Recitation 2

Neural Networks

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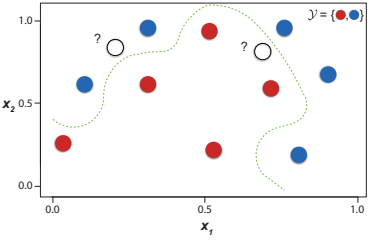
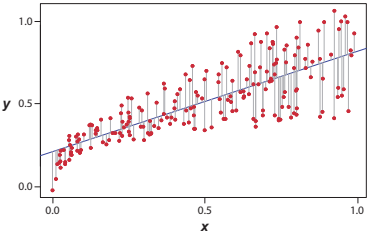
Recap of Recitation 1

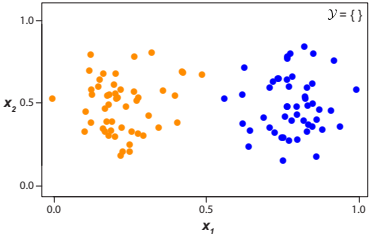
Classification



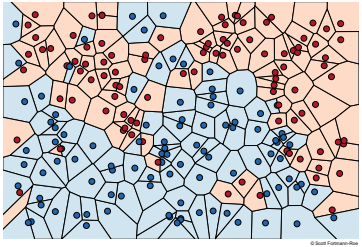
Regression



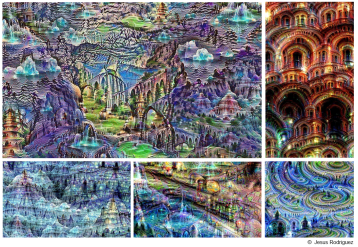
Unsupervised learning



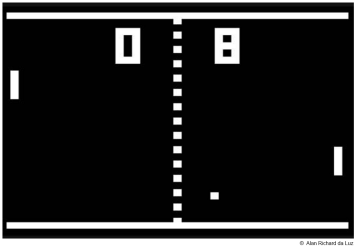
Non-parametric models



Generative models



Reinforcement learning



Recap of Recitation 1

Empirical risk associated with hypothesis $h(\boldsymbol{x})$:

$$\mathcal{R}_{\text{emp}}(h) = \frac{1}{N}\sum_{i=1}^{N} \mathcal{L}(h(\boldsymbol{x}^{(i)}), \boldsymbol{y}^{(i)})$$

Minimize $\mathcal{R}_{\text{emp}}(h)$ to find $\hat{h}$:

$$\hat{h} = \underset{h \in \mathcal{H}}{\text{argmin}}\, \mathcal{R}_{\text{emp}}(h)$$

Recitation 1:

$$\begin{aligned} \boldsymbol{x}^{(i)} \in \mathcal{X}, \boldsymbol{y}^{(i)} \in \mathcal{Y} \quad & \text{(input space, label space)} \\ \mathcal{L}(h(\boldsymbol{x}^{(i)}), \boldsymbol{y}^{(i)}) \quad & \text{(loss functions)} \\ \text{argmin}_{h \in \mathcal{H}} \quad & \text{(optimizers)} \end{aligned}$$

Recitation 2:

$$\mathcal{H}$$

ML: Define $\mathcal{H}$, obtain $\hat{h}$

$\mathcal{H} \subset \mathcal{F}$, where $\mathcal{F}$ is the set of all functions mapping $\mathcal{X}$ onto $\mathcal{Y}$.

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Problem Set 1

$$\boldsymbol{x} \in [0,1]^{784}$$
$$\hat{\boldsymbol{y}} \in [0,1]^{10}$$
$$\boldsymbol{W} \in \mathbb{R}^{784 \times 10}$$
$$\boldsymbol{b} \in \mathbb{R}^{10}$$
$$h(\boldsymbol{x}; \boldsymbol{W}, \boldsymbol{b}) = \phi_{\text{softmax}}(\boldsymbol{W}^T \boldsymbol{x} + \boldsymbol{b})$$
$$\mathcal{H} = \{h(\boldsymbol{x}; \boldsymbol{W}, \boldsymbol{b}) | \boldsymbol{W} \in \mathbb{R}^{784 \times 10}, \boldsymbol{b} \in \mathbb{R}^{10}\}$$

