Background

Machine Learning

Linear classifiers: Given input x/weights W, outputs f(x, W)=Wx+b

- Predict a vector (corresponding to class scores)
    - Bias trick to incorporate biases as last column of weights
- Is a single-layer NN (perceptron); outputs linear predictions
    - Separates space of inputs into different decision regions
    - Cannot predict from nonlinear relationships, XOR
- Intuitively: learns one "template" per class, then measures correlation between template and input image
    - Drawback: Cannot handle multiple modes of data, intra-class variation
- Variations
    - Linear regression: $y = Wx + b$
    - Logistic regression: $y = \sigma(Wx + b)$
    - Softmax regression: $z = Wx + b \implies y_i = \frac{e^{z_i}}{\sum_j e^{z_j}}$

Finding a good W: via a ***loss function*** to quantify performance of W

- Loss function averaged across all samples in dataset
- Example loss functions
    - Linear regression: L2 distance $\frac{1}{2}(s_i - y_i)^2$
    - Logistic regression: cross-entropy loss $L = -\log\left(\frac{\exp(s_{y_i})}{\sum_j \exp(s_j)}\right)$
        - Log of predicted probability (via softmax) of true class
        - Binary cross-entropy/BCE: $BCE(p, y) = -(y\log(p) + (1-y)\log(1-p))$
    - Multiclass SVM: hinge loss $L = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$
        - Sum of predicted score - true score, max with 0 (wants to make true class' score higher than all other classes)

Optimization: Finding the set of weights minimizing loss

- Via ***gradient descent*** (negative gradient - direction of steepest descent)

- Computing gradients: **numeric gradient** vs **analytic gradient**
    - **Numeric gradient** - approximate & slow convergence, but easier to implement
    - **Analytic gradient** - exact & fast, but more error-prone
        - Used in practice; numeric gradient used as a check (gradient check)
- ***Gradient descent***: at each step, move in the direction of negative gradient
    - Hyperparameters: weight initialization method, # steps, learning rate
    - Challenges: gradient may become zero or vanish, may become stuck in local mins
- *Interpretation*: loss over dataset computes the expected value of loss over real-world distribution of values (x, y)

Issue: *Batch gradient descent* (computing gradient over full batch) is expensive for large batches

- Can use ***stochastic gradient descent***/**SGD** - GD on minibatches (batch size as hyperparameter)
- Normal SGD results in noisy gradient; can use ***momentum*** (add a weighted running mean of gradients to SGD update) for less noisy optimization
    - Momentum: $v_t = \nabla f(x_t) \mapsto v_t = \rho v_t + \nabla f(x_t)$

  AdaGrad: scale gradient element-wise based on historic sum of squares
    - $s_t = s_{t-1} + g_t^2 \implies w_t = w_{t-1} - \frac{\eta}{\sqrt{s_t + \epsilon}} g(t)$
    - Acts as a form of per-parameter/adaptive learning rate
    - Lowers magnitude of steps along "steep" directions; boosts magnitude of steps along "flat" directions
- **RMSProp/weighted AdaGrad**: adds a decay rate for historic gradient term
    - $s_t = \gamma s_t + (1 - \gamma) g_t^2$
- **Adam**: "almost" RMSProp + momentum
    - Update step is (almost) momentum SGD update with RMSProp magnitude scaling
    - Bias correction - accounts for first/second moment estimates starting at 0
        - Divides momentum, RMSProp terms by $1 - \beta_1^t, 1 - \beta_2^t$ respectively

Adam:

```
input : $\gamma$ (lr), $\beta_1, \beta_2$ (betas), $\theta_0$ (params), $f(\theta)$ (objective)
initialize : $m_0 \leftarrow 0$ ( first moment), $v_0 \leftarrow 0$ (second moment
for $t = 1$ to $\ldots$ do
    $g_t \leftarrow \nabla_\theta f_t(\theta_{t-1})$
    $m_t \leftarrow \beta_1 m_{t-1} + (1 - \beta_1) g_t$
    $v_t \leftarrow \beta_2 v_{t-1} + (1 - \beta_2) g_t^2$
    $\widehat{m_t} \leftarrow m_t / \big(1 - \beta_1^t\big)$
    $\widehat{v_t} \leftarrow v_t / \big(1 - \beta_2^t\big)$
    $\theta_t \leftarrow \theta_{t-1} - \gamma \widehat{m_t} / \big(\sqrt{\widehat{v_t}} + \epsilon\big)$
return $\theta_t$
```

Overfitting occurs when model performs well on training data, but poorly on unseen data

→ ***Regularization*** incorporates an additional term $\lambda R(W)$ in loss function to incentivize less complex learned models; helps to combat overfitting

- Decreases performance on training set in exchange for better performance on validation, test sets
- Simple approach: L1/L2 regularization on magnitude of weights
    - More complex: dropout, batchnorm, cutout, mixup, etc.
    - *Interpretation*: encodes some form of "preference" regarding model weights
        - Ex: L2 prefers more "spread out" weights
- Note: L2 regularization (encodes penalty in loss itself) vs weight decay (adds additional $-\lambda w$ term in update step directly)
    - Equivalent for SGD + variants, but different for adaptive methods (e.g. AdaGrad) - weight decay is not included in adaptive sums, but L2 is

2nd-order optimization: rather than just the gradient, use gradient + Hessian to make quadratic approximation of loss landscape (look at 2nd-order Taylor expansion, use Newton's method)

- Issue: Inverting Hessian (Newton's method) is expensive, O(N^3)
- Can use Quasi-Newton methods: approximate inverse Hessian via rank-1 updates O(N^2)
    - L-BFGS - doesn't store full inverse Hessian (low memory use), but only works well for full batch setting; does not transfer well to minibatch
- In practice: 1st-order in most cases; L-BFGS when doing full batch updates

Machine Learning (Misc.)

- ***Hyperparameters***: choices made before learning regarding parameters (rather than being learned from data)
    - Evaluate via split train/validation/test datasets
    - k-fold cross validation for small datasets
- ***Curse of dimensionality***: Number of points needed for uniform coverage of space increases exponentially with input dimension
- ***Normalization***: can normalize datasets relative to known statistics (mean + stdev, e.g.) for easier learning & better transfer across datasets

Neural Networks

Issue: Linear classifiers can only learn linear decision boundaries

- Can use feature transforms - linear boundaries in transformed space correspond to nonlinear boundaries in original space
    - *Issue*: Requires knowing (fixed) feature transforms beforehand
    - Ex: color histogram/histogram of oriented gradients (HoG) as image features
- Image features via bag of words/BoW approach - extract random patches from image & cluster to form "codebook of visual words"
    - Use codebook as image encoding, a new ML model (e.g. SVM) from classification

Neural networks incorporate a nonlinear ***activation function*** between linear layers

- ***Multi-layer perceptron/MLP*** - use multiple fully-connected layers (rather than regression/single-layer)
    - Later layers use features from previous layer's activation
    - Weakly inspired by brain structure
    - Universal approximator (similar to k-NN)
- *Ex.* (Activation functions)
    - **ReLU**: $f(x) = \max(0, x)$/ **Leaky ReLU**: $f(x) = \max(0.2x, x)$
    - **Sigmoid**: $\sigma(x) = 1/(1 + e^{-x})$
    - **Tanh**: $\tanh(x) = (e^{2x} - 1)/(e^{2x} + 1)$
    - **Softplus**: $\log(1 + \exp(x))$

Convex functions: intuitively, look like a "multidimensional bowl"

- Generally easy to optimize, can derive convergence guarantees
    - In optimization, prefer to minimize convex functions if possible
- Linear classifier loss functions are convex; but neural networks are generally non-convex (few/no convergence guarantees, but decent empirical behavior)

Backpropagation

When training neural networks, need to compute gradients

- Can construct *computational graphs* - indicating operations from inputs to outputs
- ***Backpropagation***: can use the Chain Rule to derive gradients of the loss function with respect to every weight in network
    - From weights at end of network, “backpropagate” derivatives to further-back weights (from last layer to first layer)
    - Chain rule: Downstream gradient $\frac{\partial f}{\partial y} = \frac{\partial q}{\partial y} \cdot \frac{\partial f}{\partial q}$ (local * upstream gradients)
    - First perform forward pass (computing $f(x, w)$), then use backward pass to compute gradients for every weight
- Patterns in gradient flow:
    - Add gates distribute the upstream gradient to both elements of input
    - Copy gate adds upstream gradients to find singular downstream gradient
    - Multiplier gate multiplies upstream gradient with multiplicands
    - Max gate gives downstream gradient equal to upstream (for taken branch), 0 for branches not taken
- Pytorch *autograd* - uses forward, backward methods to compute gradients automatically

Backpropagation with vectors: rather than local gradients (i.e. vectors), multiply by local Jacobian matrices (2D) instead

- Jacobians indicate how much each element of inputs influence output
- Jacobians are sparse (all off-diagonal entries 0), large; therefore, can compute matrix product implicitly (via normal multiplication operators, without constructing full matrix)
- For backprop with matrices, use multi-dimensional Jacobian

Convolutional Neural Networks

Image classification: Given an image and a set of K possible classes, output the class that matches that image

- A fundamental CV task
- Challenges: viewpoint & intraclass variations, interclass similarities, occlusion, domain changes, etc.

