CS 760: Machine Learning
Neural Networks III

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Outline

- **Review & Regularization**
  - Forward/backwards Pass, Views, L1/L2 Effects
- **Other Forms of Regularization**
  - Data Augmentation, Noise, Early Stopping, Dropout
- **Convolutional Neural Networks**
  - Convolution Operation, Intuition

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Review: Backprop

- Forward pass:

$$L(f_{\text{network}}(x), y)$$

- Let's unwrap this:

$$L(r^k(W^k r^{k-1}(W^{k-1} \cdots r^2(W^2 r^1(W^1 x)) \cdots)), y)$$

Activation function **Layer k**

Linear transformation, **Layer k**

Activation function **Layer 1**

Linear transformation, **Layer 1**

Review: Forward/Backward Passes

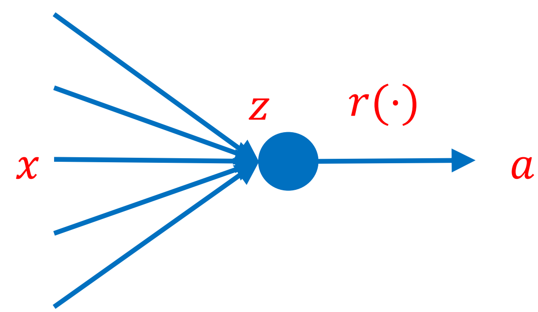
- Forward pass:

$$L(r^k(W^k r^{k-1}(W^{k-1} \cdots r^2(W^2 r^1(W^1 x)) \cdots)), y)$$

- For convenience,

$$a^j = r^j(W^j r^{j-1}(W^{j-1} \cdots r^2(W^2 r^1(W^1 x)) \cdots))$$

$$z^j = W^j r^{j-1}(W^{j-1} \cdots r^2(W^2 r^1(W^1 x)) \cdots)$$



Review: Backward Pass

- Backward pass. Say we compute gradient w.r.t. x

$$\frac{\partial L}{\partial a^k}\frac{\partial a^k}{\partial z^k}\frac{\partial z^k}{\partial a^{k-1}}\frac{\partial a^{k-1}}{\partial z^{k-1}}\frac{\partial z^{k-1}}{\partial a^{k-2}}\cdots\frac{\partial a^1}{\partial z^1}\frac{\partial z^1}{\partial x}$$

- Can write this with matrix notation
  - Writing it forward, this is equivalent

$$\nabla_x L = (W^1)^T(r^1)'\cdots(W^{k-1})^T(r^{k-1})'(W^k)^T(r^k)'\nabla_{a^k}L$$

Linear derivative

Activation function derivative

Review: Backpropagation

- Backward pass. Say we compute gradient w.r.t. x

$$\nabla_x L = (W^1)^T (r^1)' \cdots (W^{k-1})^T (r^{k-1})' (W^k)^T (r^k)' \nabla_{a^k} L$$

- Let's write this recursively:

$$\delta^j = (r^j)' (W^{j+1})^T \cdots (W^{k-1})^T (r^{k-1})' (W^k)^T (r^K)' \nabla_{a^k} L$$

- Easy to set up a recursion (start at k, go down) :

Start at j layer here

$$\delta^{j-1} = (r^{j-1})' (W^j)^T \delta^j$$

Review: Backpropagation

- Let's write this recursively:

$$\delta^j = (r^j)'(W^{j+1})^T \cdots (W^{k-1})^T (r^{k-1})'(W^k)^T (r^K)' \nabla_{a^k} L$$

- Easy to set up a recursion (start at k, go down) :

$$\delta^{j-1} = (r^{j-1})'(W^j)^T \delta^j$$

- How do we get our gradients for weights?

$$\nabla_{W^j} L = \delta^j (a^{j-1})^T$$

Review: Regularization, Bayesian Prior View

- Recall our MAP version of training. Bayes law:

$$p(\theta \mid \{x_i, y_i\}) = \frac{p(\theta)p(\{x_i, y_i\}|\theta)}{p(\{x_i, y_i\})}$$

- MAP:

$$\max_\theta \log p(\theta \mid \{x_i, y_i\}) = \min_\theta - \underbrace{\log p(\theta)}_{\textbf{Regularization}} - \underbrace{\log p(\{x_i, y_i\} \mid \theta)}_{\textbf{MLE loss}}$$

- L2: Corresponds to normal $p(x \mid y, \theta)$, **normal prior** $p(\theta)$

Choice of View?

- Typical choice for optimization: soft-constraint

$$\min_{\theta} \hat{L}_R(\theta) = \hat{L}(\theta) + \lambda R(\theta)$$

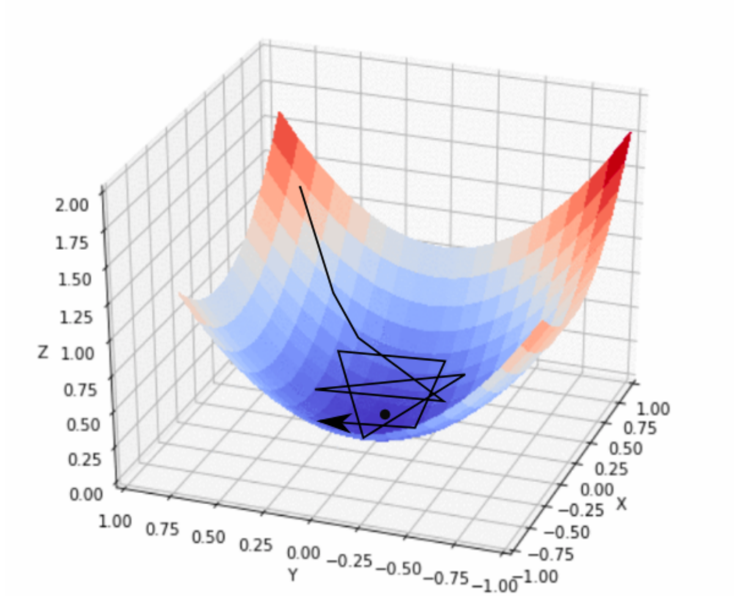
- Hard constraint / Bayesian view: conceptual / for derivation
- Hard-constraint preferred if
  - Know the explicit bound $R(\theta) \leq r$
- Bayesian view preferred if
  - Domain knowledge easy to represent as a prior

Examples: L2 Regularization

- Again,

$$\min_{\theta} \hat{L}_R(\theta) = \hat{L}(\theta) + \frac{\lambda}{2}||\theta||_2^2$$

- Questions: what are the
  - Effects on (stochastic) gradient descent?
  - Effects on the optimal solution?



L2 Regularization: **Effect on GD**

- Gradient of regularized objective

$$\nabla \hat{L}_R(\theta) = \nabla \hat{L}(\theta) + \lambda\theta$$

- Gradient descent update

$$\theta \leftarrow \theta - \eta\nabla \hat{L}_R(\theta) = \theta - \eta\,\nabla \hat{L}(\theta) - \eta\lambda\theta$$

$$= (1 - \eta\lambda)\theta - \eta\,\nabla \hat{L}(\theta)$$

- In words, **weight decay**

L2 Regularization: **Effect on Optimal Solution**

- Consider a quadratic approximation around θ^*

$$\hat{L}(\theta) \approx \hat{L}(\theta^*) + (\theta - \theta^*)^T \nabla \hat{L}(\theta^*) + \frac{1}{2}(\theta - \theta^*)^T H (\theta - \theta^*)$$

- Since θ^* is optimal, $\nabla \hat{L}(\theta^*) = 0$

$$\hat{L}(\theta) \approx \hat{L}(\theta^*) + \frac{1}{2}(\theta - \theta^*)^T H (\theta - \theta^*)$$

$$\nabla \hat{L}(\theta) \approx H(\theta - \theta^*)$$

L2 Regularization: **Effect on Optimal Solution**

- Gradient of regularized objective: $\nabla \hat{L}_R(\theta) \approx H(\theta - \theta^*) + \lambda\theta$

