Machine Learning

Early DL: perceptrons, neocognitron (like CNN), LeNet

Kullback-Leibler between distrs: $D\_KL(P \,||\, Q) = \Sigma\_y\, P(y) \log(P(y) \,/\, Q(y))$

Terms: hyperparameters, train/val/test, curse of dimensionality, dataset normalization

- Batchnorm: like dataset normalization, but without prior dataset statistics

Linear classifiers: $Wx + b$ (intuitively: learns one "template" per class); logistic ($\sigma(\cdot)$), softmax $e^{zi}/\Sigma_j e^{zj}$

- Losses: L2, CE (logistic) = $-\log(\exp(s_{yi})/\Sigma_j \exp(s_{yj}))$, hinge (SVM) $\Sigma_{j!=yi}\, max(0,\ s_j - s_{yi} + 1)$

Optimization: Gradient descent (neg. gradient = dir. of steepest descent) (hyperparam: LR, weight init. method)

- Analytic gradient (exact, error-prone) vs. numeric (noisy, slow, easy - use to check analytic)
- Batch GD (expensive) vs SGD (GD on minibatches)
- GD strategies:
  - Momentum for GD: $v\_t = \nabla f(x\_t) \Rightarrow v\_t' = \rho v\_(t-1) + \nabla f(x\_t)$
  - AdaGrad: scale gradient $g(t)$ element-wise by historic sum of squares (acts as per-element LR)

    $s\_t = s\_(t-1) + g\_t\hat{}2 \Rightarrow w\_t = w\_(t-1) - (\eta \,/\, \sqrt{s\_t + \epsilon}) \cdot g(t)$
  - RMSProp/weighted AdaGrad: decay for past gradient $s\_t = \gamma \cdot s\_(t-1) + (1-\gamma) g\_t\hat{}2$
  - Adam: almost RMSProp + momentum (+bias correction)

input : γ (lr), β_1, β_2 (betas), θ_0 (params), $f(\theta)$ (objective)
initialize : $m_0 \leftarrow 0$ (first moment), $v_0 \leftarrow 0$ (second moment

for $t = 1$ **to** ... **do**
$g_t \leftarrow \nabla_\theta f_t(\theta_{t-1})$
$m_t \leftarrow \beta_1 m_{t-1} + (1-\beta_1) g_t$
$v_t \leftarrow \beta_2 v_{t-1} + (1-\beta_2) g_t^2$
$\widehat{m_t} \leftarrow m_t/(1-\beta_1^t)$
$\widehat{v_t} \leftarrow v_t/(1-\beta_2^t)$
$\theta_t \leftarrow \theta_{t-1} - \gamma \widehat{m_t}/(\sqrt{\widehat{v_t}} + \epsilon)$

return θ_t

- 2nd-order: invert Hessian -> use L-BFGS (only if doing full batch updates)

Regularization: L1/L2, dropout, batchnorm, cutout, mixup (encodes preference for weights), data augmentation

Linear classifiers: learn linear boundaries (feature transforms for nonlinear)

- Bag of Words: Extract random patches for image, cluster to form "codebook of visual words" (use as encoding for new model, e.g. SVM for classification)

Neural Networks

Train via backprop - use the chain rule to derive gradients of loss with respect to every weight in network

- Can construct computational graph (indicating operations from inputs to outputs); fwd -> bwd pass
- Chain rule: downstream gradient $\partial f/\partial y = (\partial q/\partial y) \cdot (\partial f/\partial q)$) upstream x local gradients
- Gradient flow: add distributes up grad to both eles; copy adds both up grad; multiplier multiplies up grad with multiplicand (a*b -> a input multiplies by b); max gate passes through up grad for taken branch, 0 for others
- Backprop with vectors: look at N-d Jacobians instead

Convolutional NN

Convolutional layer: slide kernel over image spatially (convolution as cross-correlation)

- Filter contains same # channels + same dim (besides # filters) as image; # filters = # output channels
- Shapes: $(N, C\_in, H, W) \rightarrow (N, C\_out, H', W')$, convolution shape: $H' = (H - K + 2P)/S + 1$
- Later layers: resolution decreases, # channels increases (local -> complex features)

