Feature learning, neural networks and backpropagation

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(Slides credit to David Rosenberg, He He, et al.)

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Today's lecture

- Neural networks: huge empirical success but poor theoretical understanding

- Key idea: representation learning

- Optimization: backpropagation + SGD

Feature engineering

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- For example, we can use a feature map that defines a kernel, e.g., polynomials in x

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- Example: predicting how popular a restaurant is

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  - $h_2([\text{zip code}]) = \text{walkable}$
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- A final *linear* predictor uses the **intermediate features** computed by the h_i's:

$$w_1 \cdot \text{food quality} + w_2 \cdot \text{walkable} + w_3 \cdot \text{noisy}$$

- Suppose that our input features indicate light at a two points in space (0 = no light; 1 = light)

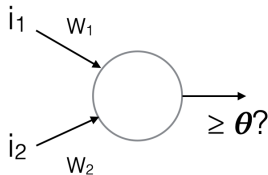- How can we build a perceptron that detects when there is light in both locations?

$$w_1 = 1, w_2 = 1, \theta = 2$$
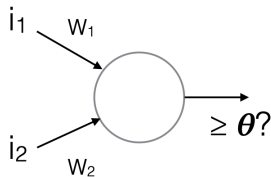
i_1	i_2	$w_1 i_1 + w_2 i_2$
0	0	0
0	1	1
1	0	1
1	1	2

Limitations of a perceptrons as logical gates

- Can we build a perceptron that fires when the two pixels have the same value ($i_1 = i_2$)?

Positive: (1, 1)   (0, 0)

$$w_1 + w_2 \geq \theta, \quad 0 \geq \theta$$
$$w_1 < \theta, \quad w_2 < \theta$$

Negative: (1, 0)   (0, 1)
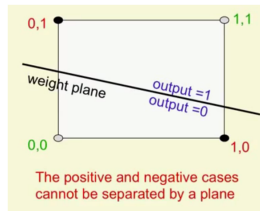
If θ is negative, the sum of two numbers that are both less than θ cannot be greater than θ

The positive and negative cases cannot be separated by a plane

Multilayer perceptron

- Fire when the two pixels have the same value ($i_1 = i_2$)

	i_1	i_2	h_1	h_2	h_1	h_2	o
			Hidden layer input		Hidden layer output		
x_1	0	0	0	0	0	1	1
o_1	0	1	1	-1	0	0	0
o_2	1	0	1	-1	0	0	0
x_2	1	1	2	-2	1	0	1

(for x_1 and x_2 the correct output is 1; for o_1 and o_2 the correct output is 0)

Multilayer perceptron

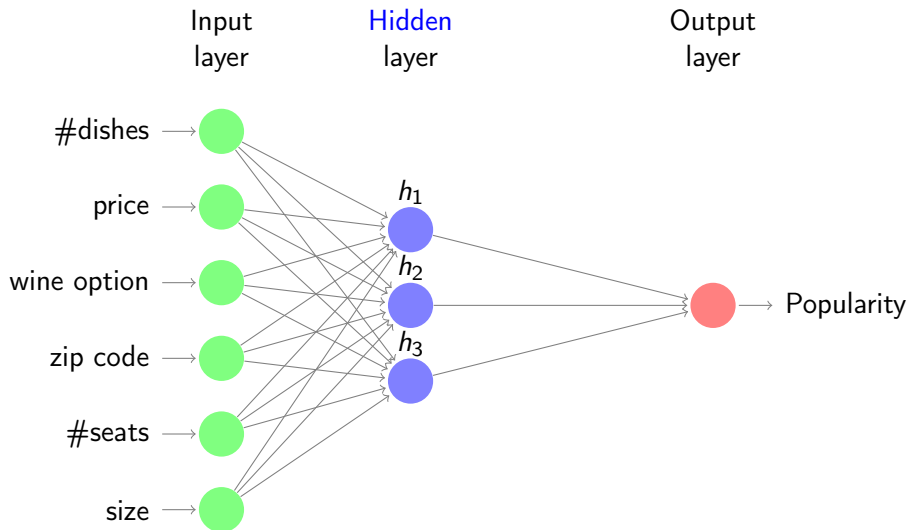- Recode the input: the hidden layer representations are now linearly separable
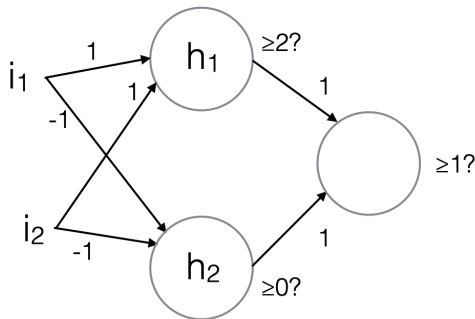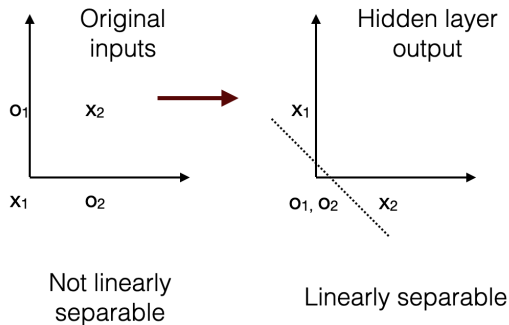
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	i_1	i_2	h_1	h_2	h_1	h_2	o
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Original inputs