- On the optimal θ_R^*: $0 = \nabla \hat{L}_R(\theta_R^*) \approx H(\theta_R^* - \theta^*) + \lambda\theta_R^*$

$$\theta_R^* \approx (H + \lambda I)^{-1} H \theta^*$$

- H has eigendecomp. $H = Q\Lambda Q^T$, assume $(\Lambda + \lambda I)^{-1}$ exists:

$$\theta_R^* \approx (H + \lambda I)^{-1} H \theta^* = Q(\Lambda + \lambda I)^{-1} \Lambda Q^T \theta^*$$

- Effect: **rescale along eigenvectors of $\boldsymbol{H}$**

L2 Regularization: **Effect on Optimal Solution**

Effect: rescale along eigenvectors of H

Visual Example:

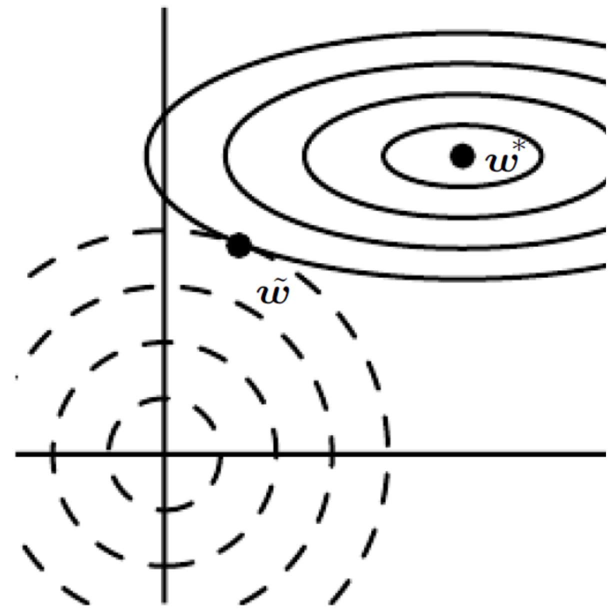


Figure from *Deep Learning*,
Goodfellow, Bengio and Courville

L1 Regularization: **Effect on GD**

$$\min_{\theta} \hat{L}_R(\theta) = \hat{L}(\theta) + \lambda ||\theta||_1$$

- Effect on (stochastic) gradient descent:
- Gradient of regularized objective

$$\nabla \hat{L}_R(\theta) = \nabla \hat{L}(\theta) + \lambda \text{sign}(\theta)$$

where **sign** applies to each element in θ

- Gradient descent update

$$\theta \leftarrow \theta - \eta \nabla \hat{L}_R(\theta) = \theta - \eta \nabla \hat{L}(\theta) - \eta \lambda \text{sign}(\theta)$$

L1 Regularization: **Effect on Optimal Solution**

- Again,

$$\hat{L}(\theta) \approx \hat{L}(\theta^*) + \frac{1}{2}(\theta - \theta^*)^T H(\theta - \theta^*)$$

- Further assume that H is diagonal and positive $(H_{ii} > 0, \forall i)$
    - **not true in general** but assume for getting some intuition

- The regularized objective is (ignoring constants)

$$\hat{L}_R(\theta) \approx \sum_i \frac{1}{2} H_{ii}(\theta_i - \theta_i^*)^2 + \lambda|\theta_i|$$

L1 Regularization: **Effect on Optimal Solution**

- The regularized objective is (ignoring constants)

$$\hat{L}_R(\theta) \approx \sum_i \frac{1}{2} H_{ii}(\theta_i - \theta_i^*)^2 + \lambda|\theta_i|$$

- The optimal θ_R^*

$$(\theta_R^*)_i \approx \begin{cases} \max\left\{\theta_i^* - \frac{\lambda}{H_{ii}}, 0\right\} & \text{if } \theta_i^* \geq 0 \\ \min\left\{\theta_i^* + \frac{\lambda}{H_{ii}}, 0\right\} & \text{if } \theta_i^* < 0 \end{cases}$$

- Compact expression for the optimal θ_R^*

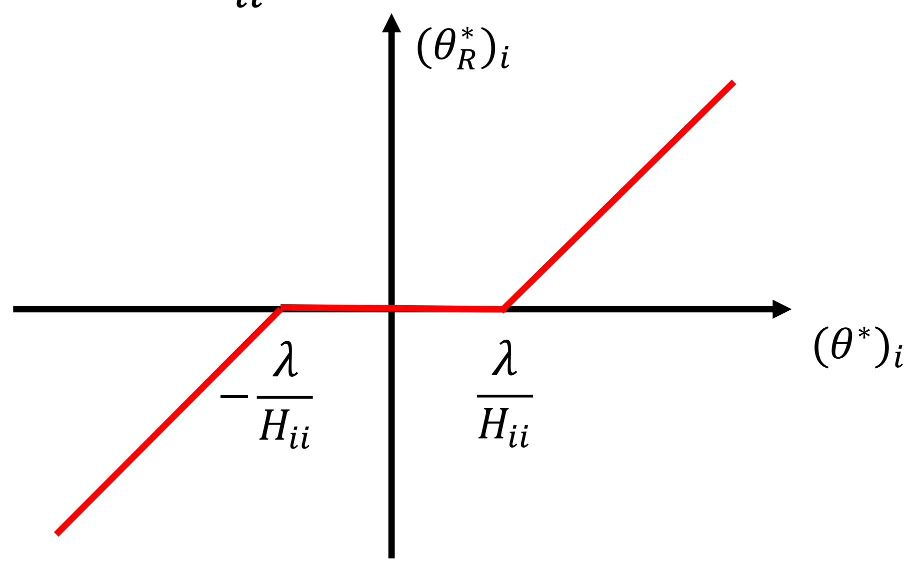
$$(\theta_R^*)_i \approx \operatorname{sign}(\theta_i^*) \max\{|\theta_i^*| - \frac{\lambda}{H_{ii}}, 0\}$$

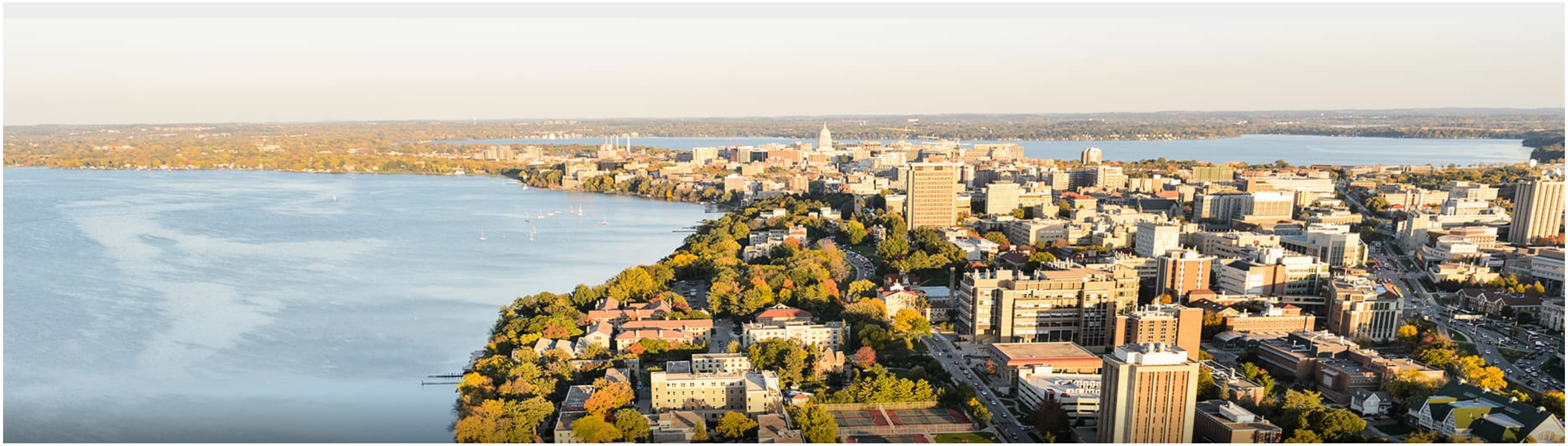
L1 Regularization: **Effect on Optimal Solution**

- The optimal θ_R^*

$$(\theta_R^*)_i \approx \begin{cases} \max\left\{\theta_i^* - \frac{\lambda}{H_{ii}}, 0\right\} & \text{if } \theta_i^* \geq 0 \\ \min\left\{\theta_i^* + \frac{\lambda}{H_{ii}}, 0\right\} & \text{if } \theta_i^* < 0 \end{cases}$$

- Effect: **induces sparsity**





Break & Quiz

Q1-2: Which of the following statement(s) is(are) TRUE about regularization parameter λ ?