Stacked convolutional layers correspond to single larger convolutional layer (convolution - linear classifier)

- Padding to preserve feature map size; $P = (K - 1)/2$ preserves input shape
- Each convolution adds $K - 1$ to size of receptive field (total size: $1 + L \cdot (K - 1)$)
- Downsample with strided convolution (reduces # conv layers needed for receptive field)

Pooling: alternative way to downsample (hyperparam: kernel size, stride, pool function)

- Ex: max pool (take max within receptive field as output) -> gives invariance to small spatial shifts
- Pooling shape: $H' = (H - K)/S + 1$

Batch norm: $x' = (x - E[x])$ / $\sqrt{Var[x]}$ (normalize layer outputs across a batch to be zero mean, unit stdev)

- Testing: use running average μ, σ^2 from training (normalize each dim of input N-d vector x separately)
- Can learn D-dim scale, shift parameters γ, β for more info → $y\_i, j = γ\_j \cdot x'\_i, j + β\_j$
- Batch-norm for CNNs: spatial batchnorm (batchnorm across each channel: take slices (N, H, W))
- Benefits: faster training/cvgnce, more robust to init., acts as regularization, can fold into conv layer during test
  - Provides robustness to internal covariate shift (change in distribution of network activations)
- Types of norm layers: batchnorm, layernorm/1D (for each input, compute mean/std across entire dim of input), instance/2D (for each input, compute mean/variance for each channel, separately)

Computing parameters: (rec: 4 bytes/float for memory)

- # params: total # weights + # biases [conv layer: $C\_out \cdot C\_in \cdot K + K \cdot C\_out$, kernel size K]
- Floating point ops/FLOPs: number of output elems * number of ops/elem [conv: $(C\_out, H', W') \cdot (C\_in, K, K)$]

Modern architectures: (from LeNet)

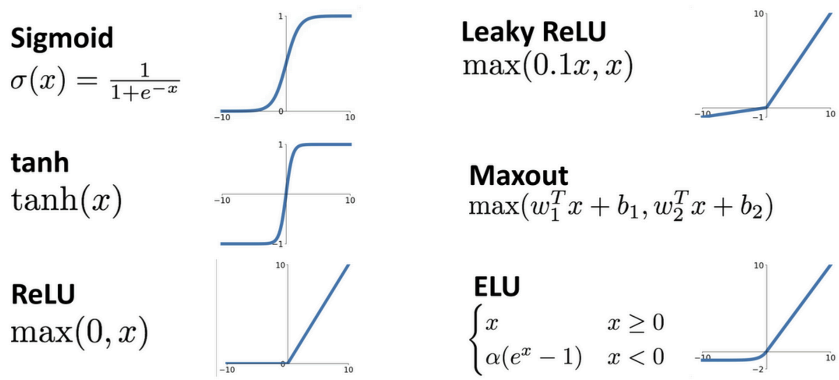
- AlexNet: sigmoid -> ReLU, more training; (most mem in early convs; FLOPs in convs; params in FC)
  - ZFNet (changed kernel stride sizes), VGG (more regular design, much larger, high mem + FLOPs)
- GoogLeNet: stem network for early downsampling; glbl avg pool (take avg of each feature map as class score) instead of end FC (less params); Inception module: local unit with parallel branches (diff-sized convs)
  - Very eff; Hack: auxiliary classifiers (outputting classifications early) to help propagate gradients
- ResNets: residual connection to help deep networks learn identity (resblocks: 1st 0.5x size, 2x channels)
  - Eff + acc; Bottleneck block: replace 2 3x3 convs with 1x1->3x3->1x1 (more layers, cheaper)
  - Variations: (block design: ReLU after instead of before)
    - ResNeXt: G-many conv paths in parallel in res block, add w/ residual at end
      - Grouped conv: parallel conv layers work on subsets of channels (e.g. C / N), produce C_out/N channels each -> parallelize for less RAM cost
    - Squeeze-and-Excite/SENet: glbl pool + 2x FC + σ within res block, * with res output