Image classifiers

- *k-Nearest Neighbors/k-NN*: Find k nearest points to input in the memorized dataset
    - O(1) training, O(N) testing
    - Image classification via pixel distance (questionable metric)
        - Alt: k-NN on ConvNet features (works well)
    - Is a universal approximator (can represent [almost] any function)
- Regular neural networks (MLPs)
- Convolutional neural networks (CNNs)

Convolution & Normalization Layers

Issue: Regular neural networks (i.e. MLPs) don't explicitly consider the spatial structure of images; act only via local matrix/vector products + activation function

- Within an MLP, have no interaction between adjacent input elements within a layer

Solution: can define new spatial operations tailored to image format: ***convolution*** & ***pooling layers***

Convolution layers convolve input image with a filter/kernel

- Filter contains same depth/# channels as input image; "slide" over image spatially (take dot products) to produce *activation map*
    - Kernel dimension corresponds to number of dimensions of input (e.g. 2D input gives 2D kernel; 3D input gives 3D kernel)
    - Can use multiple filters; each produces a single channel in output
    - Also use a bias vector (one scalar per filter, same size as activation map)
    - Shapes: $(N, C_{in}, H, W) \rightarrow (N, C_{out}, H', W')$

- Convolution as cross-correlation: dot product performs a matching between filter, scanned elements (higher -> better match)

Can stack multiple convolutional layers (with activations in between)

- Multiple convolution layers, stacked, correspond to a single larger convolution
    - Each convolution layer is a linear classifier
- Add ***padding*** around input (consisting of zeros) to preserve size of feature map with each convolution layer
    - Can set $P = (K-1)/2$ [K the kernel size] to preserve input shape
- Further-back convolution layers correspond to convolutions of/depend on larger portions of the region (have larger receptive fields)
    - Each convolution adds $K-1$ to size of ***receptive field***
        - Receptive field size: $1 + L \cdot (K-1)$
    - Initial layers learn local features (e.g. local image templates, edges); higher layers learn more complex features
- *Issue*: for large images, need many layers for receptive fields to "see" whole image
    - Can downsample inside network to reduce # layers needed
        - ***Strided convolutions*** - convolutions take larger steps between dot products to produce a smaller activation map
    - For later layers in network: spatial size decreases (via pooling), but number of channels increases (preserving total volume)
- Output size: $H' = (H - K + 2P)/S + 1$ (and similar for W')

Pooling layers: alternative way to downsample feature map

- ***Max pooling*** - takes maximum of values within receptive field as output value
    - Results in <u>invariance to small spatial shifts</u>
- Hyperparameters: kernel size, stride, pooling function
    - Output size: $H' = (H - K)/S + 1$

<u>Convolutional Neural Networks (CNNs)</u>

Classic architecture (*LeNet/AlexNet*):

1. [Conv, ReLU, Pool] N times

2. Flatten
3. [FC, ReLU] N times
4. FC to produce output

Issue: Deep networks are difficult to train, susceptible to "*internal covariate shift*"
Solution: Use ***batch normalization*** - normalize layer outputs to make them have zero mean, unit variance across a batch

- Formula: $\hat{x} = \frac{x-E[x]}{\sqrt{Var[x]}}$ (differentiable, for backprop)
    - Each dimension of input x is normalized separately
        - Use (running) average μ_j, σ_j^2 of mean/variance values observed in training during testing
- Can learn scale, shift parameters γ, β [dim D] to keep more information than pure zero mean/unit variance
    - Final output: $y_{i,j} = \gamma_j \hat{x} i, j + \beta_j$
- Batch norm for convolutional networks - *spatial batchnorm*
    - Perform batch-norm across each channel (for $(N, C, H, W$ shape, perform batchnorm across slices (N, H, W))
- Makes deep networks much easier to train:
    - Allows higher learning rates, faster convergence
    - Makes networks more robust to initialization
    - Acts as a form of regularization during training
    - During testing (parameters fixed), is a linear operator; can incorporate into convolutional layer directly
- *Issues*: not well-understood theoretically, can behave weirdly during training/testing (causes bugs)

Computing parameters

- Number of params - sum of total number of weights in network + number of biases
    - Single convolutional layer: $C_{out} \cdot C_{in} \cdot K \cdot K + C_{out}$
- 4 bytes per element (per float) gives memory
- Floating point operations/FLOPs: number of output elements * ops per output element

- Single convolutional layer: $(C_{out} \times H' \times W') \cdot (C_{in} \times K \times K)$

Types of normalization layers

1. Batch normalization (above)
2. *Layer (1D) normalization*: for each input in batch, compute mean/variance across entire dimension of input (channel + height, width, etc.)
3. *Instance (2D) normalization*: for each input in batch, compute mean/variance (for each channel, separately) across entire dimension of input

Inductive bias - encoding some hypothesis about network function into network architecture

Modern CNN Architectures

AlexNet (2012) - [Conv, ReLU, Pool] into [FC, ReLU]

- First major instance of deep CNNs for classification, achieved 1st place on ImageNet
    - From LeNet: deeper & larger, ReLU instead of sigmoid activationo, larger dataset + more training cycles
    - Architecture (i.e. layer kernel sizes, e.g.) via trial and error
- Notable characteristics:
    - Most memory usage in early convolutional layers; FLOPs in convolutional layers
    - Nearly all parameters in fully-connected layers
- Succeeded by similar, deeper networks (**ZFNet**, **VGG**)
    - *ZFNet*: changed kernel stride sizes
    - ***VGG***: more regular design: all conv are 3x3/pad 1, max pool 2x2 stride 2; double # channels after each pool
        - 2 3x3 convolutions have same receptive field as 5x5, but fewer parameters & faster to compute
        - Significantly larger than AlexNet

GoogLeNet - introduced improvements on AlexNet

- Aggressive downsampling at input via *stem network* to decrease computation, memory
- *Inception module* - local unit with parallel branches (multiple parallel convolutional layers with different dimensions, followed by concatenation); repeated throughout network
- ***Global average pooling*** (**GAP**) followed by linear layer (rather than FC layers) at end; requires significantly less parameters
- Hack: auxiliary classifiers (intermediate "classifiers" computing loss) in middle stages of network
    - Since propagating loss across entire network depth is not clean process (before batchnorm)

<u>ResNet</u>

Issue: With batchnorm, can train deeper and deeper networks; however, CNN (i.e. AlexNet & similar) performance actually decreases with deeper models (rather than shallow models)

- Initial guess was that model was overfitting; however, training error is also worse on deeper models (not just test) -> deeper modes are underfitting
- Hypothesis: deeper models harder to optimize, can't easily learn identity functions to emulate shallow models
    - Deeper models should be able to learn shallow model + successive layers of identity to match shallower models' training error

Residual networks add an extra "additive shortcut" between convolutional blocks to make learning identity functions easier

- *Residual blocks*: $x \mapsto f(x)$ becomes $x \mapsto f(x) + x$
    - Each residual block - first block halves resolution, doubles # channel

ResNet - stack of residual blocks (similar to VGG)

- Like GoogleNet - stem network at start for downsampling, global average pooling to replace FC layers at end
- *Bottleneck block*: replaces two 3x3 convs (within each residual block) with 1x1 -> 3x3 -> 1x1 convolutions
    - More layers for less computational cost
    - ResNet-50 - replaces ResNet-34 basic blocks with bottleneck blocks
- ResNets are able to train very deep networks, perform better than shallow ones
    - Still widely used today