A. *λ is the tuning parameter that decides how much we want to penalize the flexibility of our model.*
B. *λ is usually set using cross validation.*

1. True, True
2. True, False
3. False, True
4. False, False

Q1-2: Which of the following statement(s) is(are) TRUE about regularization parameter λ ?

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1. True, True ⬅
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- The optimization problem can be viewed as following:

$$\text{minimize}(\text{Loss}(\text{Data}|\text{Model}) + \lambda\ \text{complexity}(\text{Model}))$$

- If the regularization parameter is large then it requires a small model complexity
- We have learned how to use cross validate to set hyperparameters including regularization parameters.

Q2-1: Select the correct option about regression with L2 regularization (also called *Ridge Regression*).

A. *Ridge regression technique prevents coefficients from rising too high.*

B. *As $\lambda \rightarrow \infty$, the impact of the penalty grows, and the ridge regression coefficient estimates will approach infinity.*

1. Both statements are true.
2. Both statements are false.
3. Statement A is true, Statement B is false.
4. Statement B is true, Statement A is false.

Q2-1: Select the correct option about regression with L2 regularization (also called *Ridge Regression*).

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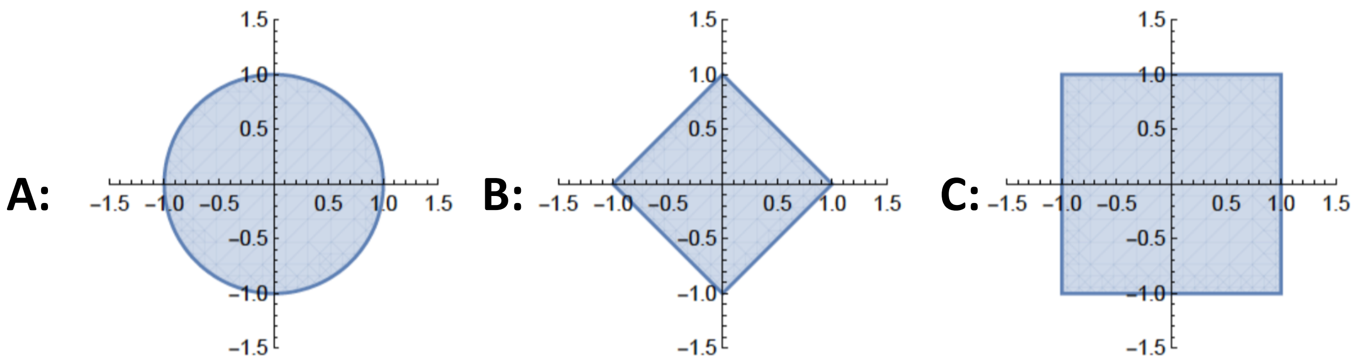
Q3-1: Following figure shows 3-norm sketches: $||x||_p<1$ for p = 1, 2, ∞. Recall that $||x||_\infty = \max\{|x_i| \text{ for all } i\}$



1. A: 1, B: 2, C: ∞
2. A: 2, B: 1, C: ∞
3. A: 2, B: ∞, C: 1
4. A: ∞, B: 2, C: 1

Q3-1: Following figure shows 3-norm sketches: $||x||_p<1$ for p = 1, 2, ∞.
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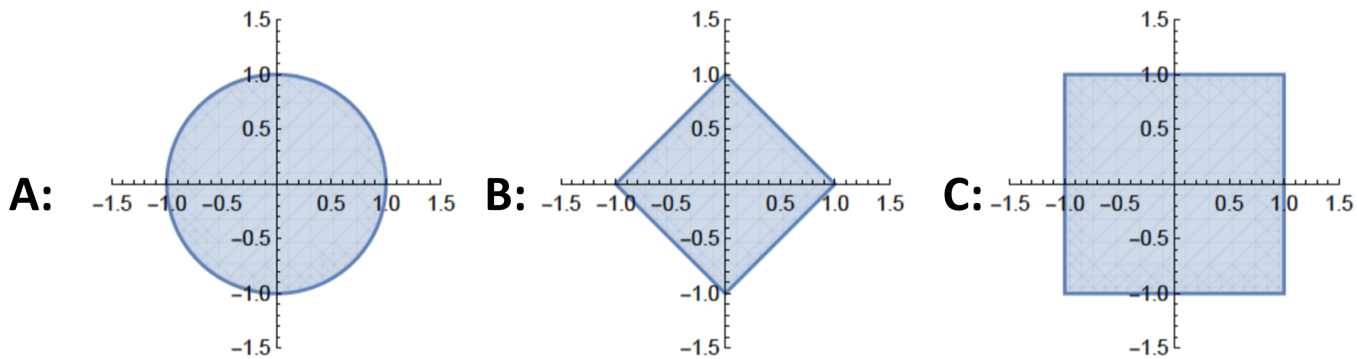

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Data Augmentation

Augmentation: transform + add new samples to dataset

- Transformations: based on domain
- Idea: build **invariances** into the model
  - **Ex**: if all images have same alignment, model learns to use it
- Keep the label the same!

Data Augmentation: Examples

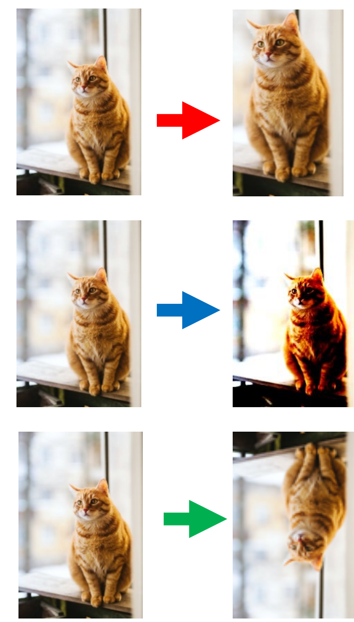
Examples of transformations for images

- **Crop** (and zoom)
- **Color** (change contrast/brightness)
- **Rotations+** (translate, stretch, shear, etc)

Many more possibilities. Combine as well!

Q: how to deal with this at **test time**?

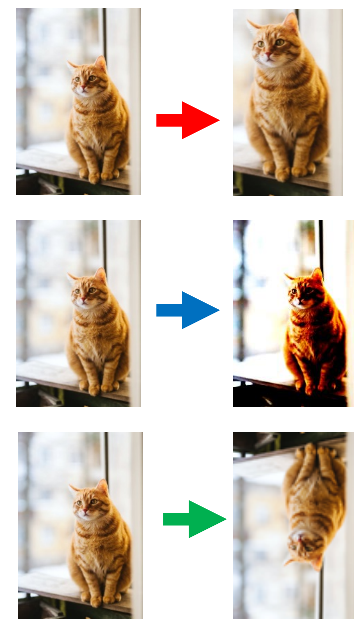
- A: transform, test, average



Combining & Automating Transformations

One way to automate the process:

- Apply every transformation and combinations
- **Downside:** most don't help…



Want a good policy, ie, 

- Active area of research: search for good policies

1. **Ratner et al**: "Learning to Compose Domain-Specific Transformations for Data Augmentation"
2. **Cubuk et al**: "AutoAugment: Learning Augmentation Strategies from Data"

