

1 Connectionism

1.1 Perceptron

Threshold Unit $f[w, b](x) = \text{sign}(x \cdot w + b)$ with **Decision Boundary** $x \cdot w + b = 0$. $-\frac{b}{\|w\|}$ is the signed distance of the hyperplane from 0.
Geometric Margin $\gamma[w, b](x, y) = \frac{y(x \cdot w + b)}{\|w\|}$.
Maximum Margin Classifier $(w^*, b^*) \in \text{argmax}_{w, b} \gamma[w, b](\mathcal{S})$, with margin $\gamma[w, b](\mathcal{S}) := \min_{(x, y) \in \mathcal{S}} \gamma[w, b](x, y)$.

Perception Learning

if $f[w, b](x) \neq y: w \leftarrow w + yx, b \leftarrow b + y$.
Aims to find some solution; assumes version space is non-empty. Does not aim for small err.
 $w_0 \in \text{span}(x_1, \dots, x_s) \Rightarrow w_t \in \text{span}(x_1, \dots, x_s) \forall t$

Convergence - Novikoff's Theorem

- If $\exists w^*, \|w^*\| = 1$, s.t. $\gamma[w^*](\mathcal{S}) = \gamma > 0 \Rightarrow w_t \cdot w^* \geq t\gamma$.
- Let $R = \max_{x \in \mathcal{S}} \|x\|$. Then $\|w_t\| \leq R\sqrt{t}$.
 $\cos \angle(w^*, w_t) = \frac{w^* \cdot w_t}{\|w^*\| \|w_t\|} \geq \frac{\gamma}{\sqrt{t}R} = \sqrt{t} \frac{\gamma}{R} \leq 1 \Rightarrow t \leq \frac{R^2}{\gamma^2}$.

Cover's Theorem for $\mathcal{S} \subset \mathbb{R}^n, |\mathcal{S}| = s$

$C(\mathcal{S}, n)$: # of ways to separate \mathcal{S} in n dimensions.
Position of pts does not matter (as long as they are in general position). $C(s+1, n) = 2 \sum_{i=0}^{n-1} \binom{s}{i}$, $C(s, n) = 2^s$ for $s \leq n$. Phase transition at $s = 2n$. For $s < 2n$ empty version space is the exception, otherwise the rule.

1.2 Hopfield Networks

$E(X) = -\frac{1}{2} \sum_{i \neq j} w_{ij} X_i X_j + \sum_i b_i X_i$, where $X_i \in \{\pm 1\}$. $w_{ij} = w_{ji}, w_{ii} = 0$.

Hebbian Learning

Choose patterns $\{x^t\}_{t=1}^s \in \{\pm 1\}^n$, compute weights once using them: $w_{ij} = \frac{1}{n} \sum_{t=1}^s x_i^t x_j^t$, $w_{ii} = 0$. For inference, update X iteratively: $X_i^{t+1} = \text{sign}(\sum_j w_{ij} X_j^t + b_i)$ asynchronously.
Capacity for random, uncorrelated patterns: $s_{\max} \approx 0.138n$. Requiring pattern to be retrieved with high probability: $s \leq \frac{n}{2 \log_2 n}$.

If $X = \text{diag}(1, \dots, 1)$, no reconstruction happens. Under async update step, any Hopfield network is guaranteed to converge.

2 Feedforward Networks

2.1 Linear Models

Linear regression (MSE)
 $L[w](X, y) = \frac{\|Xw - y\|^2}{2n}$, $\nabla_w L = \frac{X^T X w - X^T y}{n}$.
Moore-Penrose inverse solution
 $w^* = X^+ y \in \text{argmin}_w L[w](X, y)$, where $X^+ = \lim_{\delta \rightarrow 0} (X^T X + \delta I)^{-1} X^T$ Moore-Penrose inverse.

Stochastic gradient descent update $w_{t+1} = w_t + \eta(y_{i_t} - w_t^T x_{i_t}) x_{i_t}, i_t \sim \mathcal{U}([1, n])$.

Gaussian noise model $y_i = w^T x_i + \varepsilon_i, \varepsilon_i \sim \mathcal{N}(0, \sigma^2)$, LSQ equivalent to NLL of gaussian noise model.

Ridge regression $h_\lambda[w] = h[w] + \frac{\lambda}{2} \|w\|^2, w^* = (X^T X + \lambda I)^{-1} X^T y$.