<u>Complexity of convolutional models</u>

- VGG - highest memory + most operations
- GoogLeNet - very efficient (low # ops)
- AlexNet - low # operations, large # operations
- ResNet - moderately efficient (operations + parameters), higher accuracy
    - Can train very deep networks (to the point of diminishing returns)
    - Good standard choice of architecture
- Later: vision transformer (ViT) matches ResNets, outperform with more data

Improving residual networks

- Block design
    - Pre-activation: ReLU inside residual (rather than after) to ensure block can learn true identity
- *ResNeXt* - rather than single path of convolutions within bottleneck block, compute G-many paths in parallel, add together with residual at end
    - Grouped convolution - rather than all convolutional kernels touching all channels, have parallel convolution layers each working on a subset of channels (e.g. # channels / N)
        - Each parallel layer produces C out / N output channels
        - Allows for parallelization, distributing RAM cost
    - ResNeXt - add groups to improve performance, maintain computational complexity
- *Squeeze-and-Excitation/SENet* - adds "squeeze and excite" branch (global pooling + 2x FC + sigmoid) within each residual block; multiplies with residual output
    - Adds form of global context to each residual block

Other forms of convolutional networks

- *Densely connected neural networks*: introduce dense blocks, where each layer is connected to every other layer (essentially: concatenate outputs from all past layers to current layer's input at every step)
    - Alleviates vanishing gradient by strengthening propagation + encourages feature reuse across layers
- *MobileNets* - tiny networks (memory-wise)
    - Replaces standard convolution block with "depthwise convolution" (grouped convolution, # groups = # channels) block + pointwise 1x1 conv block
        - Reduces number of parameters dramatically (divides by C)
    - Used in mobile devices; related: ShuffleNet

Neural architecture search - automated process for designing NN architectures

- Controller network outputs network architecture, samples & trains child networks from controller; after each batch, perform policy gradient step on controller & repeat
- Outputs good architectures after a long time, but very expensive to perform
    - Can use to find efficient CNN architectures

Training Neural Networks

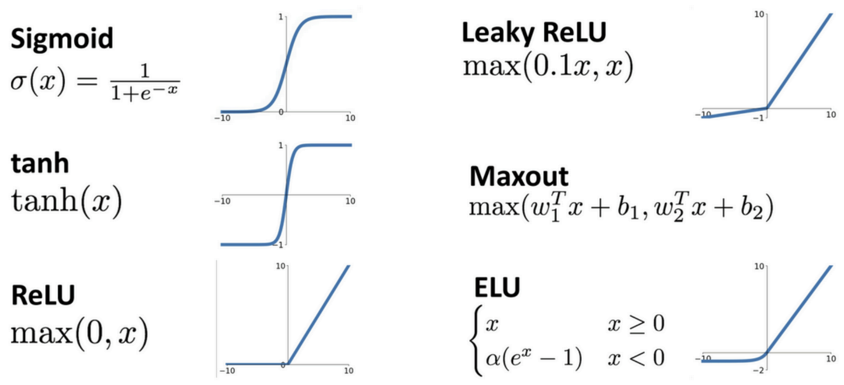
Initialization

Notable activation functions:

1. ***Tanh*** - squashes numbers to [-1, 1]
    a. Zero-centered (good), but kills gradients when saturated (bad)
2. ***ReLU***
    a. Advantages: does not saturate in + region, very efficient, converges fast in practice
    b. Disadvantages: no zero-centered output, gradient 0 for all x<0 (no updates)
3. ***Leaky ReLU***
    a. Advantages of ReLU + no vanishing gradients
4. *Exponential Linear Unit/ELU*: $f(x) = x$ for $x > 0$, $f(x) = \alpha(e^x - 1)$ for $x \leq 0$
    a. Benefits of ReLU + closer to zero mean + negative saturation regime compared to leaky ReLU (some robustness to noise)
    b. More expensive to compute (requires exp)
5. *Scaled Exponential Linear Unit/SELU*
    a. $selu(x) = \lambda x$ if $x > 0$, $selu(x) = \lambda\alpha(e^x - 1)$ if $x \leq 0$
    b. Scaled version of ELU, better for deep networks; is "self-normalizing" (can train deep SELU networks without batchnorm)
6. *Gaussian Error Linear Unit/GELU*:
    a. $X \sim N(0,1) \implies gelu(x) = xP(X \leq x) = \frac{x}{2}(1 + erf(x/\sqrt{2})) \approx x\sigma(1.702x)$
    b. Multiplies input by 0 or 1 at random; large values more likely to be multiplied by 1, small values by 0 (data-dependent dropout)
    c. Common in transformers

ReLU used in most cases (Leaky ReLU/ELU/SELU in limited cases)

- Sigmoid, tanh not generally used except to squash the output



Weight Initialization: How to initialize weights?

- Initialize all 0 causes all gradients to be the same; no "symmetry breaking"
- Initialize with small random numbers (Gaussian with zero mean, 0.01 stdev) works okay for small networks, but has problems for deeper networks
    - All activations tend to zero for deeper network layers
- Similar, but with 0.05 stdev -> all gradients saturate (local gradients zero, no learning)
- "*Xavier initialization*" - stdev = 1/sqrt(Din) - scales activations nicely for all layers
    - Conv layers: Din is $K^2 \cdot C_{in}$
    - Derivation: Sets value such that variance of output = variance of input (assuming x, w are i.i.d. zero-mean)

- ReLU initialization: Xavier assumes zero-centered activation function -> doesn't work, gradients vanish
    - *Kaiming initialization*: stdev = sqrt(2/Din) works well
- For residual networks, intiailizing with Kaiming method causes variance to grow with each block (due to residual connection)
    - *Solution*: first conv with Kaiming, second conv to zero in each residual block

Regularization

- Commonly used: L2 regularization, L1 regularization, Elastic net (L1 + L2)
- ***Dropout***: in each forward pass, randomly set some neurons to 0
    - Probability of dropping as hyperparameter; commonly 0.5

        - Forces network to have redundant representation; prevents co-adaptation of features (i.e. each neuron in a layer encoding an entirely separate feature)
            - Alt: dropout trains a large ensemble of models that share parameters
        - Used on FC layers for early networks, e.g. AlexNet/VGG (where most parameters located); GoogLeNet, ResNet, etc. use global average pooling (no dropout needed)
- ***Data augmentation***: when training for image classification, can perform various transformations to image (simulates training on a larger dataset)
    - Ex: horizontal flip, random crops/scales
    - More complex: color jitter, shearing, lens distortions, etc.

Intuitively, augmentation adds some randomness during training

- More approaches:
    - *Stochastic depth*: skip some residual blocks in ResNet during training
        - Use whole network during testing
    - *Cutout*: set random regions of images to 0 during training
        - Works well for small datasets; less common for larger datasets
    - *Mixup* - train on random blends of images
        - Ex: 40% dog, 60% cat (pixel-wise) has target label 0.4 dog, 0.6 cat
        - Scale blend probability from a beta distribution Beta(a,b) to keep blend weights close to 0, 1

General lessons for training NNs:

1. Batch normalization/data augmentation generally good ideas
2. Dropout for large FC layers

Training

Learning rate schedules: rather than a fixed learning rate, can instead vary learning rates over time

- *Step* (most common): reduce learning rate at a few fixed points
    - Ex: ResNet multiples LR by 0.1 after epochs 30, 60, 90
- *Cosine*: $\alpha_t = \frac{1}{2}\alpha_0 \left(1 + \cos\left(\frac{t\pi}{T}\right)\right)$
- *Linear*: $\alpha_t = \alpha_0 \left(1 - \frac{t}{T}\right)$
- *Inverse sqrt*: $\alpha_t = \alpha_0 / \sqrt{t}$

<u>How long to train?</u>: Want to avoid overfitting

- ***Early stopping*** - stop training model when accuracy on validation set decreases
    - Alt: keep training, but store model snapshot that worked best on validation
- Alt approach: first stop training when accuracy on validation set decreases, and record that iteration #; then train train + val dataset together, stopping at previous best iteration

Choosing Hyperparameters

Can model hyperparameter choice as Bayesian optimization problem

Grid search: can choose several values for each hyperparameter (e.g. learning rate + weight decay), evaluate all possible choices on the hyperparameter grid

- Often space choices log-linearly
- Alt: via random search (log-uniform on a certain interval, run many different trials)
    - In case where one parameter is known to be more important than th either: ranodm search samples more values of that parameter than grid
- Facebook: one single learning rate & weight decay works well across many different models/architectures (via large-scale empirical random search)

Choosing hyperparameters (in general)