Hidden layer output

Not linearly separable

Linearly separable

Decomposing the problem into predefined subproblems
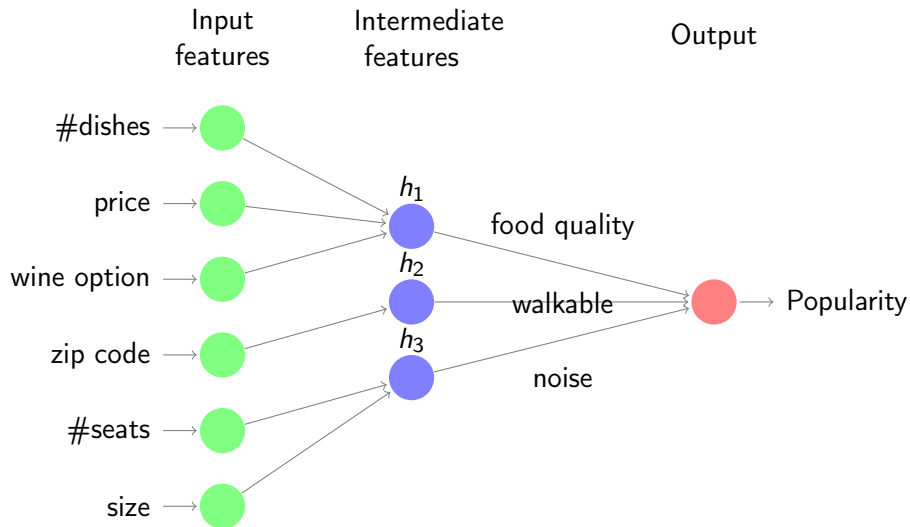
Learned intermediate features

Neural networks

Key idea: learn the intermediate features.

Feature engineering Manually specify $\phi(x)$ based on domain knowledge and learn the weights:
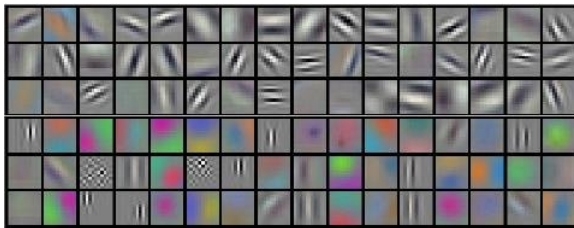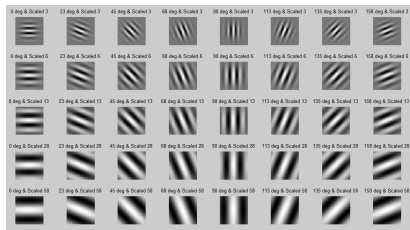
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Feature learning Learn both the features (K hidden units) and the weights:

$$h(x) = [h_1(x), \ldots, h_K(x)], \tag{3}$$

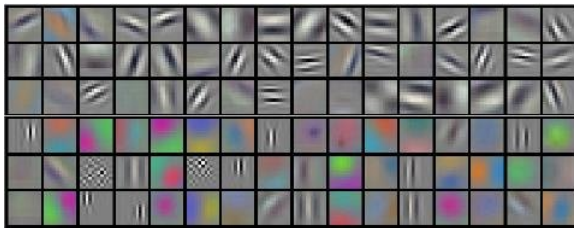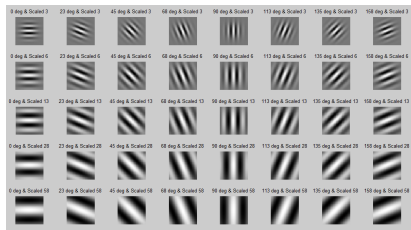$$f(x) = w^T h(x) \tag{4}$$

Feature learning example

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- Neural networks take in images and can learn the filters that are the most useful for solving the tasks. Likely more efficient than hand engineered features.
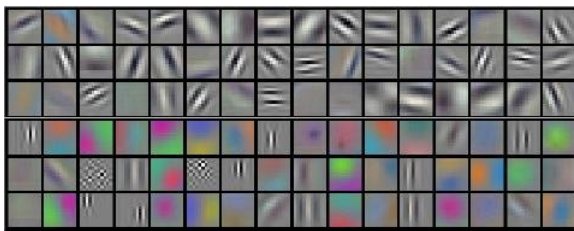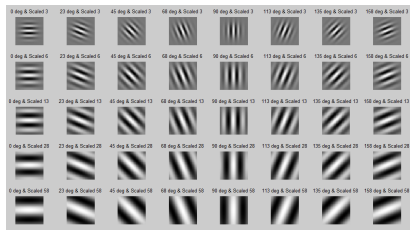
Inspiration: The brain

- Our brain has about 100 billion (10^{11}) neurons, each of which communicates (is connected) to $\sim 10^4$ other neurons, with non-linear computations.
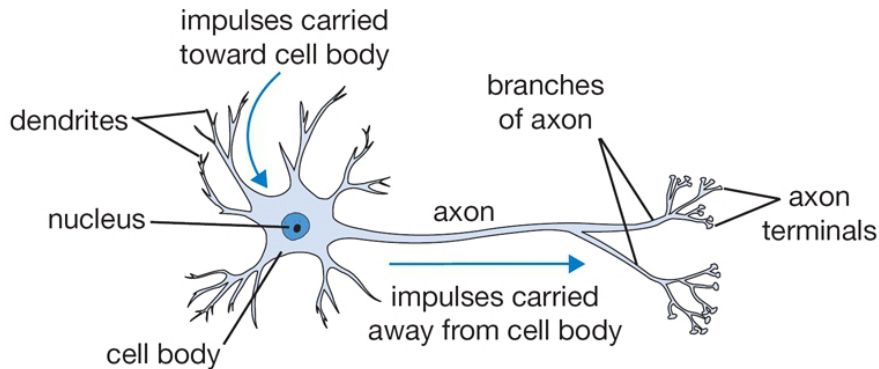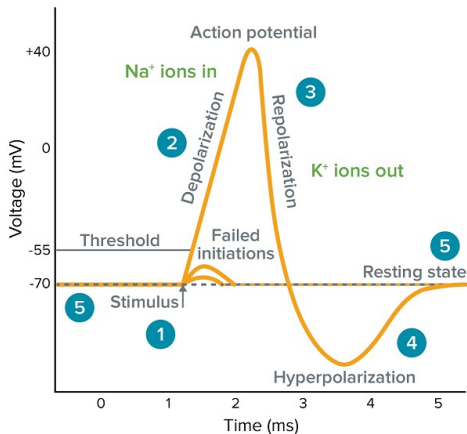

Figure: The basic computational unit of the brain: Neuron

Inspiration: The brain

- Neurons receive input signals and accumulate voltage. After some threshold they will fire spiking responses.