Data Augmentation: Other Domains

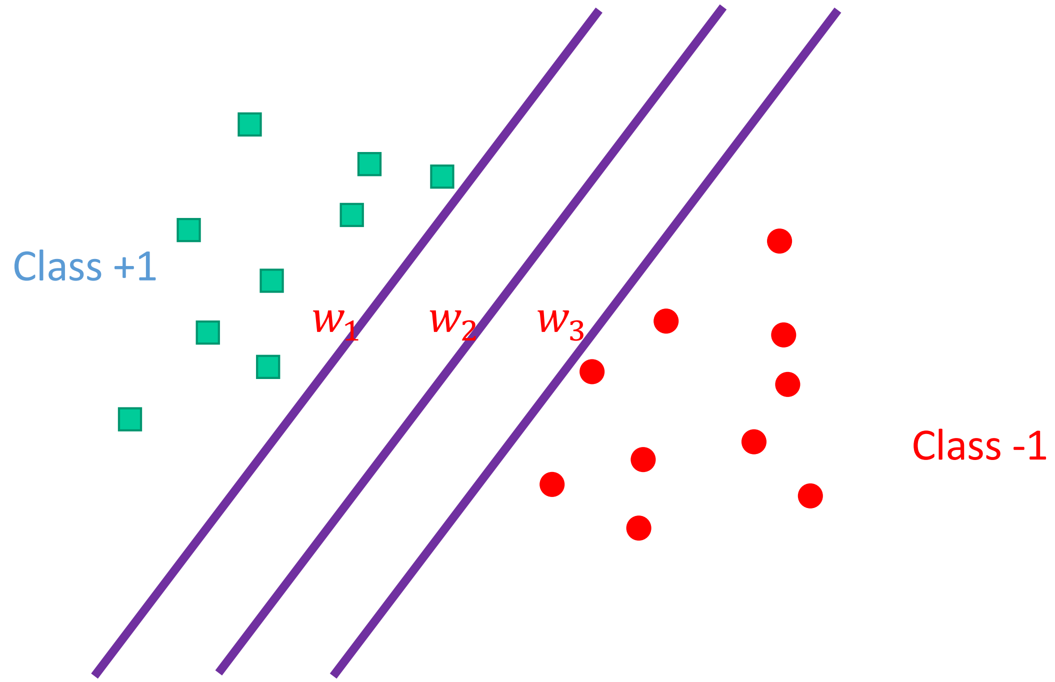
Not just for image data. For example, on text:

- Substitution
  - E.g., “It is a **great** day” ➔ “It is a **wonderful** day”
  - Use a thesaurus for particular words
  - Or, use a model. Pre-trained word embeddings, language models
- Back-translation
  - “Given the low budget and production limitations, this movie is very good.” ➔ “There are few budget items and production limitations to make this film a really good one”

Xie **et al**: “Unsupervised Data Augmentation for Consistency Training”

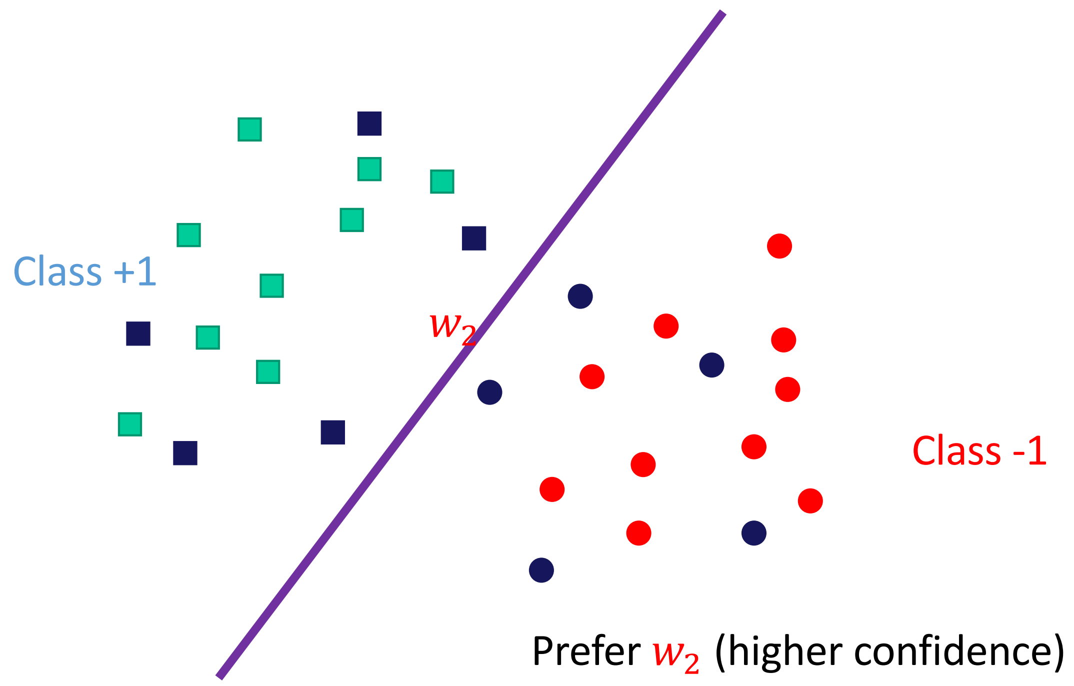
Adding Noise

- What if we have many solutions?



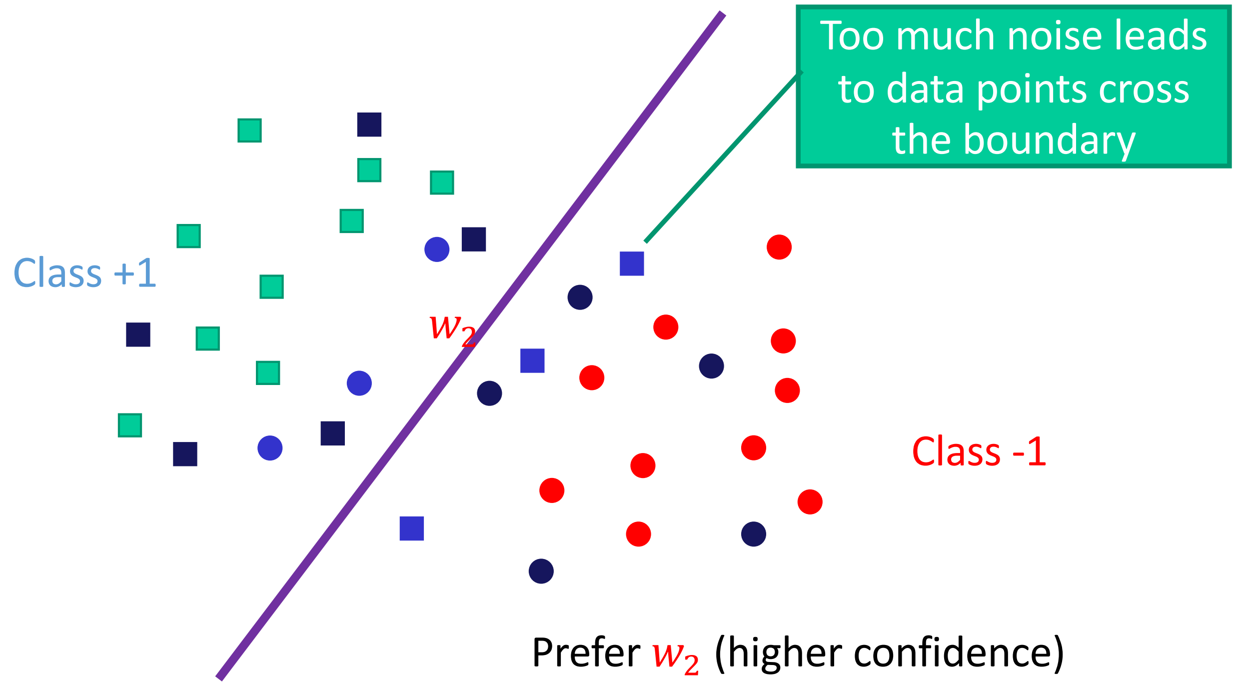
Adding Noise

- Adding some amount of noise helps us pick solution:



Adding Noise

- Too much: hurts instead



Adding Noise: Equivalence to Weight Decay

- Suppose the hypothesis is $f(x) = w^T x$, noise is $\epsilon \sim N(0, \lambda I)$
- After adding noise, the loss is

$$L(f) = \mathbb{E}_{x,y,\epsilon}[f(x+\epsilon) - y]^2 = \mathbb{E}_{x,y,\epsilon}[f(x) + w^T\epsilon - y]^2$$

$$L(f) = \mathbb{E}_{x,y,\epsilon}[f(x) - y]^2 + 2\mathbb{E}_{x,y,\epsilon}[w^T\epsilon(f(x) - y)] + \mathbb{E}_{x,y,\epsilon}[w^T\epsilon]^2$$

$$L(f) = \mathbb{E}_{x,y,\epsilon}[f(x) - y]^2 + \lambda\left||w|\right|^2$$

Early Stopping

- **Idea**: don't train the network to too small training error
  - Larger the hypothesis class, easier to find a hypothesis that fits the difference between the two
  - So: do not push the hypothesis too much; use validation error to decide when to stop