1. First, check initial loss (turn off weight decay, sanity check loss at initialization)
2. Next, overfit a small sample (try to train to 100% accuracy on a small sample of training data, e.g. 5-10 minibatches)
    a. Use to tune architecture, LR, weight initialization (no regularization yet) until loss zeroes out
3. Use architecture from previous step with all training data + small weight decay, use to tune learning rate
    a. Want learning rate that makes loss drop significantly within ~100 iterations
4. Use coarse grid, train for 1-5 epochs to test learning rate, weight decay
5. Refine grid, train longer without learning rate decay
6. Look at learning curves to qualitatively assess training progress/challenges & repeat

After Training

Model ensembles: can train multiple independent models and average results at test time for a slight boost in performance

- Take average of predicted probabilities & argmax

Transfer Learning

Rather than using a lot of data to train/use CNNs, use a pretrained CNN on a standard dataset (e.g. ImageNet) and use extracted features (before FC layers) on a new dataset

- Remove FC layers at end of CNN & replace with a new set of FCs (using same conv layers + weights as before); then, train CNN for new task
    - Works well for training on new datasets without having to retrain feature extractor
    - Can lower learning rate (e.g. 1/10 of LR used in original training), freeze lower layers during fine-tuning process
- Amount of additional layers + finetuning depends on size of new dataset, similarity to ImageNet
    - For very different datasets + small dataset, may need to add more layers or cut off & retrain some earlier layers
- Allows for transferring improvements in CNN architectures from image classification, e.g., to downstream tasks by replacing CNN feature extractor with a newer one
    - Can use as feature extractor for object detection, e.g.
- Reduces training time needed

Another approach - rather than training the CNN feature extractor on a large labeled dataset (hard to find), can instead train on large unlabeled datasets (unsupervised representation learning)

- Weakly supervised learning

Visualizing & Understanding Neural Networks

3 perspectives:

- Understanding network as a whole
- Looking at feature spaces
- Looking at individual units

Can visualize convolutional filters in CNN

- Lower layers correspond to local features of image
- Higher layers - not interesting

Looking at features - collect feature vectors from running network on many images, then use k-NN to compare features in feature space

- Can use dimensionality reduction (e.g. PCA) to visualize

Maximally activating patches **-** pick a layer & channel, then run many images through the network and find the image patches that have the highest value for that channel

- Use guided backprop to visualize

Annotating interpretation of images

- Within classified image, cut out the region (during annotation) corresponding to a label
- Can dissect networks to find "interpretable units" corresponding to each label; use IoU to evaluate (semantic segmentation)

Multimodal neurons in CNNs - some neurons in CNNs become object detectors for specific classes of object

Saliency **-** want to determine which pixels most affect the output

- **Saliency via occlusion**: Mask part of image before feeding to CNN & determine how probabilities change
- **Saliency via backprop**: Compute probabilities (forward pass) and compute gradient of (unnormalized) class score with respect to each pixel (absolute value)
- Saliency maps act as form of segmentation without supervision

- Not a perfect interpretability metric

Class activation mapping **(CAM)**

- Rather than summing all entries (across the image) in final FC layer to produce a given class's score, simply output matrix of final FC values as that class's CAM
- Can use as a form of weakly-supervised localization/object detection, interpretability
    - Only applies to last conv layer, but recent CNNs use global average pooling anyway

Gradient-weighted class activation mapping (Grad-CAM)

- Generalization of CAM:
    - Pick any layer's activations, compute gradient of class score with respect to activations
    - Use GAP on gradients to get weights, use ReLU to compute activation map
- Can also utilize for other kinds of vision models (e.g. image captioning)

Visualizing CNN features: *gradient ascent*

- Computes the synthetic image that maximally activates a neuron
    - Starting with zero image, keep forward passing & stepping input image in direction of positive gradient (of neuron value w.r.t. image pixels)
        - L2 regularization on generated image pixels; also periodically Gaussian blur + clip pixels with small values t0 0, small gradients to 0
    - Can use to visualize intermediate features at each layer
        - "Multifaceted visualization" (using more careful regularization, enter bias) for even nicer results
    - Can perform gradient ascent by training a deep generator network (prior) for the synthetic image, followed by the CNN
        - Can backpropagate through the CNN and generator network
- Adversarial usage: given an arbitrary image, start with an arbitrary category and modify image (via gradient ascent) to maximize class score until network is fooled

Feature inversion - given a CNN feature vector for an image, find a new image with a similar feature vector that "looks natural" (via some regularization)

DeepDream - try to amplify neuron activations at some layer in the network

- Given an image and layer: perform forward pass, then set gradient of chosen layer equal to its activation & backprop
- Trippy output

Texture synthesis: given a sample patch of some texture, try to generate bigger image with same texture

- Via nearest neighbors: generate pixels one at a time in scanline order; form neighborhood of already-generated pixels and copy NN from input
- Via neural networks - reshape features from C x H x W to C x HW and compute Gram matrix $G = FF^T$
    - Neural texture synthesis: use a pretrained CNN & run input texture forward through CNN, recording activations on every layer
    - At each layer, compute Gram matrix
    - Initialize generated image from random noise , pass through CNN, compute Gram matrices
    - Compute weighted sum of L2 distance between Gram matrices, backprop to get gradient on image, and make gradient step (& repeat)
- Higher layers recover larger features from input texture
- Can use for style transfer - texture transfer + Gram reconstruction
    - Matches features from content image / Gram matrices from style image
    - Adjust weight-to-style loss coefficients
    - Can mix style from multiple images via weighted average of Gram matrices

Style transfer requires many forward/backward passes through VGG (slow)

- Solution: train another neural network to perform style transfer
    - Fast neural style transfer - train a feedforward network for each style, compute same losses as before -> stylize images via single forward pass (after training)
        - Uses instance normalization
- Can train one network for multiple styles via conditional instance normalization (learning separate scale, shift parameters per style)

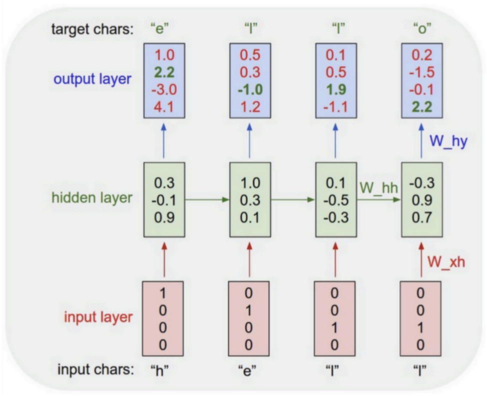
RNNs & Attention

Rather than "one-to-one"/feedforward models (seen previously), look at *sequence models* (one to many/many-to-one/many-to-many)

- Ex: for image captioning (image -> sequence of words), video classification (sequence-to-label), machine translation (sequence-to-sequence)
    - Per-frame video classification

Recurrent neural networks (**RNNs**) - store an "internal state", update as sequence is processed

- New state is function of old state & input vector at some time step $h_t = f_W(h_{t-1}, x_t)$
    - Same function (i.e. model) f_W, set of parameters W at every time step



Vanilla RNN - state consists of a single hidden vector h_t

- $h_t = \tanh(W_{hh}h_{t-1} + W_{xh}x_t + b_h)$, $y_t = W_{hy}h_t + b_y$
- Ex (language modeling): Given characters $1, 2, t-1$, model predicts character t
    - Character at time t is function of hidden state + preceding character; train model to correctly predict from existing training sequences (strings)
    - At test time: generate new text; sample characters one-by-one and feed back to model
        - At each step: input to model is output from previous sample step
        - Start with an artificial character <START>; cut off sequence when model samples <END> character
- Ex (image captioning): use feature vector from a CNN as initial hidden state for an RNN

Attention

RNNs for sequence-to-sequence prediction

1. Initially: continuously update hidden state on all characters of input sequence
2. From final hidden state, predict initial decoder state s_0 and context vector c (e.g. $c = h_T$)
3. Decoder uses context vector c, START character y_0 (plus initial state s_0) to determine decoder state s_1
4. Afterward: Keep updating decoder state $s_t = g_U(y_{t-1}, s_{t-1}, c)$ and sampling another character y_t until STOP character

Issue: input sequence bottlenecked through a fixed-size vector; may not be enough for fixed sequences
Solution: Use a new context vector at each step of decoder
At each step:

1. Use decoder state s_t to compute alignment scores $e_{t,i} = f_{att}(s_{t-1}, h_i)$ (using MLP f_{att})
    a. Initial decoder state: predicted from final hidden state h_n
2. Use softmax on alignment scores to get attention weights $a_{t,i}$
3. Compute context vector as linear combination of hidden states $c_t = \sum_i a_{t,i} h_i$
    a. $h_1, \ldots, h_n$ one hidden state per input element
4. Use context vector as input to decoder: $s_t = g_U(y_{t-1}, s_{t-1}, c_t)$
    a. Sample y_t from decoder

Intuition: context vector "attends to" (assigns higher weights $a_{t,i}$ to) the relevant part of input sequence [determined by MLP]

- Input sequence no longer bottlenecked through a single context vector; at each decoder timestep, context vector "looks at" different parts of input sequence
- Not limited to language - can use for any set of input hidden vectors h_j
    - Decoder doesn't use ordered nature of h_j's anywhere; can be unordered

Image captioning with RNNs and attention

- Use CNN to compute grid of features $h_{i,j}$ for image

- At each decoder timestep: compute alignment score for each feature $h_{i,j}$ and use to find new context vector

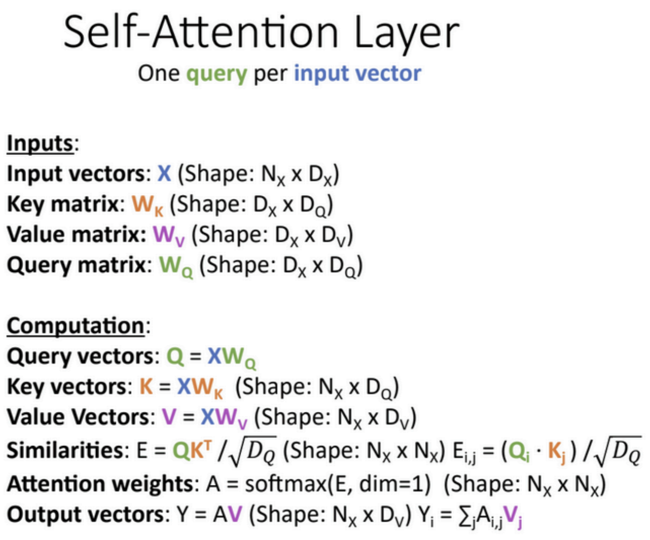
Can use attention for interpretability

- Machine translation - high attention weights correspond to relevant parts of input sentence at the current timestep/stage in translation
- Image captioning - attention weights for each word in caption correspond to the relevant part of image
- *Intuition*: works like human eye attention, picks region of focus

Types of Attention

- ***Attention layer***: uses scaled dot product to compute similarities $e = Q \cdot X / \sqrt{D_Q}$ between query vector(s) Q, input vectors X
    - Machine translation: singular query vector is decoder state; input vectors are hidden states
        - Can generalize to multiple query vectors (dot product to matrix product)
    - Scaled dot product - multiplies dot product by sqrt of query vector dimension
- *Attention layer (key-value)*
    - Add new ***key matrix*** W_K, ***value matrix*** W_V
    - Compute keys by $K = XW_K$, values by $V = XW_V$
    - Take similarities by product between query vectors Q and keys K; output vectors by $Y = AV$ (A attention weights)
- ***Self-attention***: uses query matrix W_Q to compute query vectors by $Q = XW_Q$, in addition to key & value vectors
    - One query per input vector
    - Output is permutation equivariant (permuting input gives permuted version of same output)
    - Self-attention doesn't consider order of processed vectors
        - Solution: can concatenate input with a positional encoding [vector] E to make processing "position-aware"
            - Encoding may be learned or via fixed function
- Masked self-attention (for language modeling - predicting next word)

        - Zero out all similarities with keys "further ahead" of current query vector
            - Prevents vectors from "looking ahead" in the sequence
- *Multihead self-attention*: use H independent self-attention heads in parallel
    - Copy input for each independent head; concatenate output vectors at end
    - Hyperparameters: query dimension D_Q, number of heads H

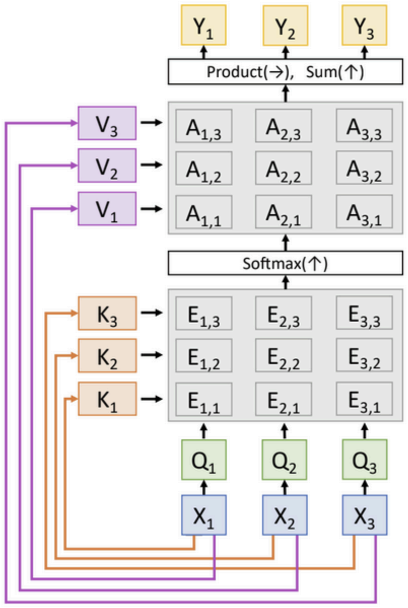


Self-Attention Layer

One query per input vector

Inputs:
Input vectors: X (Shape: $N_X \times D_X$)
Key matrix: W_K (Shape: $D_X \times D_Q$)
Value matrix: W_V (Shape: $D_X \times D_V$)
Query matrix: W_Q (Shape: $D_X \times D_Q$)

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: $N_X \times D_Q$)
Value Vectors: $V = XW_V$ (Shape: $N_X \times D_V$)
Similarities: $E = QK^T / \sqrt{D_Q}$ (Shape: $N_X \times N_X$) $E_{i,j} = (Q_i \cdot K_j) / \sqrt{D_Q}$
Attention weights: A = softmax(E, dim=1) (Shape: $N_X \times N_X$)
Output vectors: $Y = AV$ (Shape: $N_X \times D_V$) $Y_i = \sum_j A_{i,j} V_j$



CNN with self-attention

- Query, key, value matrices given by 1x1 conv with dim C' x H x W
- Use standard self-attention module plus residual connection

Three ways to process sequences

- RNN: works on ordered sequences
    - Good at long sequences (h_T "sees" whole sequence after one RNN layer), but not parallelizable (requires on sequentially finding hidden states)
- 1D convolution: works on multidimensional grids
    - Bad at long sequences (need to stack many layers for receptive field to include whole sequence), but highly parallel
- Self-attention: works on sets of vectors
    - Good at long sequences and highly parallel, but very memory-intensive

Transformers

Transformer block:

1. Self-attention (with residual connection)
2. Layer normalization
3. MLP independently on each vector (with residual connection)
4. Layer normalization & output

Transformers - sequences of transformer blocks

- Highly scalable & parallelizable
    - Only interaction between vectors happens within self-attention layers
- Multi-head attention: module for attention, runs through attention mechanisms several times in parallel & concatenates (independent) attention outputs
    - Uses a linear layer on final output to transform into expected dimension
- Effect similar to AlexNet for NLP
    - Use pretrained transformers for NLP tasks

Self-attention vs cross-attention

- Cross-attention: rather than computing queries/keys/values all from input, obtain queries from decoder and keys/values from encoder
    - Translation: decoder contains information about target language statistics; encoder contains information about source language

Attention/transformers for vision

1. Add attention to existing CNNs/CNN architectures (add between existing ResNet blocks)
    a. Still a CNN; want to replace convolution entirely
2. Replace convolution with “local attention”
    a. Attention takes center of receptive field as query, surrounding elements to find keys/values; output computed via attention
    b. Issue: hard to implement, only marginally better than ResNets
3. Standard transformer on pixels

    a. Issue: very memory-intensive, R x R image gives R^4 elements per att matrix

4. ***Vision Transformer*** (**ViT**): standard transformer on patches
    a. Divide image into smaller patches (flattened)
        i. Concatenate each patch with a learned position embedding
    b. Pass image patches as input to a standard transformer
    c. Add special extra input (classification token vector, learned, same dim as image patch); take output vector corresponding to classification token as vector of class scores
        i. No convolution layers needed (besides transformer MLPs)

<u>ViT vs ResNet</u>

- ViT performs worse on smaller datasets, but performs/scales better for larger ViTs + larger datasets
    - ViT advantage - better scalability (fairly efficient transformer memory-wise, faster to train)
- Most CNNS (e.g. ResNet): decrease resolution, increase channels for deeper layers; hierarchical structure
    - ViT: all block shave same resolution, # channels; isotropic structure

<u>Improving ViT</u>

- Regularization
    - Weight decay, stochastic depth; dropout in transformer MLP layers
- Data augmentation: MixUp, RandAugment
- Distillation:
    - Train a teacher model to classify images from ground-truth labels
    - Train a student model to match predictions from the teacher (sometimes: also ground truth labels)
        - Easier than training student from scratch
        - Can also train student on unlabeled data for semi-supervised learning
        - Can train teacher CNN -> student ViT