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- Two-layer neural network (one hidden layer and one output layer) with K hidden units:

$$f(x) = \sum_{k=1}^{K} w_k h_k(x) = \sum_{k=1}^{K} w_k \sigma(v_k^T x) \tag{6}$$

Activation Functions

- The **hyperbolic tangent** is a common activation function:
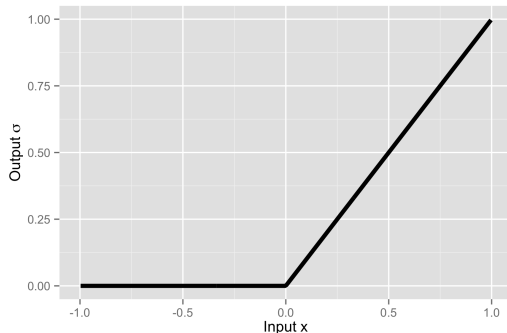
$$\sigma(x) = \tanh(x).$$
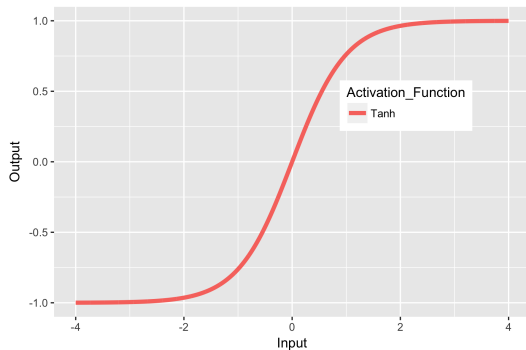
Activation Functions

- More recently, the **rectified linear** (**ReLU**) function has been very popular:
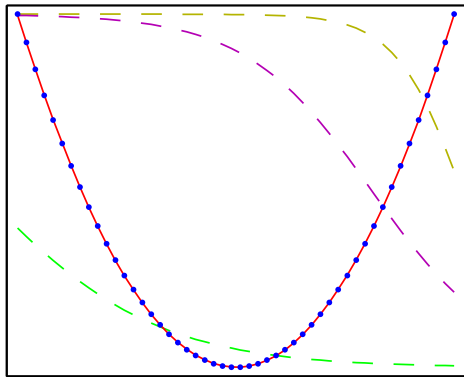
$$\sigma(x) = \max(0, x).$$

- Faster to calculate this function and its derivatives

- Often more effective in practice
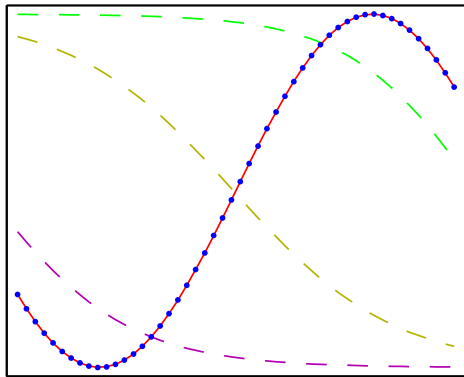
Approximation Ability: $f(x) = x^2$

- 3 hidden units; tanh activation functions

- Blue dots are training points; dashed lines are hidden unit outputs; final output in red.

From Bishop's *Pattern Recognition and Machine Learning*, Fig 5.3

Approximation Ability: $f(x) = \sin(x)$

- 3 hidden units; logistic activation function

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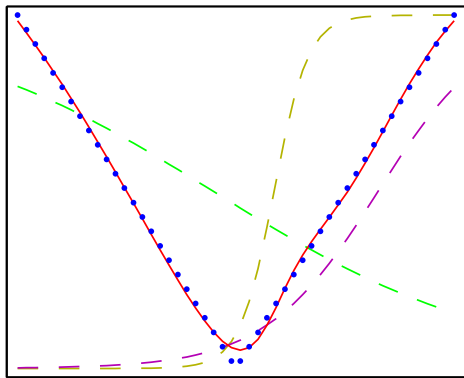# Approximation Ability: $f(x) = |x|$

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Universal approximation theorem

Theorem (Universal approximation theorem)

A neural network with one possibly huge hidden layer $\hat{F}(x)$ can approximate any continuous function $F(x)$ on a closed and bounded subset of $\mathbb{R}^d$ under mild assumptions on the activation function, i.e. $\forall \epsilon > 0$, there exists an integer N s.t.

$$\hat{F}(x) = \sum_{i=1}^{N} w_i \sigma(v_i^T x + b_i) \tag{7}$$

satisfies $|\hat{F}(x) - F(x)| < \epsilon$.

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# Universal approximation theorem

- For the theorem to work, the number of hidden units needs to be exponential in d

- The theorem doesn't tell us how to find the parameters of this network

- It doesn't explain why practical neural networks work, or tell us how to build them

Deep neural networks

- Wider: more hidden units (as in the approximation theorem).

