \(\vec{w}\))
  - Update \(\vec{w}\):
    
    \[
    \vec{w} := \begin{cases} 
    \vec{w} + \vec{\phi}(\vec{x}_i) & \text{if } y_i = 1 \\
    \vec{w} - \vec{\phi}(\vec{x}_i) & \text{if } y_i = 0
    \end{cases}
    \]
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    \end{cases}
    \]
- Initialize \(\alpha_i := 0\) for all \(i = 1, \ldots, n\)
Perceptron with feature expansion

Given: Training data $(\vec{x}_1, y_1), \ldots, (\vec{x}_n, y_n) \in \mathbb{R}^d \times \{0, 1\}$

**Perceptron** with feature map $\vec{\phi}: \mathbb{R}^d \rightarrow \mathbb{R}^D$

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    \end{cases}
    $$
- Initialize $\alpha_i := 0$ for all $i = 1, \ldots, n$
- Update with example $(\vec{x}_i, y_i)$:
  $$
  \alpha_i := \begin{cases} 
  \alpha_i + 1 & \text{if } y_i = 1 \\
  \alpha_i - 1 & \text{if } y_i = 0 
  \end{cases}
  $$
Ridge regression with feature expansion

Given: Training data \((\vec{x}_1, y_1), \ldots, (\vec{x}_n, y_n) \in \mathbb{R}^d \times \mathbb{R}\)

\[
A := \begin{bmatrix}
\leftarrow & \vec{\phi}(\vec{x}_1)^T & \rightarrow \\
\vdots & & \\
\leftarrow & \vec{\phi}(\vec{x}_n)^T & \rightarrow
\end{bmatrix} \in \mathbb{R}^{n \times D}, \quad \vec{b} := \begin{bmatrix}
y_1 \\
\vdots \\
y_n
\end{bmatrix} \in \mathbb{R}^n
\]
Ridge regression with feature expansion

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\vdots \\
y_n \end{bmatrix} \in \mathbb{R}^n
\]

Fact: \((A^T A + \lambda I)^{-1} A^T = A^T (A A^T + \lambda I)^{-1}\) for any \(\lambda > 0\)
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Fact: \((A^TA + \lambda I)^{-1}A^T = A^T(AA^T + \lambda I)^{-1}\) for any \(\lambda > 0\)

Therefore, ridge regression solution \(\vec{w}\) can be written as

\[
\vec{w} = A^T \underbrace{(AA^T + \lambda I)^{-1}\vec{b}}_{\vec{\alpha}} = \sum_{i=1}^{n} \alpha_i \vec{\varphi}(\vec{x}_i)
\]
Ridge regression with feature expansion

Given: Training data \((\vec{x}_1, y_1), \ldots, (\vec{x}_n, y_n) \in \mathbb{R}^d \times \mathbb{R}\)

\[
A := \begin{bmatrix}
\vec{\varphi}(\vec{x}_1)^T \\
\vdots \\
\vec{\varphi}(\vec{x}_n)^T
\end{bmatrix} \in \mathbb{R}^{n \times D}, \quad \vec{b} := \begin{bmatrix}
y_1 \\
\vdots \\
y_n
\end{bmatrix} \in \mathbb{R}^n
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\[
\vec{w} = A^T (A A^T + \lambda I)^{-1} \vec{b} = \sum_{i=1}^{n} \alpha_i \vec{\varphi}(\vec{x}_i)
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Moreover, matrix \(K := A A^T \in \mathbb{R}^{n \times n}\) is matrix of inner products (a.k.a. Gram matrix)

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K_{i,j} = \vec{\varphi}(\vec{x}_i) \cdot \vec{\varphi}(\vec{x}_j)
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So, compute Gram matrix \(K\) and solve linear system \((K + \lambda I)\vec{\alpha} = \vec{b}\) for \(\vec{\alpha}\)
Comparing computational costs when using degree-$k$ polynomial expansion (assume $d \ll n \ll d^k$):

- **Ridge regression with explicit feature expansion**:
  - Solving for $\vec{w}$: $O(n^2d^k)$ time
  - Each prediction: $O(d^k)$ time

- **Ridge regression using implicit representation of $\vec{w}$**:
  - Solving for $\vec{\alpha}$: $O(n^3)$ time
  - Each prediction: $O(nd)$ time
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Many other feature expansions (besides polynomial expansion) have a similar computational trick to compute dot products.
Kernels

- Many other feature expansions (besides polynomial expansion) have a similar computational trick to compute dot products.
- Conversely, many easy-to-compute “similarity functions” $k(\vec{x}, \vec{z})$ are, in fact, the dot product between certain feature expansions $\vec{\varphi}(\vec{x})$ and $\vec{\varphi}(\vec{z})$.
Many other feature expansions (besides polynomial expansion) have a similar computational trick to compute dot products.

Conversely, many easy-to-compute “similarity functions” \( k(\mathbf{x}, \mathbf{z}) \) are, in fact, the dot product between certain feature expansions \( \varphi(\mathbf{x}) \) and \( \varphi(\mathbf{z}) \).

Such similarity functions are called (positive definite) kernels.
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Such similarity functions are called (positive definite) kernels.