<u>Hierarchical ViT</u>: ***Swin transformer***

- First divide image into very small patches (e.g. 4x4), then merge (halve patch dimension) after every stage between transformer blocks
    - Merging: concatenate groups of 2x2 and linear project to half the channels
    - Results in hierarchical structure (similar to CNNs)
        - Other hierarchical transformers: MViT, Swin-V2, Improved MViT

Issue: matrices are big for earlier layers
Solution: don't use full attention, instead use attention over patches

- ***Window attention*** - rather than allowing each token to attend all other tokens, divide attention matrix into smaller M x M windows and only compute attention within each window
    - Linear in size for fixed M
    - Swin transformer - instead of positional embeddings (like ViT), encodes relative position between patches when computing attention
        - Adds bias term to similarity scores (before softmax)

Issue: no communication across windows; might lose information
Solution: alternate between normal windows and shifted windows (shifting all windows by some amount) in successive blocks

Faster & more accurate than previous models

- Can also use as backbone for downstream CV tasks (beyond classification)

<u>Improving ViT</u>

- ViT uses self-attention to mix across tokens; can try something simpler
    - MLP-Mixer: use MLP to mix across tokens (replacing self-attention)
        - All-MLP architecture
        - First applies an MLP across all N patches, then another MLP across all C channels

<u>Object detection with transformers</u>

- *DETR* (simple object detection pipeline): directly output set of boxes from transformer
    - Train using bipartite matching loss

    - Uses transformer to encode image features, then another transformer to decode & generate output vectors; from output vectors, uses FFNs to generate prediction (no object, or class + box if object)
- *Diffusion Models with Transformers* (DiT): replaces latent diffusion U-Net backbone with transformer operating on latent patches

Computer Vision

Object Detection

CV tasks:

1. Image classification
2. Semantic segmentation
3. Object detection
4. Instance segmentation

Object detection: Given an image, output a set of detected objects (consists of a label + bounding box for each object)

- Bounding box represented via coordinates (x, y, w, h)
- Loss function: Take a weighted sum of label loss (softmax) & bounding box loss (L2) as final multitask loss
- *Challenges*: Multiple outputs, multiple types of output (label + bounding box), often works on higher resolution images (compared to classification)

Object detection models

- Take feature vector from vision backbone (pretrained ResNet, e.g.) and use separate FC layers for labels, box coordinates
    - Issue: images can have more than one object; need different numbers of outputs per image depending on image contents, # of objects
- Can detect multiple objects via sliding window: apply a CNN to many different crops of image to classify crop as object vs background
    - Bounding box is the window size
- *Issue*: too many possible windows to evaluate for large images
    - ***Region proposals*** - find a small set of boxes likely to cover all objects
        - Often based on heuristics (e.g. look for "blob-like" image regions)
        - Relatively fast (e.g. selective search)

Evaluating object detectors

- Can use ***intersection over union*** (**IoU/Jaccard index**) to compare prediction, ground-truth boxes
    - Formula: (Area of intersection) / (Area of union)
    - Issue: object detectors often output overlapping detections
- Overlapping boxes (solution) - use ***non-max suppression*** (**NMS**)
    - Acts as form of post-processing: at each step, select the next highest-scoring box and eliminate all lower-scoring bounding boxes with a high IoU with current box
    - Issue: may eliminate good boxes if objects are highly overlapping (no easy solution)
- ***Mean Average Precision*** (**mAP**) - run object detector on all test images with NMS
    - For each category, compute average precision (AP) - area under Precision vs Recall curve
        - For each detection (highest to lowest score): if it matches some GT box with IoU >0.5, mark as positive and eliminate GT box; otherwise, mark negative
            - Plot points on PR curve (precision vs recall graph)
        - Aeverage precision: area under PR curve
            - AP = 1.0: hit all GT boxes with IoU >0.5, and have no "false positive" detections ranked above any "true positives"
    - Mean Average Precision: average of AP for each category
        - COCO mAP: compute mAP for multiple IoU thresholds (0.5, 0.55, etc.) and take the average

<u>**Object Detection Models**</u>

Region-Based CNN (**R-CNN**): Takes regions of interest from proposal method, transform to standard CNN input size & forward regions through CNN for classifications

- Bounding box regression: from CNN features, predict a "transform" to correct RoI to produce bounding boxes
    - Can compare with ground-truth boxes
- Running R-CNN
    - For each proposal, resize to standard input size and run independently through CNN to predict class scores & bounding boxes
    - Use scores to select subset of region proposals to output

Issue: very slow, need to perform forward pass on many regions

→ *Solution*: Run CNN before warping

Fast R-CNN: Run entire image through a CNN, then run region proposal method on CNN-output image features

- Can use any vision backbone (e.g. ResNet)
- From proposed regions; crop & resize, run through a per-region CNN network to obtain category, box transform per region
    - Can have a heavy initial backbone and relatively lightweight per-region network (even just FCs) to save redundant computation
- Significantly faster to train & run than regular R-CNN
- Q: How to crop & resize features?
    - *RoI pool* - find proposal within input image, then project onto features and “snap” to grid cells
        - Can divide into 2x2 grid of roughly equal subregions and maxpool within each subregion - ensures that region features always have same size, even if the proposed regions have different sizes
        - Issue: “snapping” may cause misalignment; method also results in different-sized subregions (in some cases)
    - *RoI align* - find proposal within input image and project
        - Rather than “snapping”, can sample features at regularly-spaced points in each subregion using bilinear interpolation
            - At each point: look at distances to four neighboring grid cells; take feature value as weighted linear combination (no snapping needed)

Issue: most of the time running Fast R-CNN is spent finding region proposals (due to needing to run on CPU); want to find a way to learn instead

Faster R-CNN: incorporates learnable region proposal network to predict proposals from features

- From feature map, region proposal network predicts proposals
    - At each point in feature map: take a fixed-size “anchor box” arond it and predict whether corresponding center point (anchor) contains an object
    - For positive boxes, also predict a box transform to convert from anchor box to object box
    - Issue: anchor box around a point may have wrong size/shape to include object

        - Solution: Use K different anchor boxes (of different shapes/sizes) at each point
- Jointly train 4 losses: RPN classification & regression + object classification & regression
- Significantly faster to run than Faster R-CNN
- Is a two-stage object detector: (i) Backbone & RPN, run once per image; (ii) Classifier for proposed regions (run once per region)
    - Q: Do we really need the second stage?

Single-stage object detection (e.g. YOLO, SSD): instead of classifying anchors in RPN as object/not object, classify as one of C categories (or background)
- May also use category-specific regression: for each non-background category, also predict a bounding box transform
- Less accurate than two-stage methods, but much faster

<u>Object detection</u>
- Better backbones are slower, but perform better
    - Recent backbones: feature pyramid networks (multiscale backbone), ResNeXt
- Single-stage methods have improved
- Very big models work better
- Test-time augmentation can help boost performance
- ICCV ‘23: object detection as a diffusion process
    - Generate an image overlaid with a random set of boxes; diffusion model will progressively refine into a better box at inference time

Semantic Segmentation

Semantic segmentation: Label each pixel with a category label (without differentiating instances)

Initial idea: sliding window

- Within an image, take a certain crop around a central pixel and classify it
- Assign pixel category to be output class from classifier
- Issue: inefficient, doesn't reuse shared features between patches

<u>Neural networks for semantic segmentation</u>

First idea: vanilla CNN with constant kernel size

Issue: convolution expensive on large images + receptive field is linear in # of convolutional layers

New idea (***encoder-decoder***): structure CNN as two stages: ***downsampling*** -> ***upsampling***

- **Downsampling -** use pooling, strided convolution to decrease resolution of features
- **Upsampling**: use **unpooling**, **transposed convolution** to increase feature resolution
    - ***Unpooling*** (e.g. 2x2 -> 4x4)
        - Naive approaches: simple (only fill in top-left corner), nearest neighbor
        - More complex: bilinear interpolation, bicubic interpolation, etc.
        - "Max unpooling": in a 2x2 maxpool, remember which position had max; during unpooling, place element into that position
    - Learnable upsampling - "***transposed convolution***"
        - Maps single pixel in input to larger kernel (3x3, e.g.) in output
            - Move one pixel in input -> 2 pixels in output, e.g.
            - Sum where outputs overlap
        - *Intuition*: can express convolution as matrix multiplication -> transposed convolution is multiplication by inverse matrix