Logistic function

$\sigma(z) = \frac{1}{1+e^{-z}}, \sigma(z) + \sigma(-z) = 1$.
 $\sigma' = \sigma(1-\sigma), \sigma'' = \sigma(1-\sigma)(1-2\sigma)$
Cross entropy loss for $y \in \{0, 1\}$
 $\ell(y, z) = -y \log \sigma(z) - (1-y) \log(1-\sigma(z)) = -\log \sigma((2y-1)z)$.

Logistic regression with Cross Entropy loss:
 $L[w] = \frac{1}{n} \sum_{i=1}^n \ell_i(y_i, w^T x_i), \nabla \ell_i = [\sigma(w^T x_i) - y_i] x_i$.

2.2 Feedforward Networks

Generic feedforward layers

$F: \overset{\text{parameters}}{\mathbb{R}^{m(n+1)}} \times \overset{\text{input}}{\mathbb{R}^n} \rightarrow \overset{\text{output}}{\mathbb{R}^m}, F[\theta](x) = \varphi(Wx + b)$.

Layer composition $G = F^L \circ \dots \circ F^1 \circ \theta^1$.
Layer activations $x^l = F^l \circ \dots \circ F^1(x) = F^l(x^{l-1}), x^0 = x, x^L = F(x)$.

Softmax $(z)_i = \frac{e^{z_i}}{\sum_j e^{z_j}}$, CE-loss in terms of log-its $\ell(y, z) = \frac{1}{\ln(2)} \left[-z_y + \ln \sum_j e^{z_j} \right]$. CE between two pmfs: $l(p; q) = -\sum_i p_i \log q_i$. CE with hard labels is NLL-loss.

Residual layer $F[W, b](x) = x + (\varphi(Wx + b) - \varphi(0))$, therefore $F[0, 0] = \text{id}$. Link that propagates x forward is called a **skip connection**. Composing residual layers: number of paths grows exponentially, can include projections for flexibility of changing dimensionality.

2.3 Sigmoid Networks

Sigmoid activation $\sigma(z) = \frac{1}{1+e^{-z}}$.
Hyperbolic tangent activation
 $\tanh(z) = \frac{e^{-z} - e^{-z}}{e^{-z} + e^{-z}} = 2\sigma(2z) - 1$.
 $\tanh'(z) = 1 - \tanh^2(z)$.

Smooth function approximation

Polynomials, ridge functions $(\varphi(a^T x + b))$ and MLPs with C^∞ activations are universal approximators.

Weierstrass: Polynomials are universal approximators of $C(\mathbb{R})$ on any given compact I .

Barron's Theorem: For $f: \mathbb{R}^d \rightarrow \mathbb{R}$ with $C_f = \int_B \|\omega\| |f(\omega)| d\omega < \infty, \exists$ width- m MLP g_m s.t.: $\int_B |f - g_m|^2 dx \leq O(\frac{1}{m})$.

2.4 ReLU(z) = max(0, z) networks

Zalavsky's Theorem: Activation patterns
 m ReLU neurons in \mathbb{R}^n . Each neuron's hyperplane $\{w_i^T x = 0\}$ partitions \mathbb{R}^n into $R(m)$ connected regions of constant activation pattern.
 $R(m) \leq \sum_{i=0}^{\min(n, m)} \binom{m}{i} \ll 2^m$.

Montufar: Connected linear regions in ReLU network $R(m, L) \geq R(m) \left\lfloor \frac{m}{n} \right\rfloor^{n(L-1)}, L$: layers, m : width.

Shekhtman: Piecewise linear functions are dense

in $C([0; 1])$. **Lebesgue:** Piecewise linear function with m pieces can be written $g(x) = ax + b + \sum_{i=1}^{m-1} c_i(x - x_i)_+$; $m+1$ parameters, a, b, c_i .
ReLU networks with 1 hidden layer are universal approximators.
Wang and Sun: Every continuous piecewise linear function $g: \mathbb{R}^n \rightarrow \mathbb{R}$ can be written as a signed sum of k -Hinges with $k \leq n+1$. A k -Hinge is a function $g(x) = \max_{j=1}^k \{w_j^T x + b_j\}$, generalizes ReLU, known as Maxout unit.

Linear Autoencoder: Optimal $A = DE$, s.t. frobenius norm reconstruction err of AX is minimized, is $D = U_k, E = U_k^\top$, not jointly convex in E and D , but individually. $\hat{X}^* = \arg \min_{\text{rank}(\hat{X})=k} \|X - \hat{X}\|_F^2 = U \Sigma_k V^\top \text{SVD}$.

3 Gradient-Based Learning

Forward mode is more memory efficient, but backward mode is more runtime efficient. Fwd is $O(\# \text{params})$, reverse is $O(d_{\text{out}})$.