- Densely connected NNs (each layer connected to all prev layers), MobileNets (replace conv with depthwise conv [group conv w/ # gps=# chnls] + ptwise 1x1 conv to reduce # params)

Neural architecture search: controller net outputs & trains child nets, updates self policy; give better archs over time

Training NNs

Activation functions (want: nonlinear, diff'tble, no vanishing gradients):



- ReLU: well-behaved derivatives, no vanishing gradients for x>0, good in practice :); no 0 init/center :(
    - Leaky ReLU (no van grads), ELU (closer to 0-cen, neg sat regime compared to LReLU; more expensive)
    - Scaled ExponentialLU/SELU: λx for $x > 0$, $\lambda\alpha(\exp(x) - 1)$ if $x \leq 0$
        - Scaled version of ELU, better for deep NNs; self-normalizing (can train w/o batchnorm)
    - Gaussian ELU/GELU: $X \sim N(0, 1) \Rightarrow selu(x) = xP(X \leq x)$ (x by 0 or 1 randomly; larger -> more probability of x1, smaller -> more P of x0 [data-dependent dropout]); used in transformers
- Sigmoid: squashes numbers (0,1) [sigmoid, tanh not typically used except to squash]
- Tanh $(\exp(2x) - 1) / (\exp(2x) + 1)$ - squashes to [-1,1] & zero-centered :), but kills gradients :(
- Softplus $\log(1 + \exp(x))$

Weight initialization

- Bad: all 0 (all gradients equal, no symmetry breaking), small rand Gaussian (activations -> 0 for deep NN), large rand Gaussian (gradients saturate -> local gradients to 0, no learning)
- Xavier initialization for 0-center: stdev = $1/\sqrt{D\_in}$ (conv layers: $D\_in = K\text{^}2 \cdot C\_in$), ReLU: $\sqrt{2/D\_in}$ [Kaiming]
    - ResNets - variance grows with residual connection -> initialize first layer with Kaiming, later w/ 0

Regularization: stochastic depth (skip some blocks randomly), cutout, mixup; dropout for large FC layers

Learning rate schedules: step (reduce at fixed points), cosine $0.5\alpha\_0(1 + \cos(t\pi / T))$, linear, inverse sqrt $\alpha\_0/\sqrt{t}$

Early stopping, or record best iter. (train w/ train, val w/ val) & repeat to iter. with train + val together

Choosing hyperparameters: grid search (log-linear scale, e.g.), random search (log-uniform on an interval)

- Random search: good if one parameter known more important (covers more total values)

Model ensembles for slightly better performance

Transfer learning: use pretrained CNN, remove FC layers, replace with new MLP head & retrain

- Advanced: lower learning rate, freeze lower layers; allows for reusing feature extraction
- Alt: instead of training feature extractor on large labeled, train on large unlabeled (unsupervised)

Understanding Neural Networks

Can visualize convolutional filters in CNN (mainly lower layers)

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

Looking at features - collect feature vectors from running on many images, k-NN/PCA to compare in feature space

Annotating interpretation of images - dissect networks to find "interpretable units" corresp. to each label

Maximally-activating patches: given layer + channel, run many images & find patches maximizing that channel val

Saliency via occlusion (mask part of image before fwd pass, see output change), backprop (compute gradient of unnormalized class scores w.r.t. each pixel); can also use saliency maps as form of unsupervised segmentation

Class-activation mapping/CAM: rather than summing all etnries (across image) in final FC layer to produce a class score, output matrix of final FC values as that class's CAM (can also use as weakly-supervised object detection)

- Issue: only works for last conv (not GAP) -> gradient-weighted CAM/Grad-CAM: pick any layer's activations, compute grad of class score w.r.t. activations, use GAP on gradients to get weights -> ReLU to find CAM

Visualizing CNN features: gradient ascent compute synthetic image maximally activating neuron

- Start with zero image, keep fwd pass & step input image in dir. of positive gradient (L2 + blur, clip also)
- Can use to visualizes; alt: train generator net (prior) for synthetic, followed by CNN (backprop CNN & gen net)
- Adversarial examples: given an arbitrary image, start with arbitrary class & grad asc to fool network
- DeepDream - try to amplify neuron activations at some layer in output -> trippy output

Feature inversion - given CNN feature vector, find new "natural-looking" image w/ similar feature vector (via regulari.)