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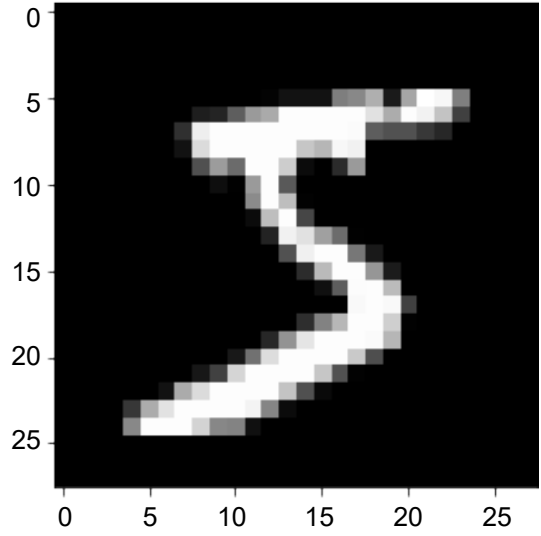
Step 2: use gradient-based optimization methods to obtain $\hat{h}$

Smartly constrain $\mathcal{H}$

What is lost when treating the pixels of an image like independent features?



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Using softmax regression, we treat the 28 by 28 2D image as a vector of 784 features, without any notion of topological distance between them.

Solution: Constrain the hypothesis space $\mathcal{H}$ in a way to *exploit the structure of the input*.

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Example 6 (3D structure): $\mathcal{X} = [0, 1]^{m \times n \times p}$, voxels (volumentric pixels) from imaging methods such as CT and MRI

Example 7 (4D structure): $\mathcal{X} = [0, 1]^{m \times n \times p \times t}$, doxels (dynamic voxels) a sequence of voxel data, e.g., time series of CT and MRI scans

Neural networks: flexibly constrain hypothesis space $\mathcal{H}$

No structure:
Dense layer (also called fully connected layer)

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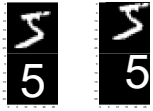
Spatial structure:
Convolutional layer (with 1D, 2D, 3D kernels): translationally equivariant through weight sharing

Input:

Filter output:



Pooling layer (with 1D, 2D, 3D kernels): (somewhat) translationally invariant through summaries

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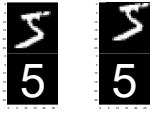
Filter output:



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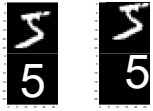

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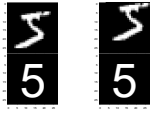
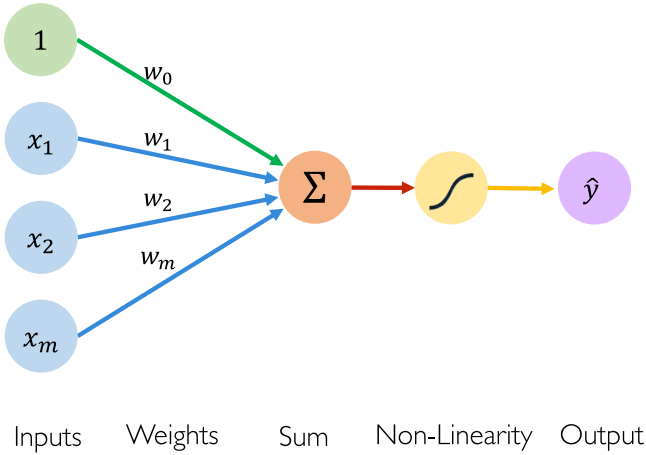
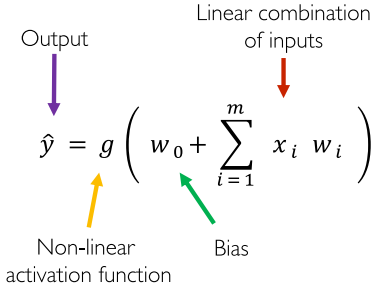


Sequential / temporal structure:
Recurrent layer (and its variants - GRU, LSTM): shares weights between time points

Perceptron





Illustrations by courtesy of [Amini and Soleimany, 2019].