Numerator layout: For $f: \mathbb{R}^n \rightarrow \mathbb{R}^m, (\frac{\partial y_i}{\partial x})_{ij} = \frac{\partial y_i}{\partial x_j} \in \mathbb{R}^{m \times n}$ and $f: \mathbb{R}^{n_1 \times n_2} \rightarrow \mathbb{R}, \nabla f(X)_{ij} = \frac{\partial f}{\partial X_{ij}} \in \mathbb{R}^{n_1 \times n_2}$.

3.1 Backpropagation

$x^\ell = \varphi(W^\ell x^{\ell-1} + b^\ell)$, $\frac{\partial \mathcal{L}}{\partial x_j} = \delta^\ell, \delta^\ell = \frac{\partial \mathcal{L}}{\partial x^\ell} \odot \varphi'(W^\ell x^{\ell-1} + b^\ell), \frac{\partial \mathcal{L}}{\partial x_j} = (W^{\ell+1})^\top \delta^{\ell+1}$.

$\frac{\partial L}{\partial x_j} = \frac{\partial L}{\partial z} \frac{\partial z}{\partial x_j}$. For $x \in \mathbb{R}^n$ different $z: \frac{\partial(Wx)}{\partial x} = W$, element wise f gives: $\frac{\partial f(x)}{\partial x} = \text{diag}(f'(x))$, $\frac{\partial \tilde{y} - y}{\partial \tilde{y}} = 2(\tilde{y} - y)^\top, \frac{\partial L}{\partial \tilde{y}} \frac{\partial(W\tilde{h})}{\partial W} = h \cdot \frac{\partial L}{\partial \tilde{y}}$.

$\frac{d}{dx} \text{softmax}(x)_i = \text{sm}(x)_i (\delta_{ij} - \text{sm}(x)_j)$

3.2 Gradient Descent

Update: $x_{t+1} = x_t - \eta \nabla f(x_t)$.

Gradient flow ODE $\frac{dx}{dt} = -\nabla f(x)$ gives ideal trajectory to be approximated by gradient descent.

Newton's method gives optimal step for quadratic model: $\Delta x = -[\nabla^2 f(x)]^{-1} \nabla f(x)$.
 $\nabla_x^2 [x^T A x + b^T x + c] = A + A^T$

Optimal LR for Convex Quadratics

For $f(x) = \frac{1}{2} x^T Q x, \eta^* = \frac{2}{\lambda_{\max}(Q) + \lambda_{\min}(Q)}$. Stability requires $\eta \leq \frac{2}{\lambda_{\max}(Q)}$. Quadratic approx. of $f: f(x + \Delta x) \approx f(x) + \nabla f(x)^T \Delta x + \frac{1}{2} \Delta x^T \nabla^2 f(x) \Delta x$. Condition number of $Q: \frac{\lambda_{\max}}{\lambda_{\min}}$

L-smooth: $\|\nabla f(x) - \nabla f(y)\| \leq L \|x - y\|$. Equivalently (if f twice diff) (for $L = 0 \Rightarrow$): $f(y) \leq f(x) + \nabla f(x)^T (y - x) + \frac{L}{2} \|y - x\|^2$. Implies $\lambda_i(\nabla^2 f(x)) \leq L$ for all EVs λ_i of $\nabla^2 f(x)$.

Convexity ($\lambda \in [0, 1]$):

$f(\lambda w + (1-\lambda)w') \leq \lambda f(w) + (1-\lambda)f(w')$.
 μ -Strong convexity: ($\mu = 0 \Leftrightarrow \text{convex} + \text{diff}$)
 $\Leftrightarrow f(y) \geq f(x) + \nabla f(x)^T (y - x) + \frac{\mu}{2} \|y - x\|^2$.

Implies $\lambda_i(\nabla^2 f(x)) \geq \mu$ for all EVs λ_i of $\nabla^2 f(x)$.
For $f: \mathbb{R} \rightarrow \mathbb{R}$, these become: $L \geq f''(x) \geq \mu \quad \forall x$.

If f μ -strongly convex, L -smooth, GD iterates x_t with $0 < \eta \leq \frac{1}{L}$ converge to unique minimizer x^* at rate $\|x_t - x^*\|^2 \leq (1 - \eta\mu)^t \|x_0 - x^*\|^2$.
If f convex, diff and L -smooth, with $\eta \leq \frac{1}{L}, f(x_t) - f(x^*) \leq \frac{1}{2\eta t} \|x_0 - x^*\|^2$.
Non-Convex case: If f diff, L -smooth, with minimum f^* , GD iterates with $\eta \leq \frac{1}{L}$ satisfy $\min_{i=0}^t \|\nabla f(x_i)\|^2 \leq \frac{2(f(x_0) - f^*)}{\eta(t+1)}$.