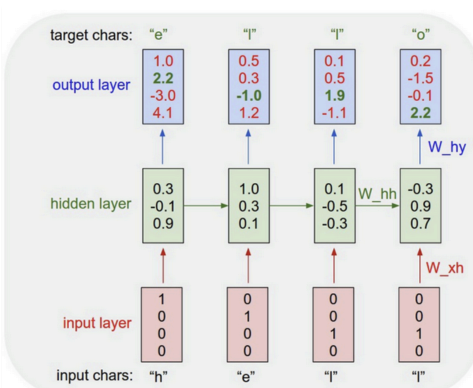
Texture synthesis: given sample patch of some texture, try to generate bigger image with same texture

- Reshape features C x H x W -> C x HW & find Gram matrix; neural texture synthesis: pretrained CNN fwd pass & find Gram matrices on every layer; initialize gen. Image from random noise, fwd pass, find Gram matrices
    - Compute weighted sum of L2 dist. between Gram matrices, backprop for gradient, make step
- Style transfer: texture transfer + Gram reconstruction (matches features from image 1, Gram Ms from image 2)
    - Fast neural style transfer - train an NN to copy style transfer (one net/style or condi. instance norm.)

RNNs

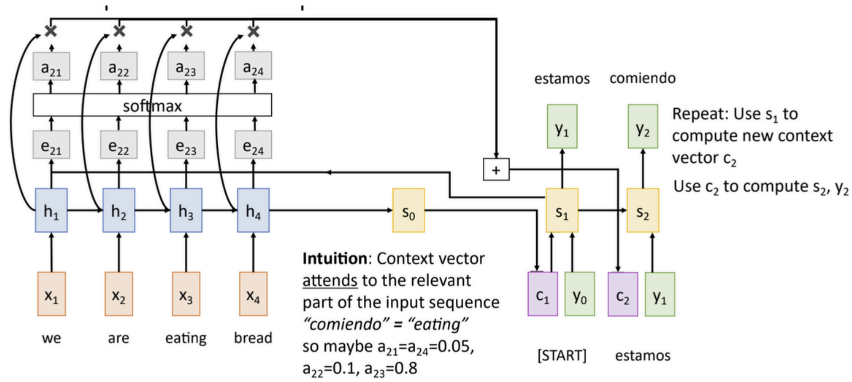
RNNs (vanilla): store state - single hidden vector h_t, new state product of old state & input vector $h_t = f_W(h_{t-1}, x_t)$

- Language modeling: given characters 1, 2, ..., t-1, char at time t is function of hidden state + preceding char
    - At test time: generate new text; sample chars 1-by-1 and feed back to model as next preceding char
    - Image captioning: use CNN feature vector as initial hidden state for RNN



RNNs w/ Attention (sequence-to-sequence) - decoder uses context vector c, preceding char $y\_(t - 1)$, preceding decoder state $s\_(t - 1)$ to update decoder state: $s\_t = g\_U(y\_(t - 1), s\_(t - 1), c)$ & sample from decoder