- Deeper: more hidden layers.
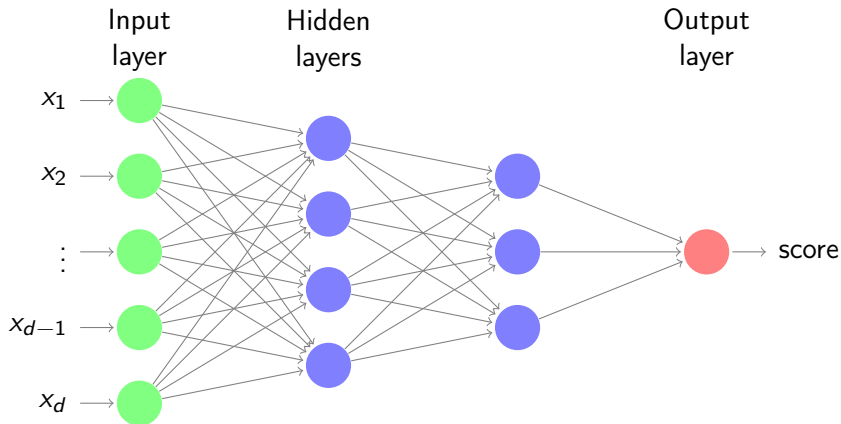
Multilayer Perceptron (MLP): formal definition

- **Input space**: $\mathcal{X} = \mathsf{R}^d$ **Output space** $\mathcal{Y} = \mathsf{R}^k$ (for k-class classification).

- Let $\sigma : \mathsf{R} \to \mathsf{R}$ be an activation function (e.g. tanh or ReLU).

- Let's consider an MLP of L hidden layers, each having m hidden units.

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- First hidden layer is given by

$$h^{(1)}(x) = \sigma\left(W^{(1)}x + b^{(1)}\right),$$

for parameters $W^{(1)} \in \mathsf{R}^{m \times d}$ and $b \in \mathsf{R}^m$, and where $\sigma(\cdot)$ is applied to each entry of its argument.

Multilayer Perceptron (MLP): formal definition

- Each subsequent hidden layer takes the *output $o \in \mathbb{R}^m$ of previous layer* and produces

$$h^{(j)}(o^{(j-1)}) = \sigma\left(W^{(j)} o^{(j-1)} + b^{(j)}\right), \text{ for } j = 2, \ldots, L$$

where $W^{(j)} \in \mathbb{R}^{m \times m}$, $b^{(j)} \in \mathbb{R}^m$.

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- Last layer is an *affine* mapping (no activation function):

$$a(o^{(L)}) = W^{(L+1)}o^{(L)} + b^{(L+1)},$$

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$$f(x) = \left(a \circ h^{(L)} \circ \cdots \circ h^{(1)}\right)(x) \tag{8}$$

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- Typically, the last layer gives us a score. How do we perform classification?

What did we do in multinomial logistic regression?

- From each x, we compute a linear score function for each class:

$$x \mapsto (\langle w_1, x \rangle, \ldots, \langle w_k, \rangle) \in \mathsf{R}^k$$

- We need to map this R^k vector into a probability vector θ.

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- The **softmax function** maps scores $s = (s_1, \ldots, s_k) \in \mathsf{R}^k$ to a categorical distribution:

$$(s_1, \ldots, s_k) \mapsto \theta = \textbf{Softmax}(s_1, \ldots, s_k) = \left(\frac{\exp(s_1)}{\sum_{i=1}^{k} \exp(s_i)}, \ldots, \frac{\exp(s_k)}{\sum_{i=1}^{k} \exp(s_i)} \right)$$

Nonlinear Generalization of Multinomial Logistic Regression

- From each x, we compute a non-linear score function for each class:

$$x \mapsto (f_1(x), \ldots, f_k(x)) \in \mathsf{R}^k$$

  where f_i's are the outputs of the last hidden layer of a neural network.

- Learning: Maximize the log-likelihood of training data

$$\underset{f_1, \ldots, f_k}{\arg\max} \sum_{i=1}^{n} \log \left[\mathsf{Softmax}\left(f_1(x), \ldots, f_k(x)\right)_{y_i} \right].$$

Interim discussion

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  Hidden layer(s) affine + *nonlinear* activation function
     Output layer affine (+ softmax)

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- Building blocks:

    Input layer no learnable parameters
    Hidden layer(s) affine + *nonlinear* activation function
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- A single, potentially huge hidden layer is sufficient to approximate any function

- In practice, it is often helpful to have multiple hidden layers

Fitting the parameters of an MLP

- **Input space**: $\mathcal{X} = \mathsf{R}$

- **Output space**: $\mathcal{Y} = \mathsf{R}$

- **Hypothesis space**: MLPs with a single 3-node hidden layer:

$$f(x) = w_0 + w_1 h_1(x) + w_2 h_2(x) + w_3 h_3(x),$$

where

$$h_i(x) = \sigma(v_i x + b_i) \text{ for } i = 1, 2, 3,$$

for some fixed activation function $\sigma : \mathsf{R} \to \mathsf{R}$.

- What are the parameters we need to fit?

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$$b_1, b_2, b_3, v_1, v_2, v_3, w_0, w_1, w_2, w_3 \in \mathbb{R}$$

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- For a training set $(x_1, y_1), \ldots, (x_n, y_n)$, our goal is to find

$$\hat{\theta} = \underset{\theta \in \mathbb{R}^{10}}{\arg \min} \frac{1}{n} \sum_{i=1}^{n} (f(x_i; \theta) - y_i)^2.$$

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- Is the loss convex in θ?
  - tanh is not convex
  - Regardless of nonlinearity, the composition of convex functions is not necessarily convex

- We might converge to a local minimum.

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- Back-propagation computes gradients for neural networks (and other models) in a systematic and efficient way

Gradient descent for (large) neural networks

- Mathematically, it's just *partial derivatives*, which you can compute by hand using the *chain rule*
  - In practice, this could be time-consuming and error-prone

- Back-propagation computes gradients for neural networks (and other models) in a systematic and efficient way

- We can visualize the process using *computation graphs*, which expose the structure of the computation (modularity and dependency)

Functions as nodes in a graph

- We represent each component of the network as a *node* that takes in a set of *inputs* and produces a set of *outputs*.