If f diff and L -smooth: $f(x) - f(x^*) \geq \frac{1}{2L} \|\nabla f(x)\|^2$.

Polyak-Lojasiewicz condition

$\frac{1}{2} \|\nabla f(x)\|^2 \geq \mu(f(x) - \min f)$ (forall x).
 μ -strong convex $\Rightarrow \mu$ -PL.

GD Convergence Rates & Learning Rates

L-smooth only: $\eta^* = \frac{1}{L}$. To reach ε -stationary point ($\|\nabla f\| \leq \varepsilon$) needs at most $\frac{2L}{\varepsilon^2} (f(x_0) - \min f)$ steps.
 μ -PL + L-smooth: Use $\eta^* = \frac{2}{L+\mu}$. Convergence: $f(x_t) - f(x^*) \leq (1 - \frac{\mu}{L})^t (f(x_0) - f(x^*))$.

3.3 Stochastic Gradient Descent

SGD variance

$V[\theta](S) = \frac{1}{s} \sum_{i=1}^s \|\nabla f[\theta](S) - \nabla f[\theta](x_i, y_i)\|^2$.

Polyak averages: $\bar{x}_{k+1} = \frac{k}{k+1} \bar{x}_k + \frac{1}{k+1} x_{k+1}$

SGD convergence rate with Polyak averaging and $\eta_k \propto \frac{1}{k}$
 $\mathbb{E}[f(\bar{\theta}_k)] - \min f \leq O(\frac{1}{\sqrt{k}})$ (general)
 $\mathbb{E}[f(\bar{\theta}_k)] - \min f \leq O(\frac{\log t}{t})$ (strongly convex)
 $\mathbb{E}[f(\bar{\theta}_k)] - \min f \leq O(\frac{1}{k})$ (additionally smooth)

Minibatch SGD: Variance \downarrow by $\propto r$. Can $\uparrow \eta \propto r$.

Var. Reduction with SVRG w/ occasional snapshot $\bar{\theta}$: $\theta_{t+1} = \theta_t - \eta [\nabla f_i(\theta_t) - \nabla f_i(\bar{\theta}) + \nabla f(\bar{\theta})]$.

3.4 Acceleration and Adaptivity

Heavy ball momentum update

$\theta_{t+1} = \theta_t - \eta \nabla f(\theta_t) + \beta(\theta_t - \theta_{t-1})$

Nesterov acceleration

$\theta_{t+1} = \theta_t + \beta(\theta_t - \theta_{t-1})$
 $\theta_{t+1} = \bar{\theta}_{t+1} - \eta \nabla h(\bar{\theta}_{t+1})$
More theoretical grounding than heavy ball.

AdaGrad updates

$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{g_t + \varepsilon}} \odot \nabla f(\theta_t),$
 $\gamma^t = \gamma^{t-1} + \nabla f(\theta_t) \odot \nabla f(\theta_t)$.

Adam updates

$m_t = \beta_1 m_{t-1} + (1 - \beta_1) \nabla f(\theta_t), \hat{m}_t = \frac{m_t}{1 - \beta_1^t}$
 $v_t = \beta_2 v_{t-1} + (1 - \beta_2) (\nabla f(\theta_t))^2, \hat{v}_t = \frac{v_t}{1 - \beta_2^t}$
 $\theta_{t+1} = \theta_t - \eta \frac{\hat{m}_t}{\sqrt{\hat{v}_t + \varepsilon}}$.

RMSprop: Adam without momentum term.

signSGD: $\theta_{t+1} = \theta_t - \eta \text{sign}(\nabla f_{i_k}(\theta_t))$.

x^4 is strictly convex but not strongly convex, since near 0 the growth of x^4 is slower than x^2 , violating the uniform lower bound on curvature.
With f L -smooth and μ -PL, GD with optimal step-size $\arg \min_\eta f(\theta_t - \eta \nabla f(\theta_t))$ converges globally at linear rate.
 $f(w) = \frac{\|Xw - y\|^2}{2} + \lambda \|w\|^2$ satisfies PL-condition.
Muon: Orthogonalize gradient, should increase the scale of other rare directions which have small magnitude in update but are important.
 $\Delta W = -\|\nabla L(W)\|_* \cdot \frac{d_{\text{out}}}{d_{\text{in}}} \cdot U^\top V \quad (\nabla L(W) = U \Sigma V^\top)$ minimizes RHS of: $L(W + \Delta W) \leq L(W) + \langle \nabla_W L(W), \Delta W \rangle_F + \frac{1}{2} \frac{d_{\text{in}}}{d_{\text{out}}} \|\Delta W\|_2^2$.
GD Trajectory always orthogonal to level set.