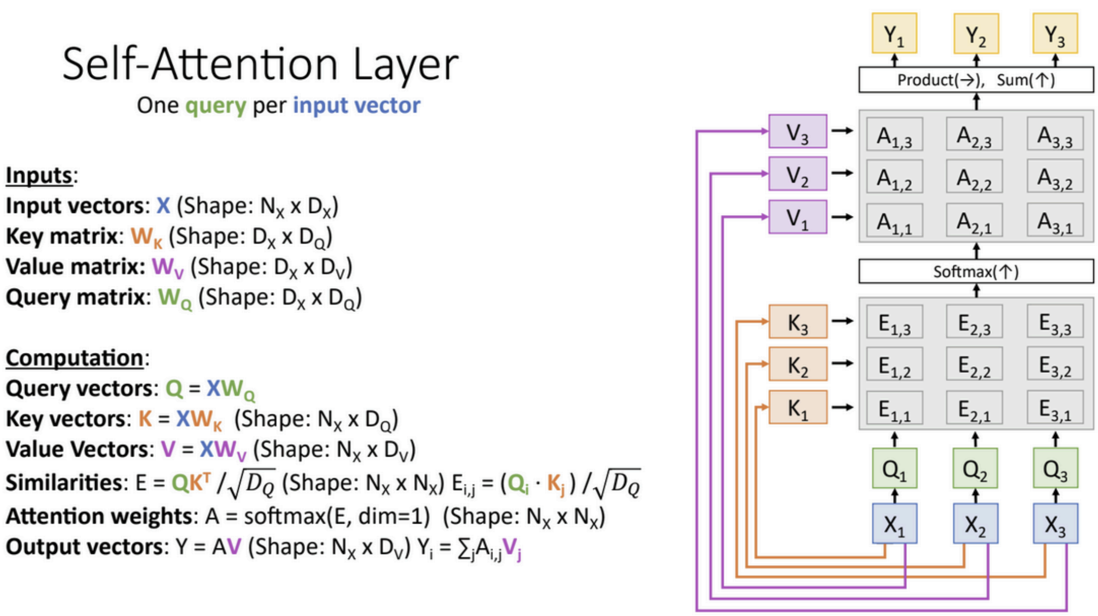
- Context vector: at each step, use decoder state s_t to compute alignment scores $e\_t, i = f(s\_(t - 1), h\_i)$ (using MLP f; s_0 from final hidden state h_n), softmax alignments for att weights, context vector as linear combination of hidden states $c\_t = \Sigma\_i\,(a\_t, i \cdot h\_i)$ -> use as input to decoder (h_i's don't need any order)



- Image captioning: use CNN to compute grid of features h_i, j -> use to compute context vector

Attention variations: (query - decoder state, input - hidden states)

- Attention: queries Q, inputs X -> scaled dot product: similarities $e = Q \cdot X/\sqrt{D\_Q}$
- Key-val attention: key, value matrices $K = XW\_K, V = XW\_V$ -> sims: prod of Q, V; output $Y = AV$
- Self-attention: uses query matrix to compute query vectors $Q = XW\_Q$, in addn. to key/value vectors
- Masked self-att: zeroes out similarities with keys "further ahead" of current query vec
- Multihead self-att: H parallel self-att heads; concatenate outputs at end



Transformers

Transformer block: self-attention w/ residual -> layernorm -> MLP (indep., on each vector) -> layernorm -> output

Transformers (sequences of transformer blocks) -> highly scalable, parallelizable (vectors only interact in self-atts)

- Multihead attention: runs parallel attentions, concatenates -> MLP on output to transform dimension
- Cross-att: instead of Q/K/V from input, Q from decoder & K/V from encoder (D: target, E: source)

Attention for vision

- Add attention to existing CNNs -> still a CNN
- Replace conv with local attention around receptive field -> not much improvement
- Standard transformer on pixels -> very memory-intensive (R x R image -> R^4 elements/attention matrix)

Vision Transformer (ViT): divide image into smaller flattened patches (concatenate with learned pos. embedding)

- Pass image patches as input to transformer; add special learned classification token (same dim as image patches) -> output vector corresp. to classification token is vector of class scores; no conv layers needed
- Scales better than ResNet for large datasets, + faster to train (but worse on small datasets)
- Distillation: Train teacher model from GT -> train student to match teacher predictions

Hierarchical ViT/Swin transformer: splitimage into patches (e.g. H/4x W/4) -> halve patch dimension between blocks

- Merging step: concatenate groups of 2x2 & linear project to half number of channels
    - Gives hierarchical structure (similar to CNNs)
- Issue: matrices big for earlier layers -> window attention: rather than all tokens attending all tokens, divide attention matrix into smaller M x M windows & only compute attention within each window linear in M)
    - Swin transformer - instead of pos. embeddings (ViT), encodes relative position btwn patches + bias
- Issue: no interaction between windows -> alternate between normal, shifted windows in each block