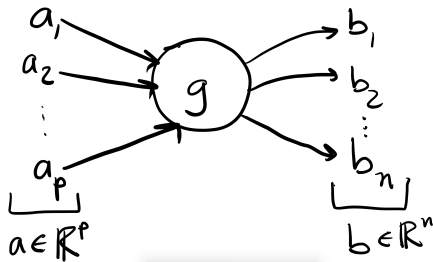- Example: $g : R^p \to R^n$.

  - Typical computation graph:
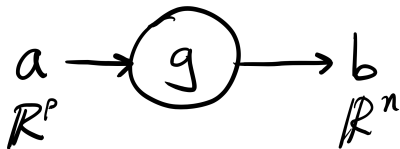
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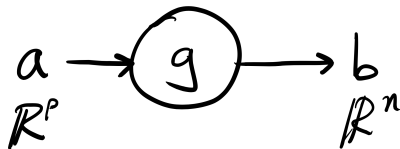
  - Broken down by component:
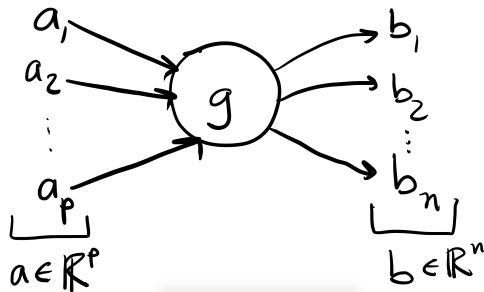
Partial derivatives of an affine function

- Define the affine function $g(x) = Mx + c$, for $M \in \mathbb{R}^{n \times p}$ and $c \in \mathbb{R}$.
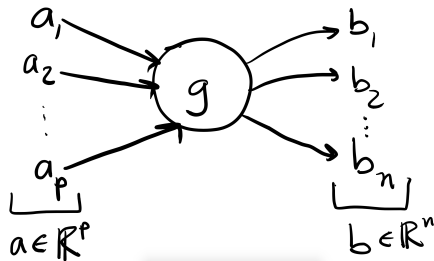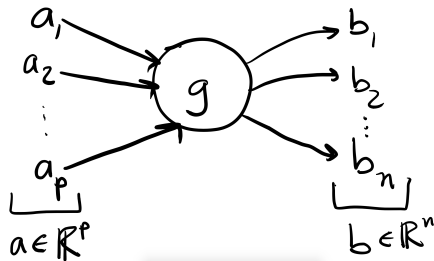
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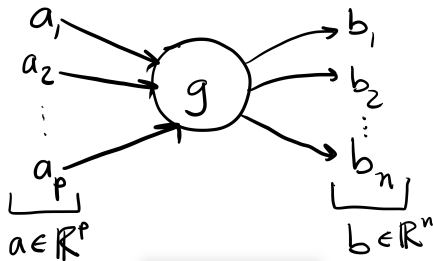
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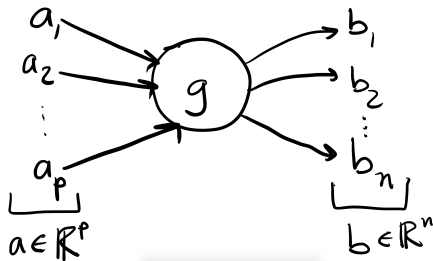
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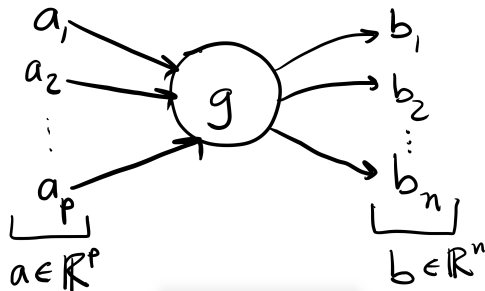$$b_i = \sum_{k=1}^{p} M_{ik} a_k + c_i.$$

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The partial derivative/gradient measures *sensitivity*: If we perturb an input a little bit, how much does the output change?

Partial derivatives in general
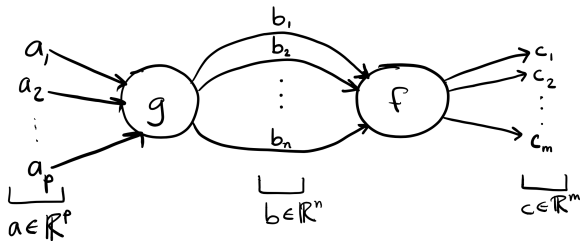
- Consider a function $g : R^p \to R^n$.

- Partial derivative $\frac{\partial b_i}{\partial a_j}$ is the rate of change of b_i as we change a_j

- If we change a_j slightly to

$$a_j + \delta,$$

- Then (for small δ), b_i changes to approximately

$$b_i + \frac{\partial b_i}{\partial a_j} \delta.$$

Composing multiple functions
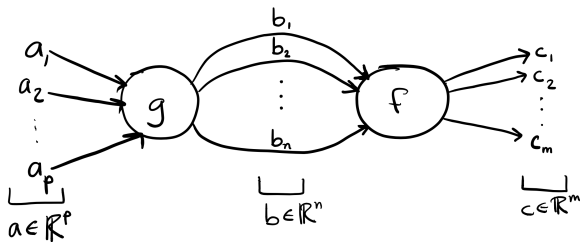
- We have $g : \mathbb{R}^p \to \mathbb{R}^n$ and $f : \mathbb{R}^n \to \mathbb{R}^m$

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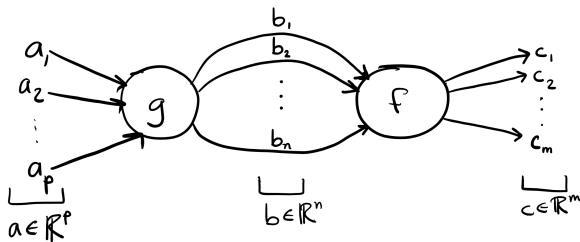- How does a small change in a_j affect c_i?