E.g., Gaussian kernel

\[
k(\vec{x}, \vec{z}) = \exp\left(-\frac{\|\vec{x} - \vec{z}\|_2^2}{2\sigma^2}\right)
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where \( \sigma > 0 \) is the “bandwidth” of the kernel (a hyperparameter).
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Technically, the feature expansion $\vec{\varphi}: \mathbb{R}^d \rightarrow \mathbb{R}^D$ may need $D = \infty$. 
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E.g., **Gaussian kernel**

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Not a problem when using **kernel methods** (i.e., versions of ridge regression, Perceptron, etc. that only compute $\vec{\alpha} = (\alpha_1, \ldots, \alpha_n)$).
Kernels

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▶ Resulting predictors with implicit representation

\[
g(\vec{x}) = \sum_{i=1}^{n} \alpha_i \, k(\vec{x}, \vec{x}_i)
\]

are called kernel machines
Neural networks
What else is there besides polynomials?

**Weierstrass approximation theorem:**
- Can approximate any continuous function using polynomials provided degree is high enough

**Stone-Weierstrass approximation theorem:**

(via Hornik, Stinchcombe, & White, 1989)

- Can approximate any continuous function using functions of form

\[ g(\vec{x}) = \sum_{i=1}^{D} \alpha_i \exp(\vec{x} \cdot \vec{w}_i) \]

provided \( D \) is large enough

- Both the \( \alpha_i \)'s and \( \vec{w}_i \)'s may need to depend on the target function
- Can replace \( \exp \) with other "activation functions" and approximation property still holds

Another interpretation:
- Can approximate any continuous function by linear function with feature expansion

\[ \vec{\phi}(\vec{x}) = (\exp(\vec{x} \cdot \vec{w}_1), \ldots, \exp(\vec{x} \cdot \vec{w}_m)) \]

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- Called a neural network
Kernel machines vs. neural networks

Kernel machine (with kernel $k$)

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

Only $\alpha_i$'s are learned

Neural network (with exp activation)

$$g(\vec{x}) = \sum_{i=1}^{D} \alpha_i \ \exp(\vec{x} \cdot \vec{w}_i)$$

Both $\alpha_i$'s and $\vec{w}_i$'s are learned
Can use $D > n$
Anatomy of a neural network

- **Top layer:** output of function
  
  \[ g(\vec{x}) = D \sum_{i=1}^{X} \alpha_i h_i(\vec{x}) + \alpha_0 \]
  
  (Sometimes also apply an activation function to output)

- **Middle layer:** hidden units (a.k.a. neurons)
  
  Each hidden unit computes composition of activation function \( \sigma_i \) with affine function of input
  
  \[ h_i(\vec{x}) = \sigma_i(\vec{x} \cdot \vec{w}_i + b_i) \]

- **Bottom layer:** input \( \vec{x} = (x_1, \ldots, x_d) \) to function

Arrows in diagram depict functional dependence

Parameters: \( \vec{w}_i \)'s, \( b_i \)'s, and \( \alpha_i \)'s
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\begin{itemize}
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\end{itemize}
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Neural network as a straight-line program

(Generalized) straight-line program that implements the neural network function:

\[ u_1 := \vec{x} \cdot \vec{w}_1 + b_1 \]
\[ v_1 := \sigma_1(u_1) \]
\[ u_2 := \vec{x} \cdot \vec{w}_2 + b_2 \]
\[ v_2 := \sigma_2(u_2) \]

\[ \vdots \]
\[ u_D := \vec{x} \cdot \vec{w}_D + b_D \]
\[ v_D := \sigma_D(u_D) \]

\[ \text{out} := \alpha_1 \times v_1 + \cdots + \alpha_D \times v_D + \alpha_0 \]
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(This is useful for the “forward pass” in autodiff!)
Neural network as a straight-line program, again

(Generalized) straight-line program that implements the neural network function:

\[
\vec{u} := W \vec{x} + \vec{b} \\
\vec{v} := \sigma(\vec{u}) \\
\text{out} := \vec{\alpha} \cdot \vec{v} + \alpha_0
\]

Parameters: \( W = [\vec{w}_1 | \cdots | \vec{w}_D]^T \in \mathbb{R}^{D \times d}, \vec{b} = (b_1, \ldots, b_D) \in \mathbb{R}^D, \vec{\alpha} = (\alpha_1, \ldots, \alpha_D) \in \mathbb{R}^D, \alpha_0 \in \mathbb{R} \)

In code above, vector-valued activation function \( \sigma: \mathbb{R}^D \rightarrow \mathbb{R}^D \) applies \( \sigma_i \) to \( i \)-th coordinate of input.
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Some other common activation functions:

- Heaviside (a.k.a. step function): \( \sigma_i(z) = \begin{cases} 1 & \text{if } z > 0 \\ 0 & \text{otherwise} \end{cases} \) (popular in 1940s)
- Sigmoid (a.k.a. logistic): \( \sigma_i(z) = \frac{1}{1 + e^{-z}} \) (popular since 1970s)
- Rectified Linear Unit (ReLU): \( \sigma_i(z) = \max\{0, z\} \) (popular since 2012)
- "Softmax": \( \sigma(\vec{z}) = \frac{e^{z_1}}{\sum_{i=1}^{D} e^{z_i}} \) (a.k.a. normalized exponential function, \( \mathbb{R}^D \rightarrow \mathbb{R}^D \); terrible naming choice)
- Max pooling: \( \sigma(\vec{z}) = \max\{z_1, \ldots, z_D\} \) (a.k.a. local max function, \( \mathbb{R}^D \rightarrow \mathbb{R}^1 \); popular in computer vision)
- Identity: \( \sigma_i(z) = z \) (you might be surprised . . . )
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\vec{u} &:= W \vec{x} + \vec{b} \\
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\end{align*}
\]

Parameters: \(W = [\vec{w}_1 | \cdots | \vec{w}_D]^T \in \mathbb{R}^{D \times d}, \vec{b} = (b_1, \ldots, b_D) \in \mathbb{R}^D, \vec{\alpha} = (\alpha_1, \ldots, \alpha_D) \in \mathbb{R}^D, \alpha_0 \in \mathbb{R}\)

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\[ \text{out} := \vec{\alpha} \cdot \vec{v} + \alpha_0 \]

Parameters: \( W = [\vec{w}_1 | \cdots | \vec{w}_D]^{\top} \in \mathbb{R}^{D \times d} \), \( \vec{b} = (b_1, \ldots, b_D) \in \mathbb{R}^D \), \( \vec{\alpha} = (\alpha_1, \ldots, \alpha_D) \in \mathbb{R}^D \), \( \alpha_0 \in \mathbb{R} \)

In code above, vector-valued activation function \( \sigma : \mathbb{R}^D \to \mathbb{R}^D \) applies \( \sigma_i \) to \( i \)-th coordinate of input

Some other common activation functions:

- **Heaviside (a.k.a. step function):** \( \sigma_i(z) = 1 \{ z > 0 \} \) (popular in 1940s)
- **Sigmoid (a.k.a. logistic):** \( \sigma_i(z) = 1 / (1 + e^{-z}) \) (popular since 1970s)
- **Rectified Linear Unit (ReLU):** \( \sigma_i(z) = \max\{0, z\} \) (popular since 2012)
- **“Softmax”:** \( \sigma(\tilde{z}) = (e^{\tilde{z}_1}, \ldots, e^{\tilde{z}_D}) / \sum_{i=1}^{D} e^{\tilde{z}_i} \) (\( \mathbb{R}^D \to \mathbb{R}^D \); terrible naming choice)
- **Max pooling:** \( \sigma(\tilde{z}) = \max\{z_1, \ldots, z_D\} \) (\( \mathbb{R}^D \to \mathbb{R}^1 \); popular in computer vision)
Neural network as a straight-line program, again

(Generalized) straight-line program that implements the neural network function:

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Parameters: \( W = [\vec{w}_1 | \cdots | \vec{w}_D]^T \in \mathbb{R}^{D \times d}, \vec{b} = (b_1, \ldots, b_D) \in \mathbb{R}^D, \vec{\alpha} = (\alpha_1, \ldots, \alpha_D) \in \mathbb{R}^D, \alpha_0 \in \mathbb{R} \)

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- Identity: \( \sigma_i(z) = z \) (you might be surprised . . .)
Modern lingo:

▶ Parameterized function = “neural network”
▶ Function template = “architecture”
More neural networks

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Second one just needs a few extra lines . . .
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To approximate certain functions, may be more size-economical to use multiple layers of hidden units
Fitting neural networks to data

**Generic strategy:**
- **Goal:** For $(\vec{X}, Y) \sim P$,

  $$\min_{f: \mathbb{R}^d \to \mathbb{R}} \mathbb{E}[\ell(Y, f(\vec{X}))]$$

  where $\ell(y, p)$ is loss function (e.g., square loss, zero-one loss, logarithmic loss)
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- **Use empirical distribution** \(P_n\) as plug-in estimate of \(P\) to get training objective \(J\)
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  (Autodiff is very helpful here!)
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Note: $J$ is typically not convex function of neural network parameters \(_\(\_\)(\_)/_\)
Practical issues: Optimization

- Objective is often not convex function of parameters, and often has saddle point at zero
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- Run SGD starting from randomly chosen parameter values

- Many heuristics available for initial parameter distribution
  - These heuristics often rely on inputs $\vec{x}$ being standardized and/or uncorrelated (PCA can help!)

- No single step size for SGD will work well for all problems
  - Many heuristics available for choosing “schedule” of step sizes

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  ![Graph showing a non-convex function with a saddle point at zero.]
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  - Entire research communities (e.g., natural language processing, computer vision, compbio) devote considerable effort to finding good architectures for their problems
  - Some choices are driven by goal of making optimization easier
    - E.g., differentiable activation functions, very wide layers of hidden units

But no panacea
Kernel machines and neural networks are powerful approaches to go beyond linear predictors.

In practice, more flexibility with neural networks (for better and/or for worse)

Autodiff and autodiff software has made a big difference.

No single solution works well for all problems.