MLP-Mixer: use MLP to mix across tokens (replacing self-attention) -> all-MLP architecture

Object detection with transformers

- DETR (simple pipeline): directly output set of bounding boxes from transformer; use transformer to encode & another to decode, generate output vectors; use FFNs to generate prediction (no object, or class + box)
- Diffusion models with Transfs (DiT): replaces latent diffusion U-Net backbone w/ transformer on latent patches

<u>Object Detection</u>

Crop (sliding window) & CNN for classification on window (bounding box: (x, y, w, h); L2 loss)

R-CNN: On proposed regions, transform/resize -> forward through CNN with classification

- CNN: predict class & bounding box correction/transform (select subset of detections to output)
- Transform: RoI pool (snap onto grid cells) vs RoI align (bilinear interp. - look at 4 nearest points x/y)

Fast R-CNN: Run CNN first -> on features: region proposal + transform + per-region CNN

Faster R-CNN: Learnable region proposal network from feature map (backbone + RPN -> per-region CNN)

- At each point in feature map: take K anchor boxes, predict if contains object (+ object box, if so)

Single-stage detection: instead of RPN output is/isn't object, predict as one of C classes (or BG) + BBox TF

Indices: IoU/Jaccard

- NMS: select next highest-scoring output box & eliminate worse boxes with significant IoU
- Mean Avg Prec/mAP: for each detection, if matches GT w/ IoU>0.5, mark (+) & eliminate GT box; else, mark (-) [avg prec: area under prec vs recall curve] -> mAP: average across all categories
    - Prec: TP / (TP + FP); recall: TP / (TP + FN); COCO mAP: avg across multiple IoU thresholds

<u>Semantic Segmentation</u>

U-Net: downsample (maxpool, strided conv) -> upsample (unpool, transpose conv)

- Unpooling: simple (only fill top-left), NNghb, interp, "max unpooling" (remember maxpool pos)
- Transpose conv: map single pixel in input to larger kernel (e.g. 3x3) in output
    - Move one input in input -> two in output, e.g.; sum where kernels overlap (int: x by A^{-1})

Other: dilated/astrous convolution (spread-out kernel pixels), pyramid structures; Cityscapes/ADE20K

Instance Segmentation

Mask R-CNN: Faster R-CNN for object detection + add segmentation mask prediction to outputs

Other tasks: panoptic (inst + sem seg), keypoint (Mask R-CNN + 1-pixel keypoint mask), Mesh R-CNN (mesh head)

Generative Models

Supervised/discriminative (learn p(y|x)) vs. unsupervised/generative (learn + sample from p(x))

- Discriminative: given images, labels compete for prob. mass vs gen: images for mass (also: cond. gen.)

Generative models:

- Explicit density: autoregressive (tractable -exact p(x)) vs approximate (VAE - variational lower bound, diffusion)
- Implicit density: GANs (don't compute p(x), only sample from it)

Autoregressive: want to learn $p(x) = f(x, W)$ -> solve $W = argmax\_W \Pi_i^N p(x^{(i)})$ for dataset $x^{(i)}$

- Idea: for multi-part inputs $x = (x1, ..., xT)$, use conditional probs $p(x) = \Pi p(xi|x1,..., x[i - 1])$
- PixelRNN: generates pixels 1-by-1 from upper left (RNN: computes hidden state based on RGB of pixels directly to left and above; for each pixel, predict RGB separately & softmax) -> issue: slow due to sequential
- PixelCNN: CNN instead of LSTM for dependency on prev. pixels (parallelizable conv, but still slow sequential)
- Pros: explicitly computes $p(x)$, good samples; cons: slow due to sequential steps

Autoencoders (unsupervised for feature extraction): train model as encoder & decoder (decoder attempts to reconstruct original input data from encoded features; e.g. encoder conv -> decoder tconv); encoder is autoenc

- Can use encoder to initializer supervised models [encoder: high -> low dim, decoder: low -> orig. dim]

Variational autoencoders/VAE: attempts to learn latent features z from input data -> sample from model to generate