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- Visualizing the **chain rule**:
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$$\frac{\partial c_i}{\partial a_j} = \sum_{k=1}^{n} \frac{\partial c_i}{\partial b_k} \frac{\partial b_k}{\partial a_j}.$$

Example: Linear least squares

- Hypothesis space $\left\{ f(x) = w^T x + b \mid w \in \mathsf{R}^d, b \in \mathsf{R} \right\}$.

- Data set $(x_1, y_1), \ldots, (x_n, y_n) \in \mathsf{R}^d \times \mathsf{R}$.

- Define
$$\ell_i(w, b) = \left[\left(w^T x_i + b \right) - y_i \right]^2.$$

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- In SGD, in each round we choose a random training instance $i \in 1, \ldots, n$ and take a gradient step

$$
\begin{aligned}
w_j &\leftarrow w_j - \eta \frac{\partial \ell_i(w, b)}{\partial w_j}, \text{ for } j = 1, \ldots, d \\
b &\leftarrow b - \eta \frac{\partial \ell_i(w, b)}{\partial b},
\end{aligned}
$$

for some step size $\eta > 0$.

- How do we calculate these partial derivatives on a computation graph?

Computation graph and intermediate variables

- For a training point (x, y), the loss is

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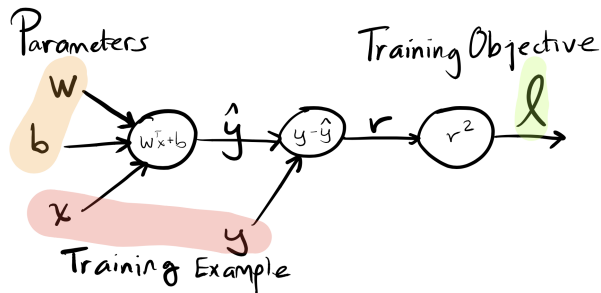
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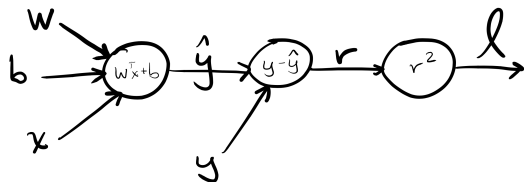(residual) $r \; = \; y - \hat{y}$

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Partial derivatives on computation graph

- We'll work our way from the output ℓ back to the parameters w and b, reusing previous computations as much as possible:
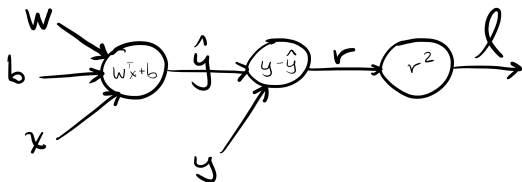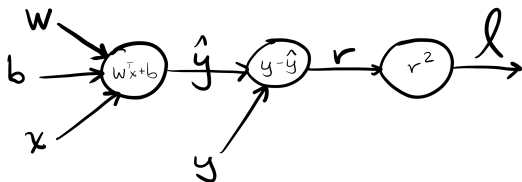
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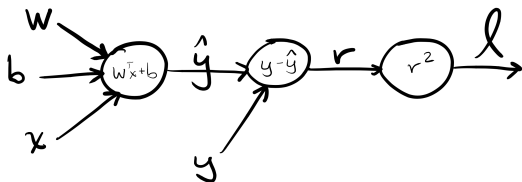# Partial derivatives on computation graph

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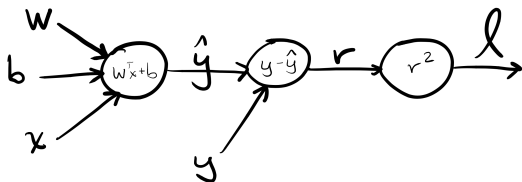
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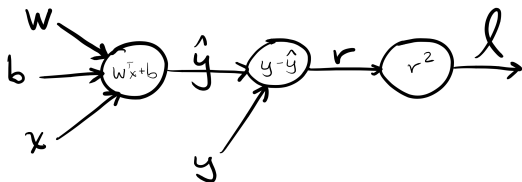
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Example: Ridge Regression

- For training point (x, y), the ℓ_2-regularized objective function is

$$J(w, b) = \left[\left(w^T x + b \right) - y \right]^2 + \lambda w^T w.$$

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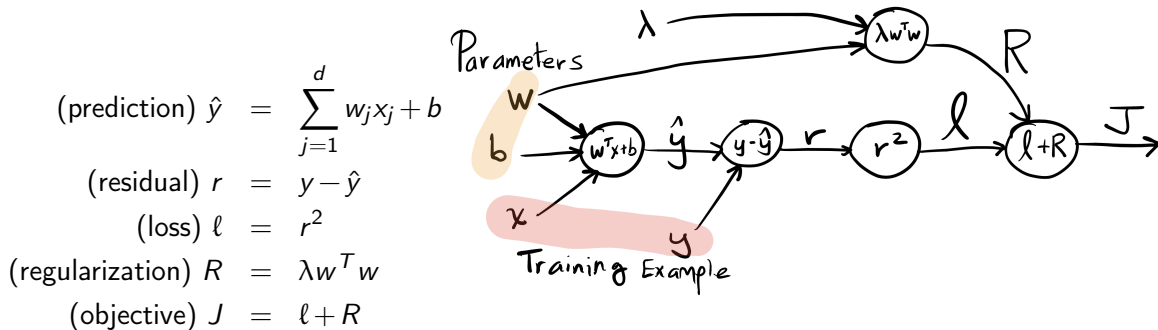\text{(loss)} \ \ell &= r^2 \\
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Partial Derivatives on Computation Graph