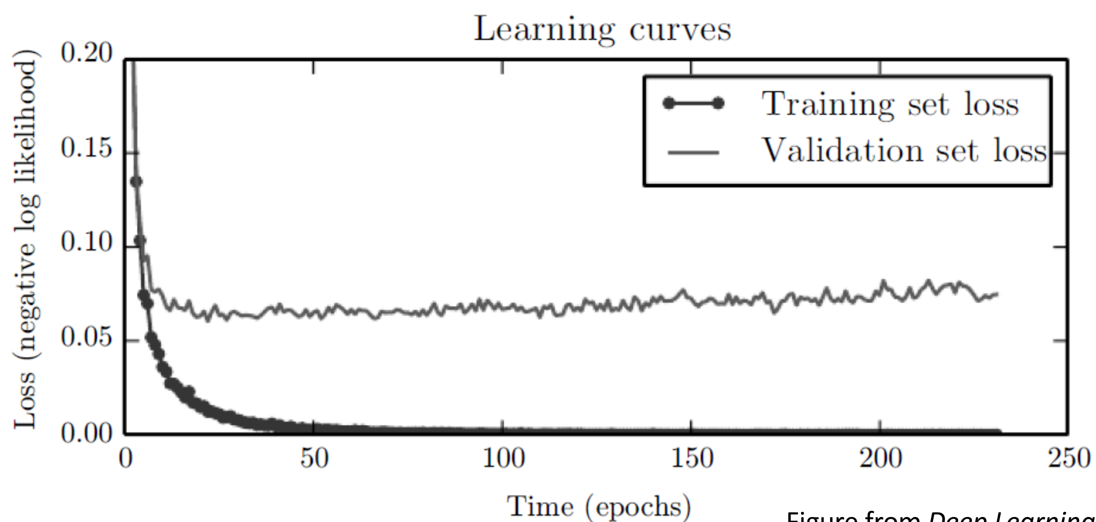
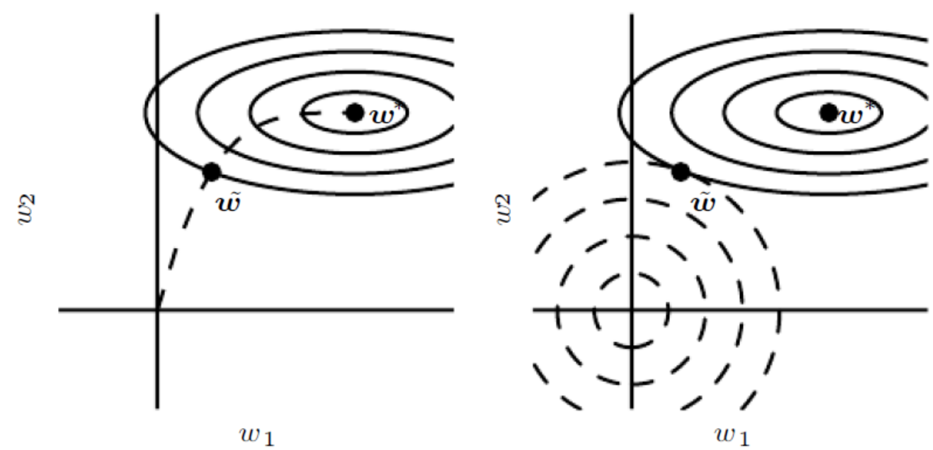


Figure from *Deep Learning*, Goodfellow, Bengio and Courville

Early Stopping

- Practically: when training, also output validation error
  - Every time validation error improved, store a copy of the weights
  - When validation error not improved for some time, stop
  - Return the copy of the weights stored



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Dropout

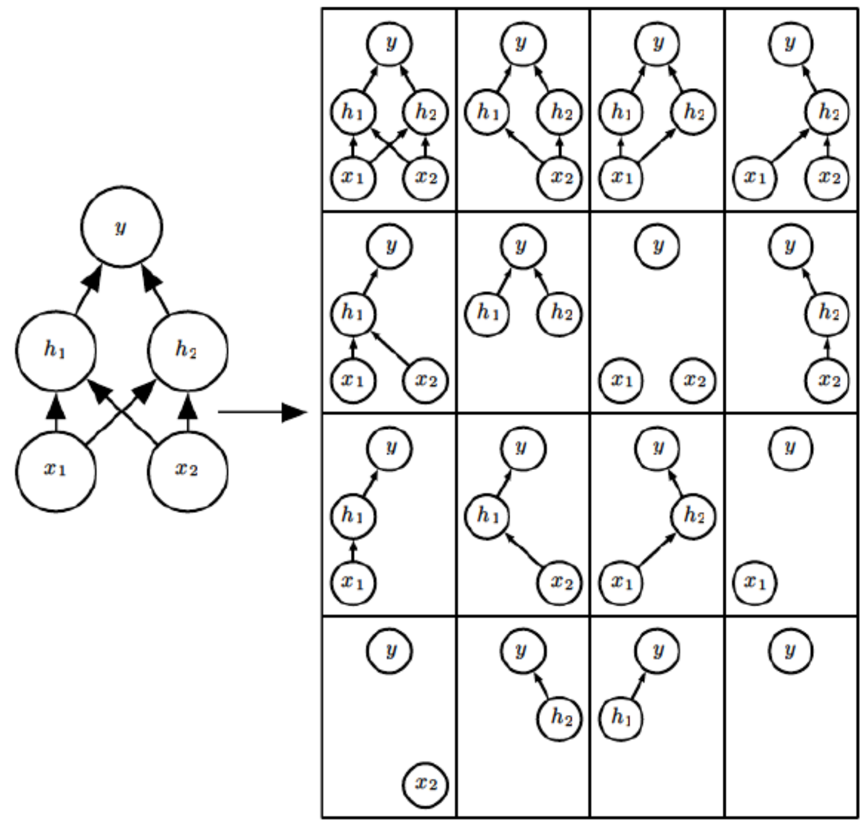
- **Basic idea**: randomly select weights to update

- In each update step
  - Randomly sample a different binary mask to all the input and hidden units
  - Multiply the mask bits with the units and do the update as usual

- Typical dropout prob: 0.2 for input and 0.5 for hidden units

Dropout

- Closely related to bagging:
  - Ensembling many models



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Batch Normalization

- If outputs of earlier layers are uniform or change greatly on one round for one mini-batch, then neurons at next levels can't keep up: they output all high (or all low) values

- Next layer doesn't have ability to change its outputs with learning-rate-sized changes to its input weights

- We say the layer has "saturated"

Batch Normalization

- Algorithm:

- (i)-(iii) like standardization of input data, but w.r.t. only the data in mini-batch. Can take derivative and incorporate the learning of last step parameters into backpropagation.