Activation function	Equation	Example	1D Graph
Unit step (Heaviside)	$\phi(z) = \begin{cases} 0, & z < 0, \\ 0.5, & z = 0, \\ 1, & z > 0, \end{cases}$	Perceptron variant	
Sign (Signum)	$\phi(z) = \begin{cases} -1, & z < 0, \\ 0, & z = 0, \\ 1, & z > 0, \end{cases}$	Perceptron variant	
Linear	$\phi(z) = z$	Adaline, linear regression	
Piece-wise linear	$\phi(z) = \begin{cases} 1, & z \geq \frac{1}{2}, \\ z + \frac{1}{2}, & -\frac{1}{2} < z < \frac{1}{2}, \\ 0, & z \leq -\frac{1}{2}, \end{cases}$	Support vector machine	
Logistic (sigmoid)	$\phi(z) = \frac{1}{1 + e^{-z}}$	Logistic regression, Multi-layer NN	
Hyperbolic tangent	$\phi(z) = \frac{e^{z} - e^{-z}}{e^{z} + e^{-z}}$	Multi-layer Neural Networks	
Rectifier, ReLU (Rectified Linear Unit)	$\phi(z) = max(0, z)$	Multi-layer Neural Networks	
Rectifier, softplus	$\phi(z) = \ln(1 + e^{z})$	Multi-layer Neural Networks	

only in output layer (why?):

- linear activation function (for regression)
- sigmoid activation function (for binary or multi-label classification)
- softmax activation function (for binary or multi-class classification)

Activation functions

- softmax (identical to sigmoid in binary classification)
- exponential linear unit (ELU)

$$\phi(z, \alpha)_{\text{ELU}} = \begin{cases} z, & \text{for } z \geq 0 \\ \alpha(e^{z} - 1), & \text{for } z < 0 \end{cases}$$

- scaled exponential linear unit (SELU)

$$\phi(z, \alpha, \beta) = \beta * \phi(z, \alpha)_{\text{ELU}}$$

- softsign

$$\phi(z) = \frac{z}{|z| + 1}$$

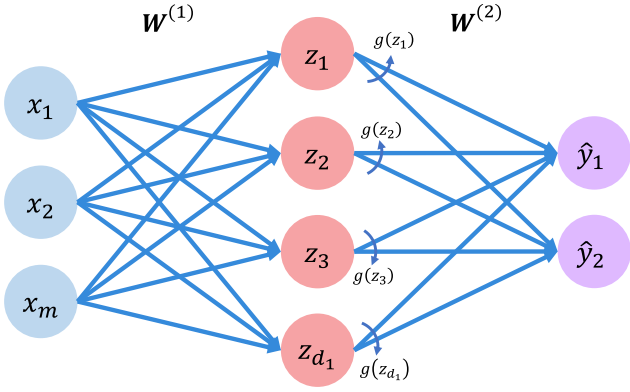
- leaky ReLU

$$\phi(z, \alpha) = \begin{cases} z, & \text{for } z \geq 0 \\ \alpha z, & \text{for } z < 0 \end{cases}$$

- parametric ReLU (PReLU, identical to leaky ReLU, but α is learned)

$$\phi(z; \alpha) = \begin{cases} z, & \text{for } z \geq 0 \\ \alpha z, & \text{for } z < 0 \end{cases}$$