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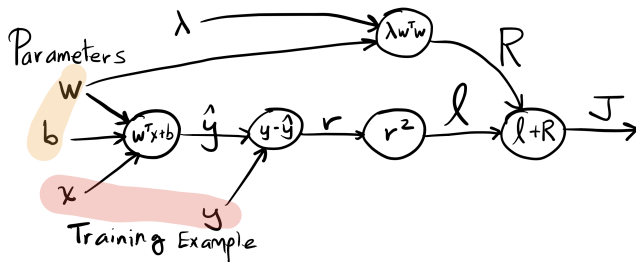
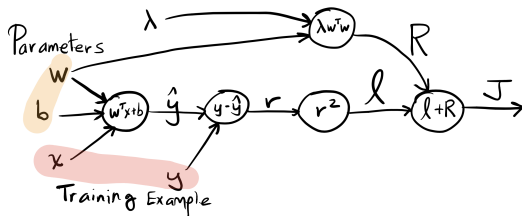$$\frac{\partial J}{\partial \ell} = \frac{\partial J}{\partial R} = 1$$

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$$\frac{\partial J}{\partial w_j} = \text{Exercise}$$

Backpropagation: Overview

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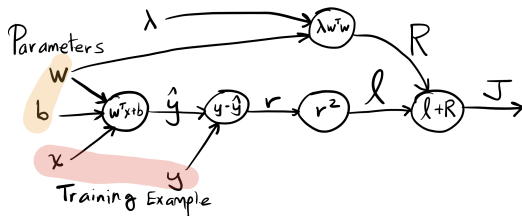

Forward pass — Compute intermediate function values, i.e. output of each node

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How do we minimize computation?

- Path sharing: each node *caches intermediate results*: we don't need to compute them over and over again

- An example of dynamic programming

Forward pass

- Order nodes by **topological sort** (every node appears before its children)

- For each node, compute the output given the input (output of its parents).

- Forward at intermediate node f_i and f_j:
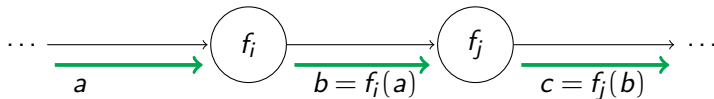
Backward pass

- Order nodes in **reverse topological order** (every node appears after its children)

- For each node, compute the partial derivative of its output w.r.t. its input, multiplied by the partial derivative of its children (chain rule)
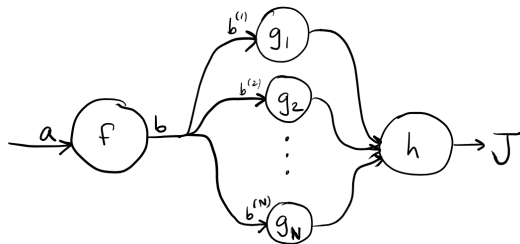
- Backward pass at intermediate node f_i:
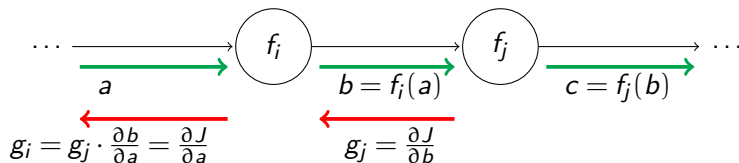
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- First sum partial derivatives from all children, then multiply.
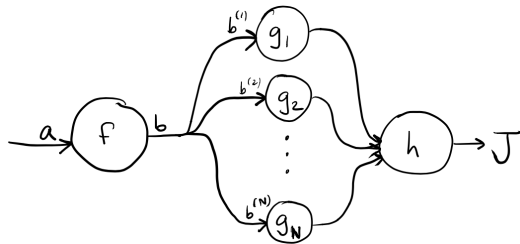
Multiple children

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- Backprop for node f:

- **Input**: $\frac{\partial J}{\partial b^{(1)}}, \ldots, \frac{\partial J}{\partial b^{(N)}}$
  (Partials w.r.t. inputs to all children)

- **Output**:

$$\frac{\partial J}{\partial b} = \sum_{k=1}^{N} \frac{\partial J}{\partial b^{(k)}}$$

$$\frac{\partial J}{\partial a} = \frac{\partial J}{\partial b} \frac{\partial b}{\partial a}$$

Why backward?

- We can write the chain rule in different orders of computation.

$$y = y(c(b(a))) \tag{9}$$

$$\tag{12}$$

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- Optimal ordering = matrix chain ordering problem. Dynamic programming solution.
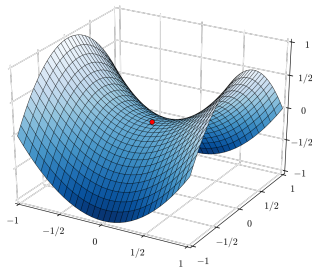
Non-convex optimization
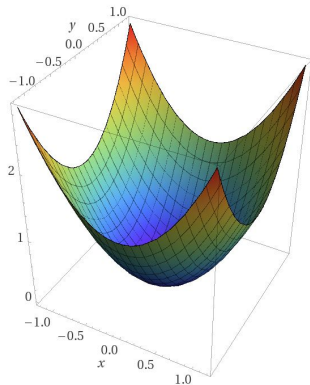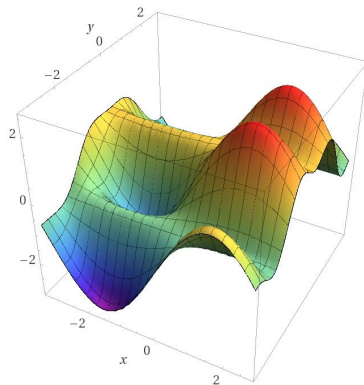
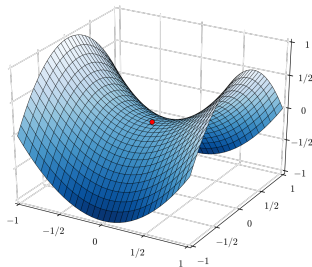- Left: convex loss function. Right: non-convex loss function.