- Note last step can completely un-do previous 3 steps

- But if so this un-doing is driven by the *later* layers, not the *earlier* layers; later layers get to "choose" whether they want standard normal inputs or not

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1\ldots m}\}$;
Parameters to be learned: γ, β

Output: $\{y_i = \text{BN}_{\gamma,\beta}(x_i)\}$

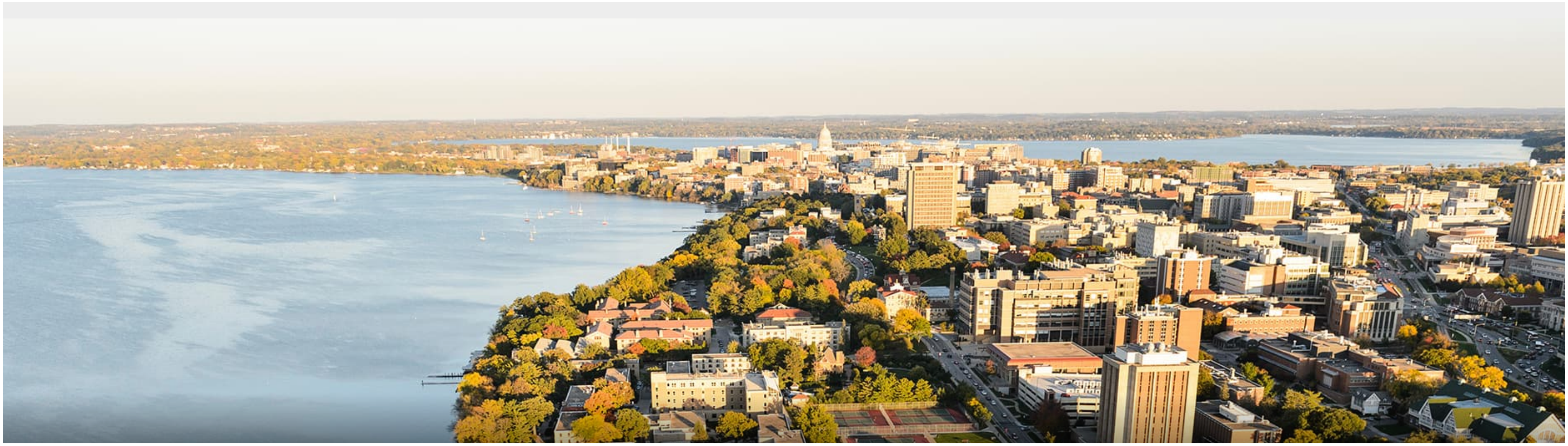
$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i \qquad \text{// mini-batch mean}$$

$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m}\sum_{i=1}^{m}(x_i - \mu_{\mathcal{B}})^2 \qquad \text{// mini-batch variance}$$

$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \qquad \text{// normalize}$$

$$y_i \leftarrow \gamma\widehat{x}_i + \beta \equiv \text{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$$

Algorithm 1: Batch Normalizing Transform, applied to activation x over a mini-batch.



Break & Quiz

Q2-2: Are these statements true or false?
(A) We need validation data to decide when to early stop.
(B) We can think early stopping as a regularization to limit the volume of parameter space reachable from the initial parameter.

1. True, True
2. True, False
3. False, True
4. False, False

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(A) We need validation data to decide when to early stop.
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1. True, True ⬅
2. True, False
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4. False, False

(A) As is shown in the lecture.
(B) That's true. Early stopping will limit the training time and thus potentially limit the space the training can search.

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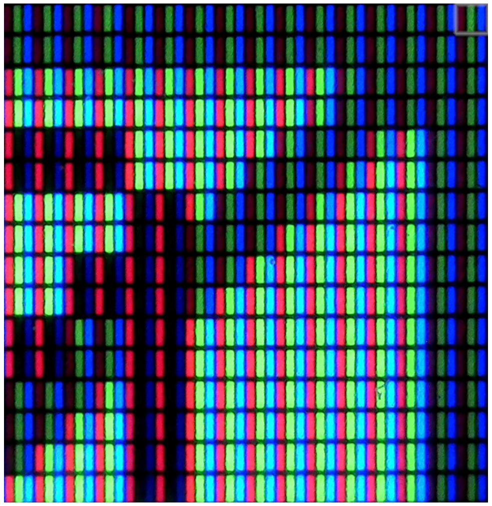
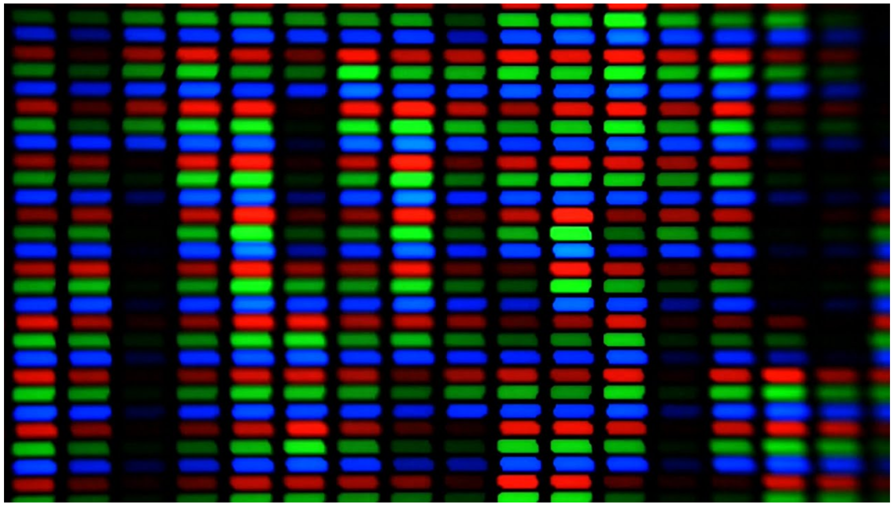
Images as Input?

- We could use the feed-forward fully-connected layers we have so far…
  - Kind of big though…
  - Also, if our images move, should the weights change?



Microsoft



PixelArt4K

Convolution Operation

- Given array u_t and w_t, their convolution is a function s_t

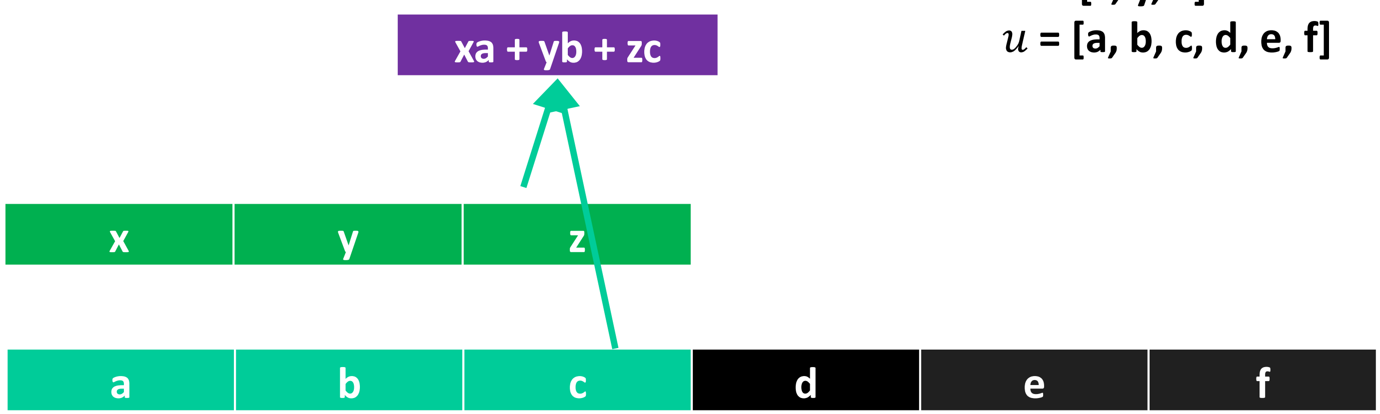
$$s_t = \sum_{a=-\infty}^{+\infty} u_a w_{t-a}$$

- Written as $s = (u * w) \quad \text{or} \quad s_t = (u * w)_t$
- When u_t or w_t is not defined, assumed to be 0

Convolution Operation

- Example:

w = [z, y, x]
u = [a, b, c, d, e, f]



Convolution Operation

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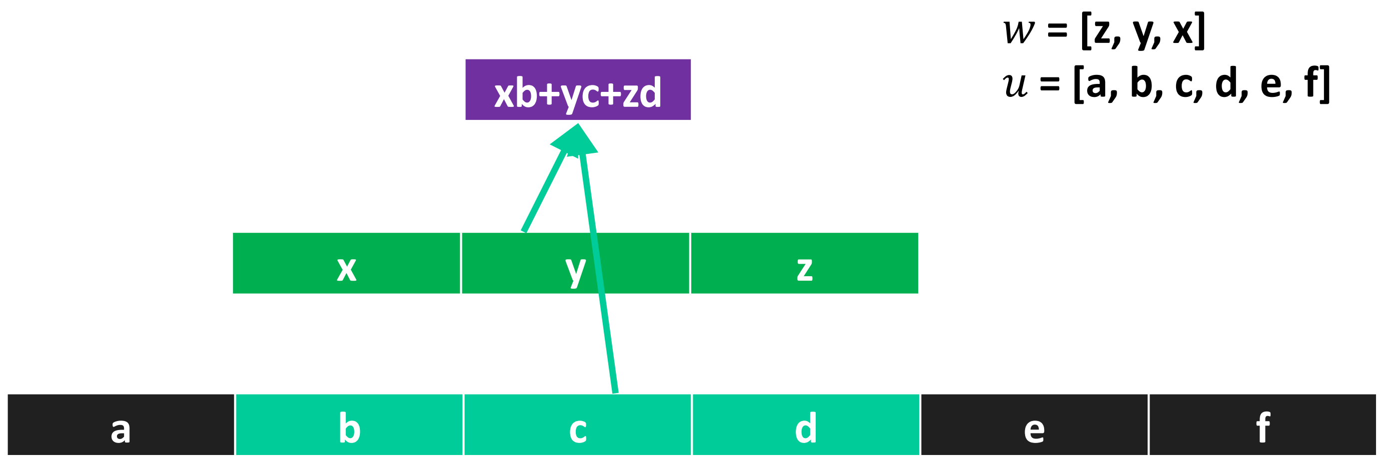