<u>Encoder-decoder networks</u>

- Want to improve encoding of spatial information (encoder), maintaining spatial structure of mask (decoder)
- Encoder

    - ***Dilated/astrous convolution*** - rather than multiplying a contiguous region of input image during convolution (3x3 kernel -> 3x3 region, e.g.), place gaps of 1 pixel between each sampled input region (3x3 kernel -> 5x5 region, e.g.)
        - Creates larger receptive field
    - Feature pyramid structures
        - *Pyramid scene parsing network/PSPnet*: use multiple differently-sized convolutions on the same set of features and fuse outputs
            - Hypothesis: different sizes encode different kinds of features
        - *Feature Pyramid Networks/FPN*: predict at each feature size (?)
- ***U-Net*** - popular network for biomedical image segmentation

Semantic segmentation datasets - Cityscapes, MIT ADE20K

- ADE20K - manually labeled over several years by a single expert annotator

Instance Segmentation

Instance segmentation: detect all objects in images + corresponding pixels

One approach - perform object detection, then predict segmentation mask for each object

- ***Mask R-CNN***: Uses Faster R-CNN approach + adds segmentation mask prediction to outputs
    - Outputs: object category, bounding box, segmentation mask

Instance vs semantic segmentation

- Instance segmentation - labels pixels + detects individual instances, but only for pixels corresponding to detected objects (not for background, sky, e.g.)
- Semantic segmentation - labels all pixels, but not instances

More advanced CV tasks

- ***Panoptic segmentation*** - label all pixels in image & separate object instances (for objects)
    - Combination of instance, semantic segmentation
- ***Human keypoints*** - detect human pose via locating a set of keypoints
    - Can extend Mask R-CNN, add keypoint positions as additional output
        - In addition to segmentation mask, output individual masks for each keypoint (K many)
        - Ground truth - one “pixel” enabled per keypoint, use softmax loss

General approach to advanced CV tasks: Add additional “heads”/outputs to Mask R-CNN

- Heads incorporated into per-region network
- Ex:
    - LSTM head for dense captioning
    - Mesh R-CNN: mesh predictor head

Segment Anything (SAM): foundation model for image segmentation

Generative Models

Supervised vs unsupervised learning

- ***Supervised learning***: Given a set of data (x, y), want to learn function mapping x to y
    - *Ex*: image classification, object detection, semantic segmentation
    - *Intuition*: Attempts to learn conditional probability distributions p(y | x)
        - Cannot sample raw distribution p(x)
- ***Unsupervised learning***: Given a set of data x (no labels), want to learn some underlying structure of the data
    - *Ex*: clustering, dimensionality reduction, feature learning, density estimation
    - Attempts to learn unconditional probability distribution p(x)
        - Allows for sampling from p(x) directly

Computer vision

- Supervised learning via ***discriminative models***
    - For classification, segmentation, etc.
    - Lots of success across many tasks
- ***Generative models*** - unsupervised learning
    - More recent interest nowadays
    - Many advances in recent years

Recall: probability mass of a given element in a distribution assigned by density function

- Discriminative models (learn p(y | x)): given an image, different labels compete for probability mass
    - Different images do not compete
    - Correct labels should be assigned more mass
        - Done via feature learning with labels
- Generative models (learn p(x)): different images compete for probability mass
    - "Reasonable" outputs should be assigned more mass
        - Trained via feature learning without labels
        - Sample to generate new data
- Conditional generative models - learn p(x | y)
    - Given a label, different images compete for probability mass

Classes of Generative Models

1. *Explicit density*: model can compute p(x) explicitly
    a. Tractable density - can compute p(x) exactly
        i. Ex: autoregressive, NADE/MADE, etc.
    b. Approximate density - can only approximate p(x)
        i. Variational: Variational autoencoder (VAE)
        ii. Markov chain: Boltzmann machine, diffusion model
2. *Implicit density*: model does not explicitly compute p(x), only samples from it
    a. Markov chain: GSN
    b. Direct: Generative adversarial networks (GANs)

Autoregressive Models

Goal: Want to write an explicit function $p(x) = f(x, W)$

- Given dataset $x^{(1)}, \dots, x^{(N)}$, train the model to solve $W^* = \arg\max_W \prod_i^N p(x^{(i)})$
- Loss function: $\arg\max_W \sum_i \log f(x^{(i)}, W)$
    - Maximum likelihood estimation
- Idea: for multi-part inputs $x = (x_1, \dots, x_T)$, model using conditional probabilities $p(x) = \prod_i^T p(x_i | x_1, \dots, x_{i-1})$

PixelRNN - generates pixels one at a time, starting from upper left corner

- Via RNN - computes hidden state for each pixel based on hidden states and RGB values from all preceding pixels (pixels directly to the left and above)
    - At each pixel, predict R, G, B separately and softmax over [0, 1, …, 255]
    - Recurrences via LSTM
- *Issue*: slow to train & test (requires $2N - 1$ sequential steps)

PixelCNN - dependency on previous pixels modeled via CNN over some context region

- Faster to train than PixelRNN (convolution parallelizable), but still slow to generate due to sequential steps

<u>**Autoregressive Models**</u>

Pros:

- Explicitly computes likelihood p(x)
- Explicit likelihood of training data gives a good evaluation metric
- Good samples

Cons:

- Sequential generation is slow

Variational Autoencoders

Variational autoencoders (**VAE**) - define an intractable density (cannot compute or optimize; only directly optimize a lower bound on density)

Regular/non-variational autoencoders: unsupervised method for learning feature vectors from raw data without labels

- Originally linear + nonlinearity; later MLP, ReLU CNN
- Want to learn useful features from data for downstream tasks; Q: how?
    - Idea: Train model as two parts: **encoder** & **decoder**
        - ***Decoder*** attempts to reconstruct original input data from encoded features
            - Loss: L2 between original, reconstructed features
            - Ex: conv layers in encoder -> transpose conv in decoder
        - ***Encoder*** portion is used as autoencoder
            - Throw away decoder after training -> encoder for downstream tasks
- Can use encoder to initialize a supervised model
    - From there, use to train on a final task (with limited data, e.g.)
        - Ex: dimensionality reduction with unsupervised learning
- Regular autoencoders not probabilistic - no way to sample new data from learned model

Variational autoencoders - probabilistic variation on regular autoencoders

- Learn latent features z from raw data -> can sample from model to generate new data
- Assumes training data $x^{(1)}, \ldots, x^{(N)}$ generated from unobserved/latent representation z
    - Intuition: x an image; z latent features used to represent image (e.g. attributes, orientation, etc.)
- After training: first sample z from prior $p_{\theta^*}(z)$, then sample x from conditional distribution $p_{\theta^*}(x|z)$
    - Assumes simple prior $p_{\theta^*}(z)$ (Gaussian, e.g.)
    - Represent $p_{\theta^*}(x|z)$ via NN (similar to autoencoder decoder network)
        - Want to sample x from Gaussian with mean $\mu_{x|z}$, diagonal covariance $\Sigma_{x|z}$
            - Diagonal prior causes dimensions of z to be independent

- *Idea*: want to learn $p_\theta(x) = \frac{p_\theta(x|z)p_\theta(z)}{p_\theta(z|x)}$
    - $p_\theta(x|z)$ via decoder network; from Gaussian prior
    - $p_\theta(z|x)$: train another network (encoder) $q_\phi(z|x)$ to learn this
        - Want $q_\phi(z|x) \approx p_\theta(z|x)$

<u>Network</u>:

- Encoder network inputs data x, gives distribution over latent codes z (learns $\mu_{z|x}, \Sigma_{z|x}$)
- Decoder network inputs latent code z, gives distribution over data x (learns $\mu_{x|z}, \Sigma_{x|z}$)
- Want to jointly train both encoder, decoder
    - Train to maximize variational lower bound on data likelihood
      $\log p_\theta(x) \geq E_{z \sim q_\phi(z|x)}[\log p_\theta(x|z)] - D_{KL}(q_\phi(z|x), p(z))$

<u>Fully-connected VAE</u>:

- Each of encoder, decoder has one initial linear layer + two parallel linear layers for μ, Σ
    - Encoder: high-dimensional x to low-dimensional μ, Σ
    - Decoder: low-dimensional z to high-dimensional μ, Σ [approx. same dim as original x