Non-convex optimization: challenges

- What if we converge to a bad local minimum?
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Non-convex optimization: challenges

- What if we converge to a bad local minimum?
  - Rerun with a different initialization

- Hit a saddle point
  - Doesn't often happen with SGD
  - Second partial derivative test

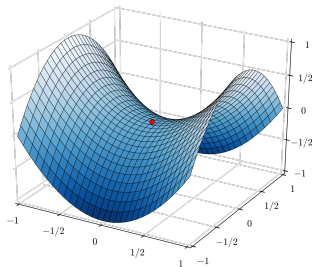Reference: Chris De Sa's slides (CS6787 Lecture 7).

Non-convex optimization: challenges

- What if we converge to a bad local minimum?
  - Rerun with a different initialization

- Hit a saddle point
  - Doesn't often happen with SGD
  - Second partial derivative test

- Flat region: low gradient magnitude
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- High curvature: large gradient magnitude
  - Possible solutions: Gradient clipping, adaptive step sizes
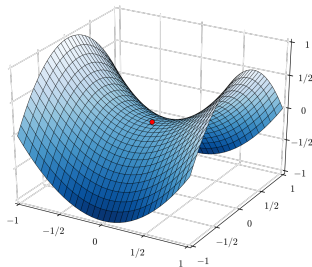
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- Learning rate decay (staircase 10x, cosine, etc.), speeds up convergence

Biological Plausibility

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- Two main problems with implementing in an asynchronous analog hardware like our brain.
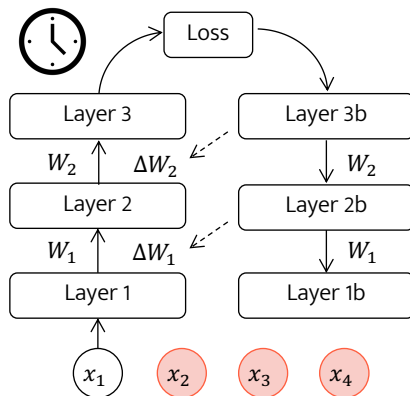
1) Weight Symmetry & Network Symmetry
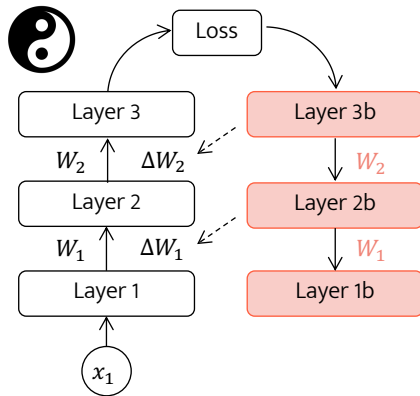
Biological Plausibility

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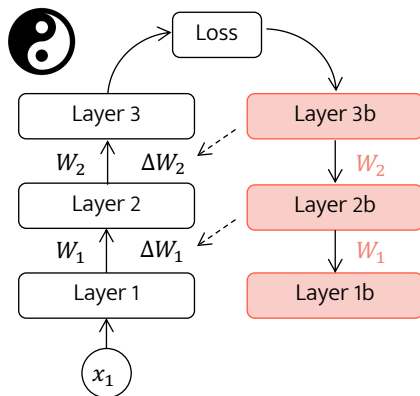
2) Global Synchronization

Review

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- It is used in gradient descent optimization for neural networks.

- Key idea: function composition and the chain rule

- In practice, we can use existing software packages, e.g. PyTorch (backpropagation, neural network building blocks, optimization algorithms etc.)

Applying Neural Networks on Images

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- Stored the intensity value pixel by pixel.

- A 28×28 image of digit 4:

Fully connected vs. locally connected

- So far we apply a layer where all output neurons are connected to all input neurons.

- In matrix form, $z = W\mathbf{x}$.

- This is also called a fully connected layer or a dense layer or a linear layer.

Fully connected vs. locally connected

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- For 200×200 image and 1000 hidden units, the matrix of a single layer will have 40M parameters!
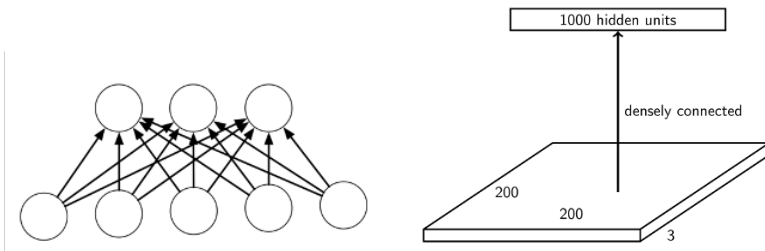
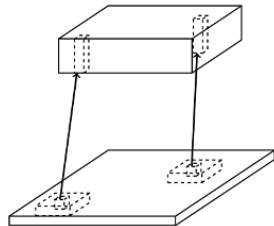# Fully connected vs. locally connected

- An alternative strategy is to use local connection.

- For neuron i, only connects to its neighborhood (e.g. [i+k, i-k])

- For images, we index neurons with three dimensions i, j, and c.

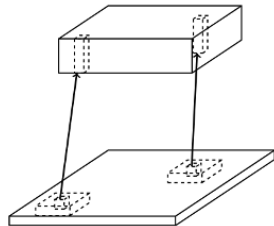- i = vertical index, j = horizontal index, c = channel index.
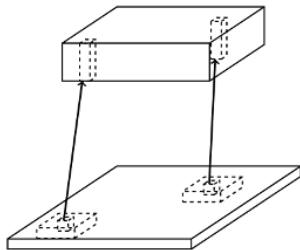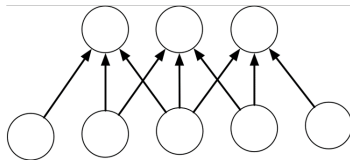
Local connection patterns

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- k is the "kernel" size - do not confuse with the other kernel we learned.

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- The spatial awareness (receptive field) of the neighborhood grows bigger as we go deeper.