4 Convolutional Networks

Convolution $(f * g)(u) = (g * f)(u)$

$= \int_{-\infty}^{\infty} f(t)g(u-t) dt = \int_{-\infty}^{\infty} f(u-t)g(t) dt$.
 $(f * g) = \text{Toeplitz-Matrix}(g)f$.

Fourier transform convolution property

$\mathcal{F}(f * g) = \mathcal{F}(f) \cdot \mathcal{F}(g)$.

Cross-correlation:

$(g * f)[u] = \sum_t g[t]f[u+t]$.

$(f(t) * g(t))(y) = (f(-t) * g(t))(y)$.
 $(f(t) * g(t))(-y) = (f(-t) * g(t))(y) = (f(t) * g(-t))(y)$.
Translation-Equivariant Operators = Convolutions.

For $x \in \mathbb{R}^D, h \in \mathbb{R}^K, x * h = W_h x$. **Toeplitz Matrix:** $W_h \in \mathbb{R}^{(D-K+1) \times D}$
 $(W_h)_{k,j} = \begin{cases} h_{K+k-j} & \text{if } k \leq j \leq k+K-1 \\ 0 & \text{otherwise} \end{cases}$ for $h \in \mathbb{R}^K$.

$\nabla_w v^\top \text{vec}(\sigma(x * w)) = \text{flip}[x] * [\text{mat}(v) \odot \sigma^*(x * w)]$, flip rows and columns.

Normal convolution of image $x \in \mathbb{R}^{d \times d}$, kernel $w \in \mathbb{R}^{q \times q} x * w$ requires $\mathcal{O}((d-q)^2 q^2)$. If w separable st $w = uv^\top, u \in \mathbb{R}^q, v \in \mathbb{R}^p, \mathcal{O}(dq(d-q))$

Output size: $H_{\text{out}} = \lfloor \frac{H_{\text{in}} + 2P - K}{S} \rfloor + 1$, Height, Input size, padding, Kernel size, stride.

4.1 Convolutional Networks

Conventions for Padding: Add zeros around input.

ConvNets for Images (r out channel, u in channel)
 $y[r][s, t] = \sum_u \sum_{i,j} w[r, u][i, j] * x[u][s+i, t+j]$.

Number of parameters of a convolutional layer
 $(|r| \times |u|) \cdot (|i| \times |j|)$: fully connected \times patch-size.

4.2 Word2Vec

Per word ω , have input embedding x_ω and output embedding y_ω .

Predict context word ν given center word ω : $P(\nu \mid \omega) = \frac{\exp(x_\omega^\top y_\nu)}{\sum_\mu \exp(x_\omega^\top y_\mu)}$.

NLL loss: $\ell_{\omega,\nu} = -x_\omega^\top y_\nu + \ln \sum_\mu \exp(x_\omega^\top y_\mu)$.
Total: $h(\{x_\omega\}, \{y_\nu\}) = \sum_{(\omega,\nu)} \ell_{\omega,\nu}$ over observed pairs. Use only input embeddings after training.

5 Geometric Deep Learning

Group is set G with a binary operation s.t.:
1) $(gh)f = g(hf)$, 2) $\exists e \in G$ s.t. $ef = fe = f$,
3) $\forall g \exists g^{-1} \in G$ s.t. $gg^{-1} = g^{-1}g = e$, 4) $gh \in G \forall g, h$. **Abelian** if $gh = hg$.

5.1 Sets and Points

Order-invariance property:

$f(x_1, \dots, x_M) = f(x_{\pi(1)}, \dots, x_{\pi(M)})$ (perturbations).

(Permutation) Equivariance property:

$f(x_1, \dots, x_M) = (y_1, \dots, y_M) \Rightarrow f(x_{\pi(1)}, \dots, x_{\pi(M)}) = (y_{\pi(1)}, \dots, y_{\pi(M)})$

Deep Sets model (invariant layer):

$f(x_1, \dots, x_M) = \rho(\sum_{m=1}^M \varphi(x_m))$.

Equivariant map construction:

$\rho: \mathbb{R} \times \mathbb{R}^N \rightarrow Y, (x_m, \sum_{k=1}^M \varphi(x_k)) \mapsto y_m$

5.2 Graph Convolutional Networks

Feature and adjacency matrices

$X = \text{mat}(x_1^\top; \dots; x_M^\top)$, $A = (a_{nm})$ with $a_{nm} = 1 \Leftrightarrow \{v_n, v_m\} \in E$.