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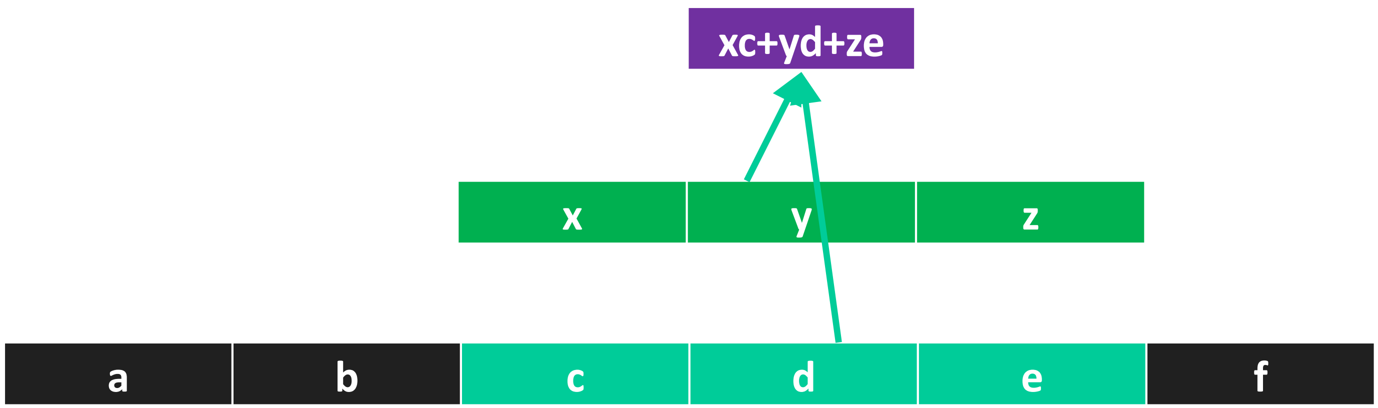

Convolution Operation

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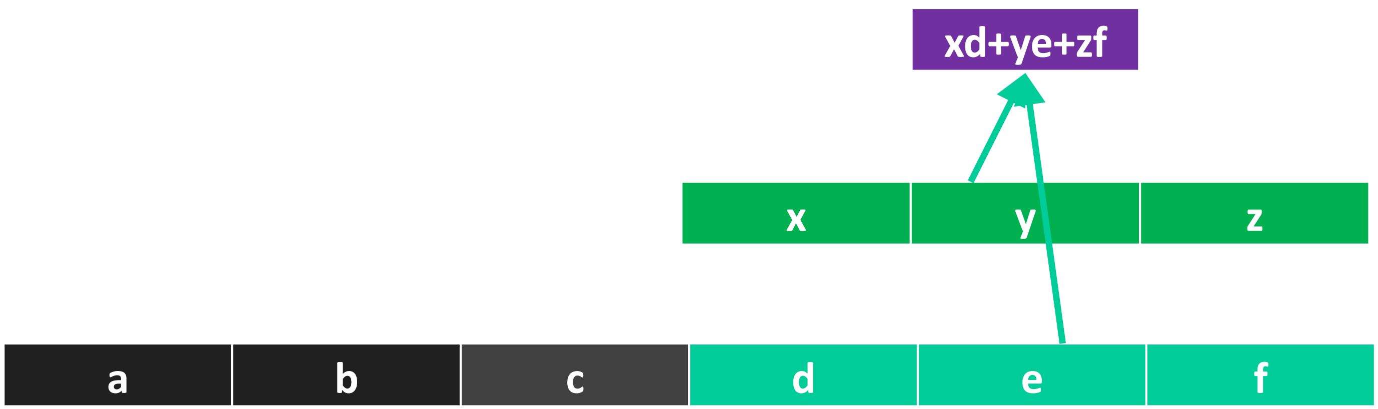
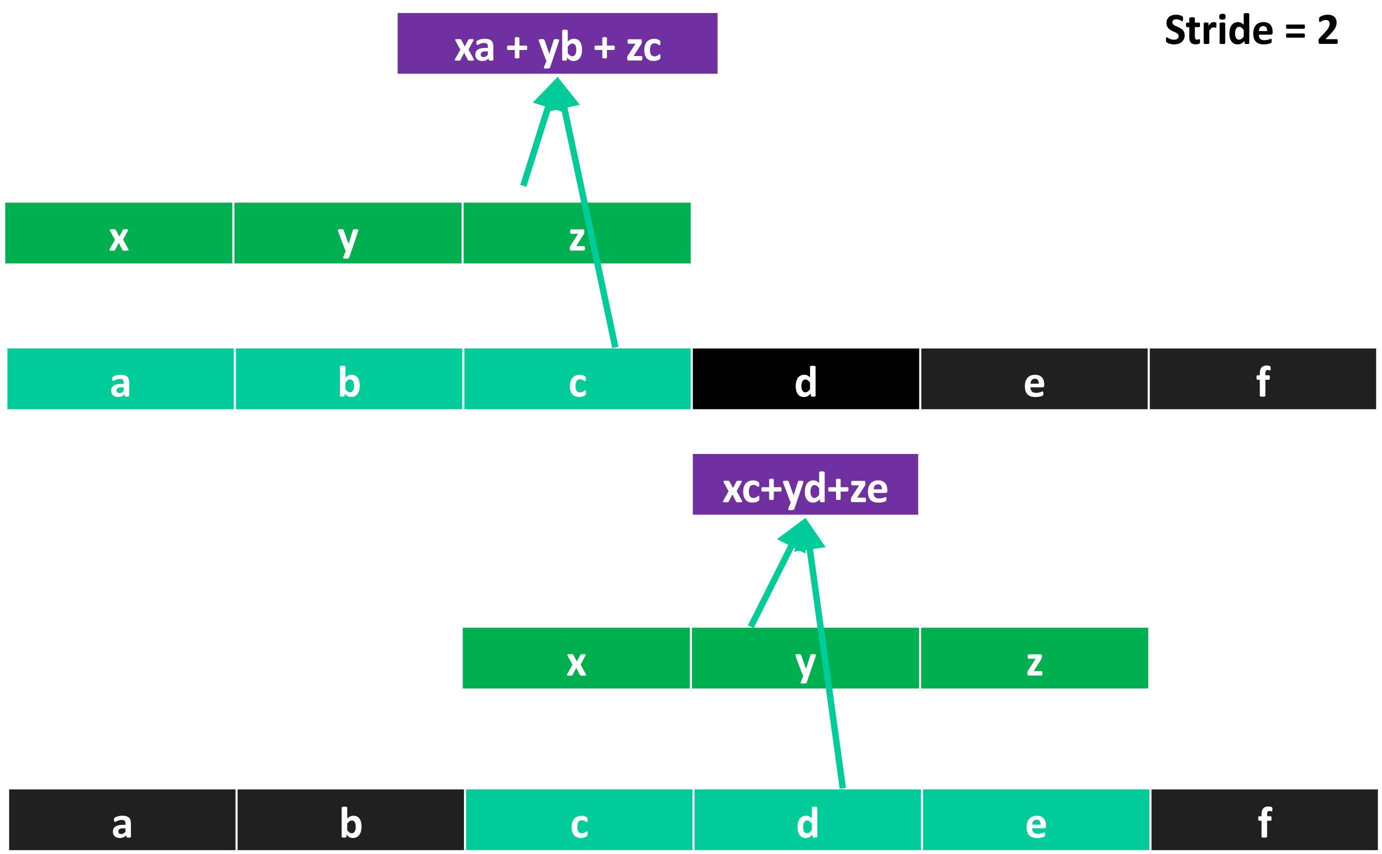