Single-layer neural network

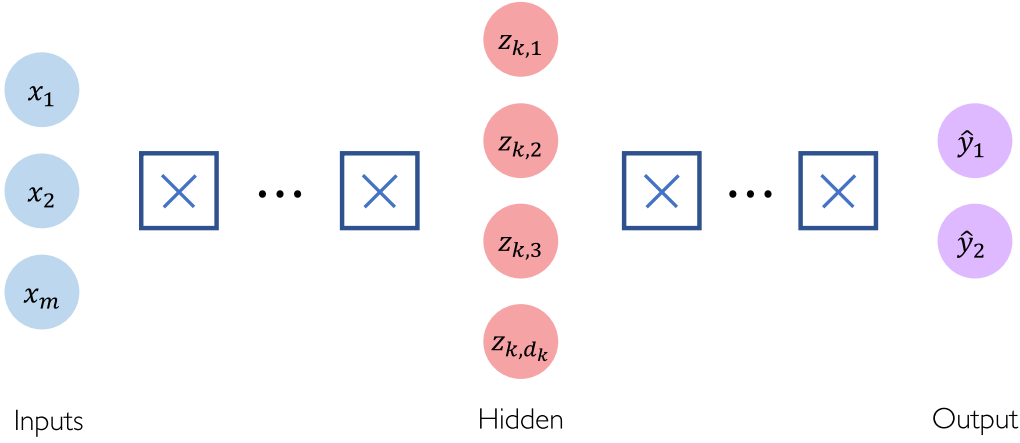


Inputs Hidden Final Output

$$z_i = w_{0,i}^{(1)} + \sum_{j=1}^{m} x_j \, w_{j,i}^{(1)} \qquad \hat{y}_i = g\left(w_{0,i}^{(2)} + \sum_{j=1}^{d_1} z_j \, w_{j,i}^{(2)}\right)$$

Multi-layer neural network

How deep is deep learning?



$$z_{k,i} = w_{0,i}^{(k)} + \sum_{j=1}^{d_{k-1}} g(z_{k-1,j})\, w_{j,i}^{(k)}$$

Dense layer in TF: low-level vs high-level

Listing 1: low-level TF (`tf.nn.*`)

```
def model(x_ph):
  ...
  w = tf.Variable(tf.truncated_normal([in_channels, out_channels]))
  b = tf.Variable(tf.constant(0.1, shape=[out_channels]))
  dense_op = tf.matmul(x_ph, w)
  dense_op = tf.nn.bias_add(dense_op, b)
  dense_op = tf.nn.relu(dense_op)
  ...
```

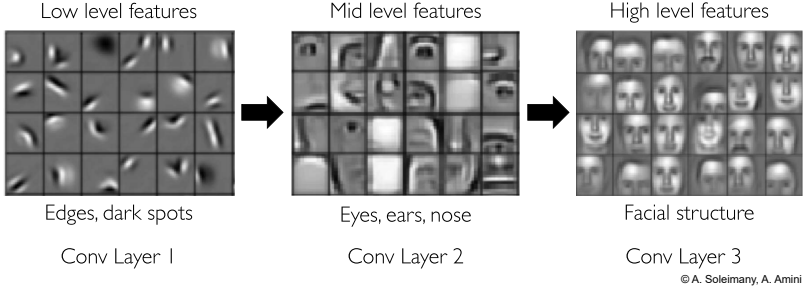
Listing 2: high-level TF (`tf.keras.*`)

```
model = tf.keras.Sequential()
# first layer
model.add(tf.keras.layers.Dense(out_channels, activation='relu', input_shape=(in_channels,)))
...
model.add(tf.keras.layers.Dense(out_channels, activation='relu'))
...
```

PS2 will be the last problem set implemented in low-level TF.

Convolutional neural networks

Idea: Learn a hierarchy of pattern detectors
Example: 3-layer convolutional neural network for face recognition



Example: In CNN for TF binding site classification, filters learn binding site motifs

Visualizations of filters and operations in latent space:

- Chris Olah's article on Distill: `https://distill.pub/2018/building-blocks/`
- OpenAI's Glow: `https://blog.openai.com/glow/`

Convolutional layer in TF: low-level vs high-level

Listing 3: low-level TF (`tf.nn.*`)

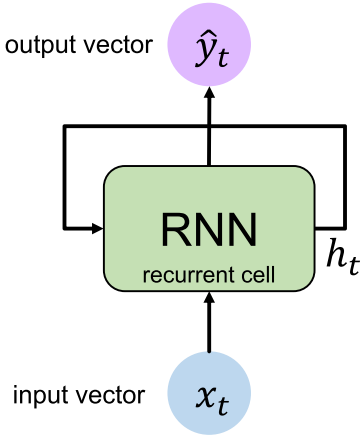
```
def model(x_ph):
  ...
  w = tf.Variable(tf.truncated_normal([filter_height, filter_width,
                                       in_channels, out_channels]))
  b = tf.Variable(tf.constant(0.1, shape=[out_channels]))

  conv_op = tf.nn.conv2d(x_ph, w, strides=[1, 1, 1, 1], padding="SAME")
  conv_op = tf.nn.bias_add(conv_op, b)
  conv_op = tf.nn.relu(conv_op)
  ...
```