Permutation matrix constraints

$P \in \{0, 1\}^{M \times M}$ with single 1 in each row and col.

Graph invariance definition

$f(X, A) \stackrel{!}{=} f(PX, PAP^\top)$, $\forall P \in \Pi_M$.

Graph equivariance definition

$f(X, A) = Pf(PX, PAP^\top)$, $\forall P \in \Pi_M$.

Node neighborhood features

$X_m = \{\{x_n : \{v_n, v_m\} \in E\}\}$, $\{\{\cdot\}\} = \text{multiset}$

Message passing scheme

$\varphi(x_m, X_m) = \varphi(x_m, \bigoplus_{x \in X_m} \psi(x))$,
 \bigoplus is some permutation-invariant operation.

Normalized adjacency matrix

$\bar{A} = D^{-\frac{1}{2}}(A + I)D^{-\frac{1}{2}}$,
 $\bar{D} = \text{diag}(d_1, \dots, d_M)$, $d_m = 1 + \sum_{n=1}^M a_{nm}$.

One GCN layer

$X^+ = \sigma(\bar{A}XW)$, $W \in \mathbb{R}^{M \times N}$.

5.2.1 Spectral Graph Theory

Laplacian operator

$\Delta f = \sum_{n=1}^N \frac{\partial^2 f}{\partial x_n^2}, f: \mathbb{R}^N \rightarrow \mathbb{R}$.

Graph Laplacian

$L = D - A$, $(Lx)_n = \sum_{m=1}^M a_{nm}(x_n - x_m)$.
 $x^\top Lx = \frac{1}{2} \sum_u \sum_v A_{uv}(x_u - x_v)^2 \geq 0$ (psd).

Normalized Laplacian

$\tilde{L} = I - D^{-\frac{1}{2}}AD^{-\frac{1}{2}} = D^{-\frac{1}{2}}(D - A)D^{-\frac{1}{2}}$.

Graph Fourier transform

$L = D - A = U\Lambda U^\top$, $\hat{f} = U^\top f$, $f = U\hat{f}$.

$\Lambda := \text{diag}(\lambda_1, \dots, \lambda_M)$, $\lambda_i \geq \lambda_{i+1}$.

Convolution: $x * y = U((U^\top x) \odot (U^\top y))$.

Filtering operation

$G_\theta(L)x = UG_\theta(\Lambda)U^\top x$

Polynomial kernels

$U(\sum_{k=0}^K \alpha_k \Lambda^k)U^\top = \sum_{k=0}^K \alpha_k L^k$

Polynomial kernel network layer

$x_i^{l+1} = \sum_j p_{ij}(L)x_j^l + b_i$,

$p_{ij}(L) = \sum_{k=0}^K \alpha_{ijk} L^k$

GNNs cannot distinguish between certain graphs that are topologically different. Unconstrained set architectures are more powerful. If **WL-test** says graphs are different, they are; but if it says they're the same, they might still be different.

6 Theory of DNNs

6.1 Statistical Learning Theory

Risk decomposition

f^* : optimal predictor over all functions,
 $f_H^* = \text{argmin}_{f \in H} \mathcal{R}(f)$, \hat{f}_H : learned from finite data.
 $\underbrace{\mathcal{R}(\hat{f}_H) - \mathcal{R}(f^*)}_{\text{excess risk}} = \underbrace{\mathcal{R}(\hat{f}_H) - \mathcal{R}(f_H^*)}_{\text{estimation error}} + \underbrace{\mathcal{R}(f_H^*) - \mathcal{R}(f^*)}_{\text{approximation error}}.$

Rademacher Complexity $G = \{g_h \mid h \in H\}$:
For $\sigma \in \{-1, 1\}$, measures how well G can fit random noise: $\mathfrak{R}_{D_n}(G) = \mathbb{E}_\sigma \left[\sup_{g \in G} \frac{1}{n} \sum_{i=1}^n \sigma_i g(z_i) \right]$.
 $\mathbb{E} \sup_{h \in H} \mathcal{R}(h) - \mathcal{R}_{D_n}(h) \leq 2\mathfrak{R}_{D_n}(G)$,
 $\mathbb{E} [\mathcal{R}(\hat{f}_H)] \leq \mathcal{R}(h_H^*) + 2\mathfrak{R}_{D_n}(G)$.

Double descent:

Beyond the interpolation point, models eventually may level out at a lower generalization error.

Implicit bias towards min norm solutions:
Any convergent algorithm with iterates in $\text{span}\{x_1, \dots, x_n\}$ finds the minimum norm solution.