- Assume training data x1,...,xN from latent rep. z (latent features; e.g. attributes, orientation, etc.)
- Idea: Learn $p_\theta(x) = (p_\theta(x|z)p_\theta(z))$ / $(p_\theta(z|x)$; $p_\theta(x|z)$ via decoder network (from Gaussian prior, e.g.); $p_\theta(z|x)$ via trained encoder $q\_\phi(z|x)$ [want to approximate $p\_\theta(z|x)$]
- Network: encoder network takes input x, gives distribution over latents z [learns $\mu[z|x]$, $\Sigma[z|x]$]
    - Decoder network takes latent z, gives distribution over x [learns $\mu[x|z]$, $\Sigma[]x|z]$]; train jointly
    - Tries to maximize varia. LB ELBO on likelihood: $\log p_\theta(x) \geq E_{z\sim q\_\phi(z|x)}[\log p_\theta(x|z] - D_{KL}(q_\phi(z|x), p(z))$
- FC VAE: each encoder, decoder is one initial linear layer + two parallel linear layers for μ, Σ
- Training VAE: run input data through encoder to get distr over latents, sample latents from encoder output -> run latent through decoder to get distr over data (want orig input data to have high probability)
    - Sampling: sample z from $p(z)$ prior, use decoder to get distr over x & sample [modify z -> change attrs]
- Pros: mathematically principled, rich latent space; cons: doesn't find $p(x)$ [only maximizes LB], bad quality

Vector-quantized VAE (VQ-VAE): VAE-like encoder generates latent space; autoregressive on latent space as decoder

- Train VAE encoder-decoder to generate grids of latent codes from input (continuous latent sp -> disc distr via vector quant.); PixelCNN to sample from latents (improves in VAE image quality)

Generative adversarial networks (GANs): train generator G to fool discriminator D

- Assume have data x from $p\_data(x)$ -> introduce latent variable z with simple prior $p(z)$, sample $z \sim p(z)$ to G and train generator to sample, fool discriminator D (D a classifier - real/fake) [global min: $pG = pdata$]
- Train D, G jointly via minimax $[min[G]\ max[D]\ V(D,\ G)]$ (note: difficult, unstable training/loss)
    - Train G to minimize $-\ \log(D(G(z)))$ to avoid vanishing gradients
- Layer-wise stochast. (StyleGAN): GAN only initial random latent input -> fixed input + new rand latent/layer
- GANs: latent space encodes semantic info, continuous (can traverse, identify subspaces)

Image-to-image transl: can use GANs to translate images between diff domains (generator takes input image as input instead of random noise; discriminator takes input paired image, generator-output image)

- Non-paired translation: CycleGAN - take two sets of images (one in each domain) w/o pairing, use cycle reconstruction loss - minimize reconstruction error from converting from one domain to other & back

Diffusion models

Training: Forward process (at each step t, add some noise ϵ_t sampled from standard normal; $x \rightarrow z\_T$) -> denoising proc. (use noise from encoding process to denoise; $z\_T \rightarrow x$)

- Markov chain process - each step depends only on output of previous step
    - Hyperparams: noise schedule β_t; at each step of diffusion proc., moves $p(x)$ toward $N(0, 1)$
- Denoising: have individual mappings $p(z[t\ -\ 1]\ |\ z[t],\ \phi[t])$ mapping noise $z[T]$ to x (via learned NN - inputs image, time embedding) -> want to learn $\Phi[1...T]\ =\ argmax\_\phi[1..T]\ (\Sigma_i^I \log[p(x1\ |\ \phi[1...T]\ )$
- In practice: use diffusion encoder/decoder as encoder/decoder in U-Net; from noise z_T, use U-Net as denoising network for each step $zt \rightarrow z(t\ -\ 1)$ [T many U-Nets; from noisy image + time enc, preds. noise]
    - After training: sample white noise, pass to decoder to generate an image

Latent diffusion: use encoder/decoder to move from pixel to latent space (like VAE); diffusion process performed within latent space, encoder/decoder convert input, output to, from pixel space to latent space (faster + more eff)

- Extensions: stable diffusion, control (ControlNet: input condition image & text prompt; incorporate image encodings into diffusion decoder stages)