Listing 4: high-level TF (`tf.keras.*`)

```
model = tf.keras.Sequential()
model.add(tf.keras.layers.Conv2D(out_channels,
                                 kernel_size=(filter_height, filter_width),
                                 strides=1,
                                 activation="relu", padding="SAME"))
...
```

Recurrent neural networks

Idea: Learn sequential / temporal relationships



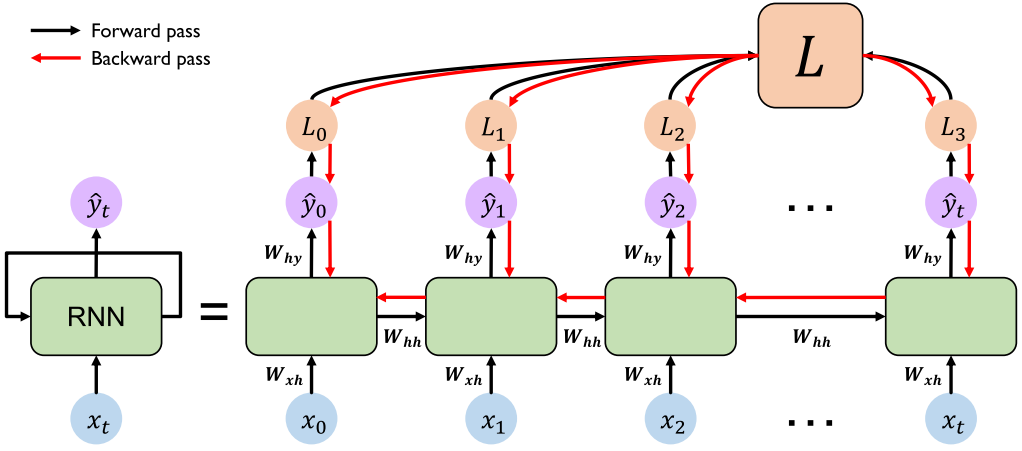
Apply a **recurrence relation** at every time step to process a sequence:

$$h_t = f_W(h_{t-1}, x_t)$$

new state — function parameterized by W — old state — input vector at time step t

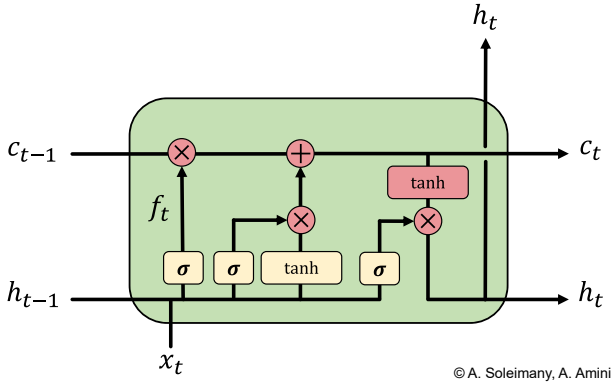
Note: the same function and set of parameters are used at every time step

RNN backpropagation through time



RNN variants GRU and LSTM

Idea: introduce memory in recurrent unit and control it via gates (forget gate, input / update gate, output gate)



Useful links:

- 6.S191 lecture on RNN, GRU, LSTM:
  `http://introtodeeplearning.com/materials/2019_6S191_L2.pdf`
- Chris Olah's article about LSTM:
  `http://colah.github.io/posts/2015-08-Understanding-LSTMs/`

LSTM layer in TF: low-level vs high-level

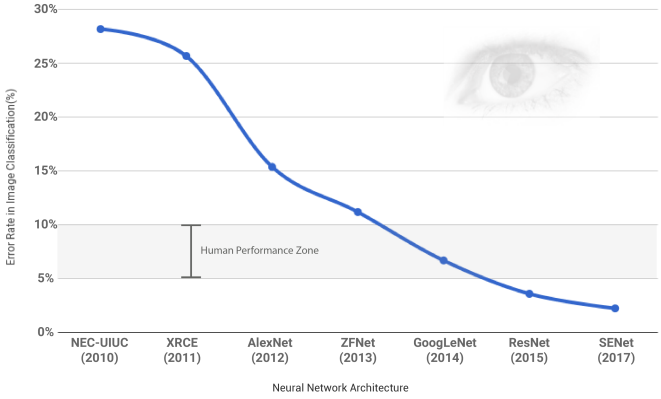
Listing 5: low-level TF (`tf.nn.*`)

```
def model(x_ph):
  # x_ph.get_shape() == [time_points * number_of_examples, in_channels]
  ...
  split_ops = tf.split(axis=0, num_or_size_splits=time_points, value=x_ph)
  lstm_cell = tf.nn.rnn_cell.LSTMCell(units)
  outputs, states = tf.nn.static_rnn(lstm_cell, split_ops, dtype=tf.float32)
  # outputs[-1] contains RNN prediction (prediction at last time point)
  ...
```