6.1.1 A PAC-Bayesian result

P prior distribution over functions before seeing data, Q posterior after training.

PAC-Bayesian theorem

Bounds generalization gap for stochastic

classifiers ($f \sim Q$): $E_Q[\mathcal{R}(f)] - E_Q[\hat{\mathcal{R}}_n(f)] \leq \sqrt{\frac{2}{n} [\text{KL}(Q\|P) + \ln(2\sqrt{n}/\varepsilon)]}$
• P : prior, Q : posterior (learned). Rate $\tilde{O}(1/\sqrt{n})$
• $\text{KL}(Q\|P)$: "information cost" of moving $P \rightarrow Q$
• Insight: generalization depends on **distance moved**, not parameter count

PAC-Bayesian for DNNs

$P = \mathcal{N}(0, \lambda I)$, $Q = \mathcal{N}(\theta, \text{diag}(\sigma_i^2))$,
 $\text{KL}(Q\|P) = \sum_i \left[\log \frac{\lambda}{\sigma_i} + \frac{\sigma_i^2 + \theta_i^2}{2\lambda^2} - \frac{1}{2} \right]$
Minimize directly: $E_Q[\hat{\mathcal{R}}] + \sqrt{\frac{2}{n} [\text{KL}(Q\|P) + \dots]}$
 \Rightarrow encourages wide/flat minima (perturbations $\theta + \varepsilon$ must also perform well)

Implementation: Reparameterization: $\tilde{\theta} = \theta + \text{diag}(\sigma_i)\eta$, $\eta \sim \mathcal{N}(0, I)$, Backprop through θ and σ .

6.2 Linearized DNNs and NTK

Training neural network $f(\theta)(x)$ can be approximated by **linearizing** around initialization θ_0 when parameters change slowly.

Linearization \rightarrow Kernel Regression:

Taylor approximation: $h(\beta)(x) = f(\theta_0)(x) + \beta \cdot \nabla f(\theta_0)(x)$, $\beta = \theta - \theta_0$.
With residuals $\tilde{y}_i = y_i - f(\theta_0)(x_i)$, training becomes **linear regression** with features $\nabla f(\theta_0)(x_i)$: $\min \|\tilde{y}_i - \beta \cdot \nabla f(\theta_0)\|$

Neural Tangent Kernel (NTK):

Definition: $k_\theta(x, x') := \nabla f(\theta)(x) \cdot \nabla f(\theta)(x')$.

Dual representation:

$h(\alpha)(x) = f(\theta_0)(x) + \sum_{i=1}^n \alpha_i k_{\theta_0}(x_i, x)$.

Optimization problem: $\min_\alpha \frac{1}{2} \|\mathbf{K}_{\theta_0} \alpha - \tilde{\mathbf{y}}\|^2$
Optimal solution (kernel regression):
 $\alpha^* = \mathbf{K}_{\theta_0}^\dagger (\mathbf{y} - f(\theta_0))$, $h^*(x) = \mathbf{k}_{\theta_0}(x)^\top \alpha^*$

Functional Gradient Flow

Training dynamics in function space:

$\dot{\mathbf{f}}(\theta) = \mathbf{K}(\theta)(\mathbf{y} - \mathbf{f}(\theta))$
• If $\mathbf{K}(\theta)$ constant \rightarrow **linear ODE** with closed-form solution
• If $\mathbf{K}(\theta)$ evolves \rightarrow **nonlinear dynamics**, feature learning

Infinite-Width Limit

Initialization: $w_{ij}^{(\ell)} \sim \frac{\sigma_w}{\sqrt{m_\ell}} \mathcal{N}(0, 1)$. Result: As width $m \rightarrow \infty$: $k_{\theta(t)} \rightarrow k_\infty$ (constant during training).
• Kernel becomes **deterministic** (depends only on architecture/init scheme)
• Training = kernel regression with frozen k_∞
• No feature learning

Finite-width: $\|\mathbf{K}(\theta_0) - \mathbf{K}(\theta(t))\| = \mathcal{O}(\frac{1}{m})$

Why Kernel Stays Constant:

Kernel grad $\nabla K = \nabla^2 f(x) \nabla f(z) + \nabla^2 f(z) \nabla f(x)$,
at $m = \infty$: $\nabla^2 f \rightarrow 0 \Rightarrow \nabla K \rightarrow 0 \rightarrow$ kernel frozen.

Lazy Training (NTK Regime)	Feature Learning (Rich Regime)
$m \rightarrow \infty$, small LR	Finite width, normal LR
\mathbf{K} const \rightarrow linear dynamics	\mathbf{K} evolves \rightarrow nonlinear
No feature learning	Learns representations
Theoretically tractable	SOTA performance

Takeaways:

Linearization turns NN training into kernel regression with features $\nabla f(\theta_0)(x)$.