<u>Training a VAE</u> (to minimize $D_{KL}(q_\phi(z|x), p(z))$)

- Run input data through encoder to get distribution over latent codes
    - Want encoder output to match prior $p(z)$
        - Has closed-form solution if q_ϕ diagonal Gaussian, p unit Gaussian
- Sample latent code z from encoder output
- Run sampled code through decoder to get a distribution over data samples
    - Want original input data to be likely under encoder-output distribution - can sample a reconstruction

<u>Sampling a VAE</u>

- Sample z from prior $p(z)$
- Run sampled z through decoder to get distribution over data x
- Sample from distribution to generate data

Can edit images after training:

- Run input data through encoder to get distribution over latent codes
- Sample code z from encoder output
    - Modify elements of sampled code as needed
        - Can use to change attributes of image, e.g.
- Run modified z through decoder to get new distribution & sample

Variational autoencoders

Pros:

- Principled approach to generatiev models
- Allows inference of latent codes q(z|x) -> can be used as feature representation elsewhere

Cons:

- Maximizes lower bound of likelihood rather than computing distribution directly
- Samples are relatively blurry/low-quality compared to SoTA

Vector-quantized VAE (**VQ-VAE**) - combines VAE and autoregressive models

- VAE-like encoder generates latent space
- Converts continuous latent space into discrete distribution (latent code) via vector quantization
    - Trains an autoregressive model on discrete distribution as decoder

Training VQ-VAE

- Train a VAE-like encoder-decoder model to generate multiscale grids of latent codes from input data
    - Decoder - train to reconstruct from latent code
- Use multiscale PixelCNN to sample in/generate from latent code space

VQ-VAE improves on VAE in terms of image quality

- Used as image generation backbone in DALL-E (translating text to images) - uses VQ-VAE to decode text embedding space to generate images

Generative Adversarial Networks (GANs)

Generative adversarial networks (**GANs**) - train two separate networks: a ***generator network*** G and a ***discriminator network*** D

- Assume have data x_i from $p_{data}(x)$, want to sample from p_{data}
    - Idea: introduce latent variable z with simple prior $p(z)$
    - Sample $z \sim p(z)$ and pass to generator network $x = G(z)$
    - Take samples x from generator distribution p_G (want: $p_G = p_{data}$)
        - Train G to "fool" discriminator D
- Discriminator is a classifier network, train to classify data as real/fake
    - Train generator network G to generate an image (taking a sample from generator distribution) and fool the discriminator

<u>**Training GANs**</u>

- Discriminator, generator trained <u>jointly</u> via *minimax* objective
    - Minimax - generator trains to minimize (maximum error across all discriminators)
    - G, D share same loss function, but opposite objectives
        - $\min_G \max_D V(D, G)$ [note: no overall loss]
- Doesn't explicitly model p(x), only samples from it
- Training GANs is difficult, unstable training + loss
    - Plot log(1-D(G(z))
    - Generator initially very bad (very easy for discriminator to distinguish - D(G(z)) near 0), improves over time
        - Issue: vanishing gradients for 0 when D(G(z)) near 0 [log(1-D(G(z)) small]
        - Solution: train G to minimize -log(D(G(z)))
- GANs provably achieve global min when $p_G = p_{data}$
    - No guarantees on convergence of G, D to optimal

Improving GANs: better loss functions, StyleGAN for higher resolution

- La begin with fixed constant input vector & add in new layer-wise random latent vectors at each layer

GANs - latent space actually encodes semantic information; can identify patterns in latent space based on semantic attributes (e.g. “man”)

- Latent space is continuous - can perform random walk to traverse
- Can identify subspaces associated with causal relations in latent space using unsupervised learning
    - Can use for manipulation

Image-to-image translation (P2P) - can use GANs to translate image types between different domains

- Generator takes input image (rather than random noise) as input; discriminator takes both input image, generator-output image
- *Issue*: for training, need image pairs (one in each domain) for paired translation
    - **CycleGAN** - take two sets of images (one in each domain) with no pairing
        - ***Cycle reconstruction loss*** - minimize reconstruction error from converting from one domain to the other & back again
- Ex: road map to fake satellite image

Diffusion Models

<u>**Diffusion models**</u>

- Training: rather than one-shot (GAN/VAE), train a model to gradually add Gaussian noise (encoder - forward/diffusion process) and then reverses/denoises the noise (decoder)
    - Decoder uses noise from encoding process to denoise
    - Markov chain process: each step depends only on output of previous step
    - After training: can sample white noise and pass to decoder to generate an image

<u>Diffusion</u> **- Forward/diffusion process**

- At each time step, at some amount of noise ϵ_t from standard normal distribution
    - Hyperparameter β_t (noise schedule) determines rate of noise blending
    - Given initial density $p(x)$, diffusion process gradually blurs distribution (moves toward standard normal distribution)
- Take T many steps $x \rightarrow z_1 \rightarrow \ldots \rightarrow z_T$
    - From input image x to z_T (approximately pure noise)

***<u>Diffusion</u>* - Reverse/denoising process**

- Want to learn series of probabilistic mappings $z_T \rightarrow z_{T-1} \rightarrow \ldots \rightarrow z_1 \rightarrow x$
    - Individual mappings: $p(z_{t-1}|z_t, \phi_t)$
    - Maps z_T (pure noise) back to input image x (during training)
    - Via learned neural network
        - Pass in image + time embedding
- Overall, want to learn: $\hat{\phi}_{1\ldots T} = \arg\max_{\phi_{1\ldots T}} \left[\sum_{i=1}^{I} \log\left[p(x_1|\phi_{1\ldots T})\right]\right]$

In practice: use diffusion encoder/decoder as encoder/decoder in U-Net model

- From noise image z_T, use U-Net as denoising network for each step $z_t \rightarrow z_{t-1}$
- After training: pass white noise image + noise concatenations as input to decoder

Latent diffusion: use encoder/decoder to move to/from pixel to latent space (similar to VAE)

- Use initial encoder to convert input x into latent space before performing forward diffusion; use final decoder to convert denoising output z back into pixel space output $\tilde{x}$

        - Performs diffusion within latent space for efficiency + speed
    - Ex: unCLIP model
        - Text encoder generates text embedding
        - Use text embedding as input to MLP generating latent code; latent code uses diffusion model as decoder (to generate images)
            - Training - use image encoder (CLIP, e.g.) to convert sampled image to image encoding; CLIP objective - match image encoding with original text encoding

Latent diffusion - extensions

- *Stable diffusion*
- Adding control to text-to-image diffusion (e.g. *ControlNet* - different visual inputs)
    - ControlNet - input condition image & text prompt together; incorporate image encodings of image into diffusion decoder stages via convolution
    - FreeControl: training-free control with any condition

Generative Models (Summary)

1. ***Autoregressive models***: directly maximize likelihood of training data
   $p_\theta(x) = \prod_{i=1}^{N} p_\theta(x_i|x_1, \ldots, x_{i-1})$
    a. Good quality, but slow & hard to scale
2. ***Variational autoencoders***: introduce latent z for interpolation/editing
    a. Maximizes lower bound
3. ***Generative adversarial networks***: don't model $p(x)$, but samples $p(x)$
    a. Good qualitative results
4. ***Diffusion models***: use long Markov chain of diffusion steps to model $p(x)$
    a. Flexible, but expensive to evaluate/train/sample

<u>Trends in CV</u>

Current trends:

- Ultra-large vision via foundation models
    - Scaling to large image datasets (OpenAI CLIP)
    - Multimodal image understanding models (LLaVA)
    - Image segmentation (SAMs)
    - Text2Image/Text2Video generation (Stable diffusion, Mochi)
    - Recognition & generation (Chameleon, Janus)
- 3D vision from multiple cameras & neural rendering
    - 3D perception with more cameras/sensors
    - 3D scanning
    - Recognizing 3D shapes (Mesh R-CNN, 3D object detection)
    - Interactive environments for embodied AI
    - Neural rendering: NeRF and Gaussian splatting for surface reconstruction & novel view synthesis from sets of images of objects/environments
        - 3D Gaussian splatting for real-time radiance fields

Challenges

- Interpretability, safety, robustness, etc.
    - Interpretability of AI model
    - AI safety in real-world applications
        - CV models fragile, easily fooled
    - Bias in visual classifiers, datasets
- Need a large amount of training data
    - Low-shot learning - learning from small datasets
    - Self-supervised learning - learning from unlabeled data