Listing 6: high-level TF (`tf.keras.*`)

```
model = tf.keras.Sequential()
...
model.add(tf.keras.layers.LSTM(units)
...
```

Why Deep Residual Networks?



Last two ILSVRC winners are networks with residual modules:

- ILSVRC 2017: SENet [Hu et al., 2018] is a ensemble of different models, highest scoring model is modified ResNeXt [Xie et al., 2017]
- ILSVRC 2016: ResNet [He et al., 2016]

- **ResNet:** to remedy vanishing gradients, introduce skip connections (bypass layers by adding identity mapping)

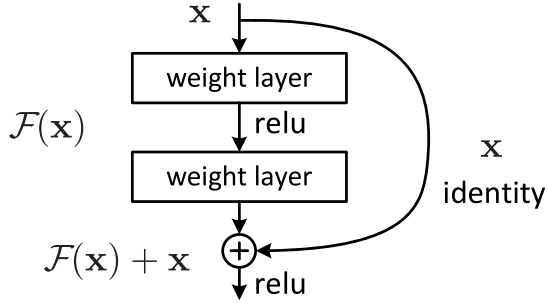


Figure 2. Residual learning: a building block.

Evolution of Deep Residual Networks

- **Wide Residual Networks:** decrease depth (number of layers), increase width (number of feature maps) in residual layers [Zagoruyko and Komodakis, 2016]
- **ResNeXt:** introduce cardinality (number of aggregated transformations), in addition to depth and width [Xie et al., 2017]

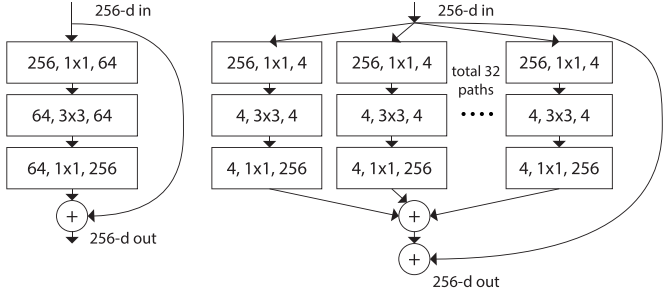


Figure 1. **Left**: A block of ResNet [14]. **Right**: A block of ResNeXt with cardinality = 32, with roughly the same complexity. A layer is shown as (# in channels, filter size, # out channels).

- **DenseNet:** each layer has direct input connections to all previous feature maps [Huang et al., 2016]

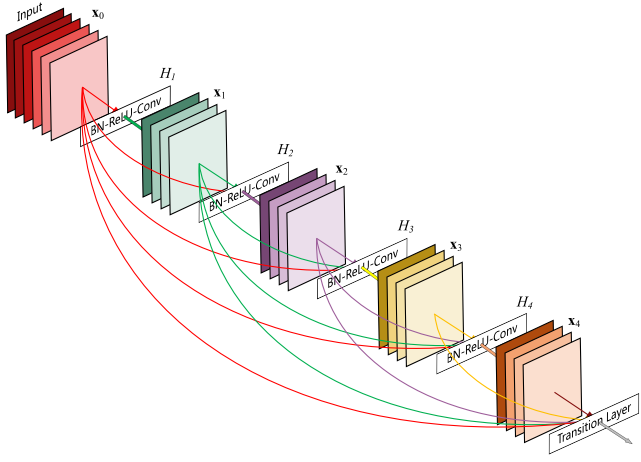


Figure 1: A 5-layer dense block with a growth rate of $k = 4$. Each layer takes all preceding feature-maps as input.

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