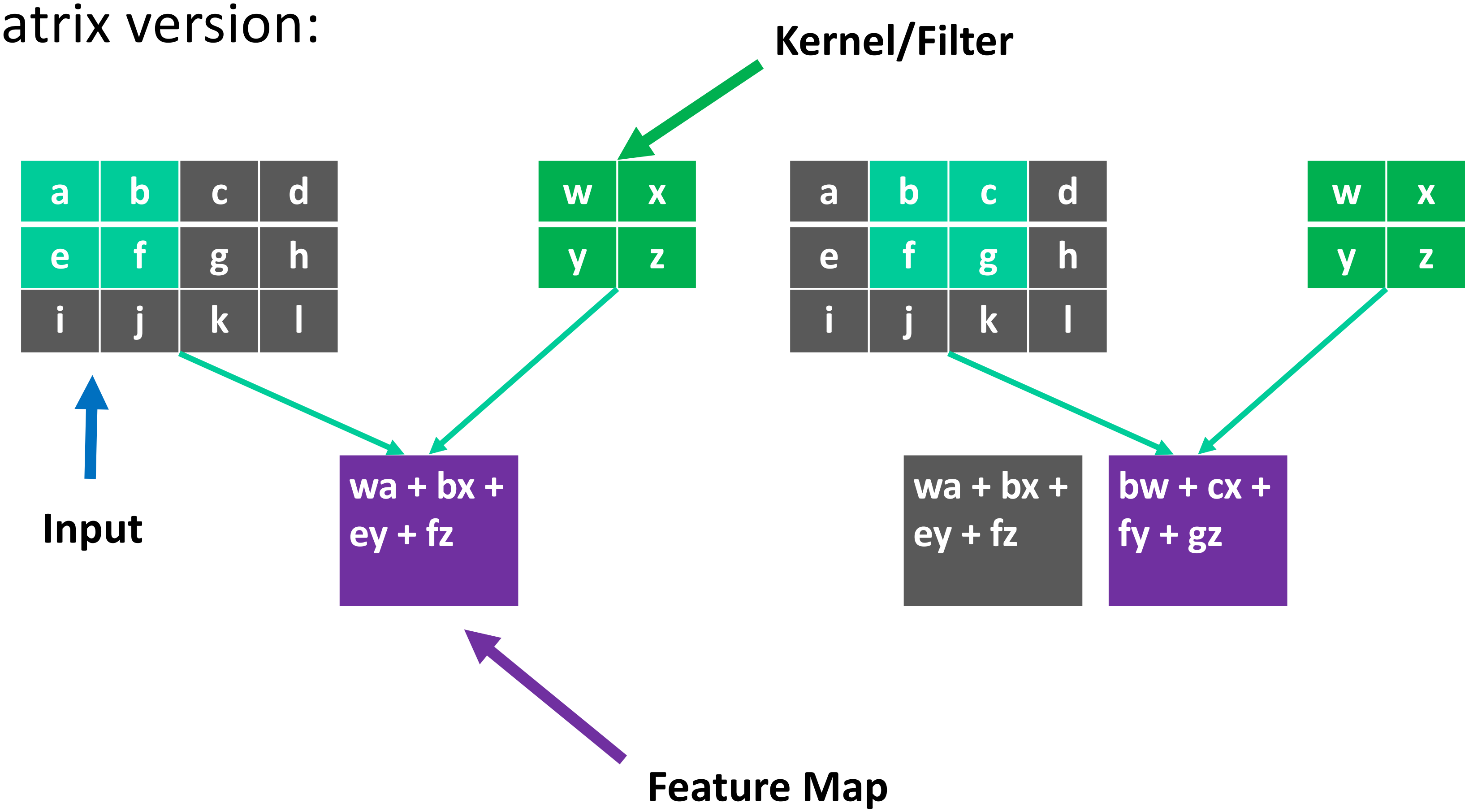
Convolution Operation

- Stride: # of positions we move per step



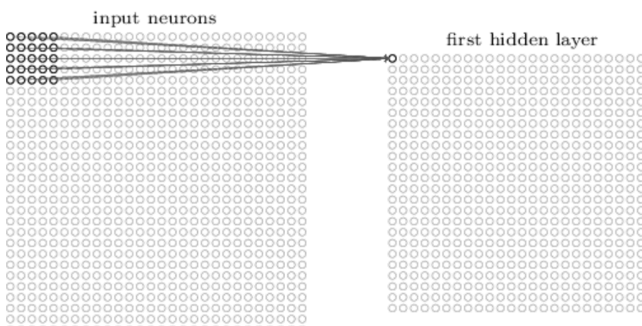
Convolution Operation

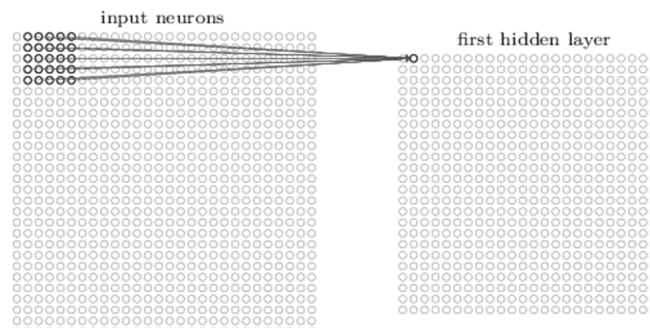
- Matrix version:



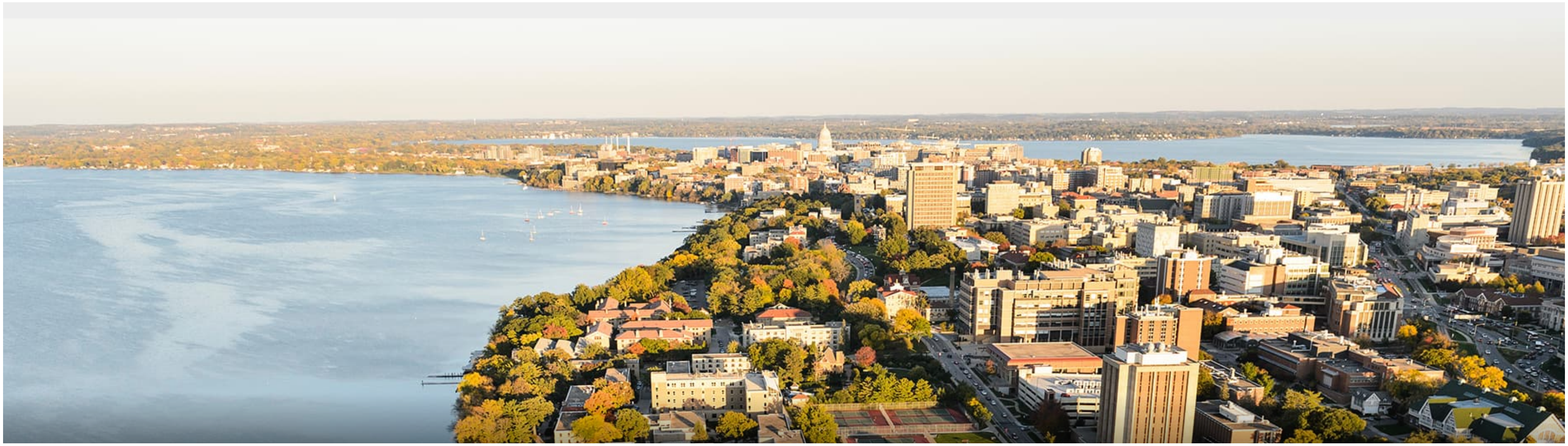
Convolution Operation

- All the units used the same set of weights (kernel)
- The units detect the same “feature” but at different locations





[Figure from neuralnetworksanddeeplearning.com]



Thanks Everyone!

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