NTK $k_\theta = \nabla f(\theta)(x) \cdot \nabla f(\theta)(x')$ governs training dynamics via $\dot{\mathbf{f}} = \mathbf{K}(\mathbf{y} - \mathbf{f})$.

Infinite width \rightarrow kernel constant \rightarrow NN = kernel machine (no feature learning).

Finite width \rightarrow kernel evolves $\mathcal{O}(\frac{1}{m}) \rightarrow$ enables feature learning.

NTK explains lazy regime but NOT why deep learning works \rightarrow real power is feature learning when kernel changes.

6.3 Random NNs and GPs

Marginals and Conditionals of MV Gaussians

Let $X \in \mathbb{R}^d \sim \mathcal{N}(\mu, \Sigma)$ with partition: $X = \begin{pmatrix} X_A \\ X_B \end{pmatrix}$, $\mu = \begin{pmatrix} \mu_A \\ \mu_B \end{pmatrix}$, $\Sigma = \begin{bmatrix} \Sigma_{AA} & \Sigma_{AB} \\ \Sigma_{BA} & \Sigma_{BB} \end{bmatrix}$

Marginal: $X_A \sim \mathcal{N}(\mu_A, \Sigma_{AA})$

Conditional: $X_B \mid X_A \sim \mathcal{N}(\mu_{B|A}, \Sigma_{B|A})$

$\mu_{B|A} = \mu_B + \Sigma_{BA} \Sigma_{AA}^{-1} (X_A - \mu_A)$

$\Sigma_{B|A} = \Sigma_{BB} - \Sigma_{BA} \Sigma_{AA}^{-1} \Sigma_{AB}$

6.3.1 Bayesian Linear Regression

Least-squares: $\hat{w} = \arg \min_w \frac{1}{2n\sigma^2} \|\mathbf{y} - \mathbf{X}w\|^2$.

Closed-form solution: $\hat{w} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$.

MLE interpretation: $y_i = x_i^\top w + \varepsilon_i$, $\varepsilon_i \sim \mathcal{N}(0, \sigma^2)$, $\mathcal{L}(w) = \log \prod_{i=1}^n p(y_i \mid x_i, w)$,
 $y_i \mid x_i, w \sim \mathcal{N}(x_i^\top w, \sigma^2)$.

Prior: $p(w) = \mathcal{N}(0, I_d)$.

Posterior: $p(w \mid \mathbf{y}, \mathbf{X}) = \frac{p(\mathbf{y} \mid \mathbf{X}, w)p(w)}{p(\mathbf{y} \mid \mathbf{X})}$.

Predictive distribution: $p(y_{n+1}) = \int p(y_{n+1} \mid w)p(w \mid \mathbf{y}, \mathbf{d}w)$.

$\Sigma_{ww} = I_d$, $\Sigma_{yw} = \mathbf{X}$, $\Sigma_{yy} = \mathbf{X}\mathbf{X}^\top + \sigma^2 I_n$.

$\mu_{w|y} = \mathbf{X}^\top \Sigma_{yy}^{-1} \mathbf{y} = (\mathbf{X}^\top \mathbf{X} + \sigma^2 I_d)^{-1} \mathbf{X}^\top \mathbf{y}$,

$\Sigma_{w|y} = I_d -$

$\mathbf{X}^\top \Sigma_{yy}^{-1} \mathbf{X} = \sigma^2 (\mathbf{X}^\top \mathbf{X} + \sigma^2 I_d)^{-1}$.

Same result as ridge: $\hat{w} = (\mathbf{X}^\top \mathbf{X} + \sigma^2 I_d)^{-1} \mathbf{X}^\top \mathbf{y}$.

Equiv. to GP with linear kernel: $f(\cdot) \sim \mathcal{GP}(0, k(\cdot, \cdot))$: $k(x, x') = \phi(x)^\top \phi(x')$, $y = f + \varepsilon$, $f \sim \mathcal{N}(0, K)$, $\varepsilon \sim \mathcal{N}(0, \sigma^2 I_n)$, posterior $p(f|y) = \mathcal{N}(\mu_{f|y}, \Sigma_{f|y})$, $\mu_{f|y} = \mathbf{K}(\mathbf{K} + \sigma^2 I_n)^{-1} \mathbf{y}$.

For $y = f(x) + \varepsilon$, $f(x) = x^\top w$, $\varepsilon \sim \mathcal{N}(0, \sigma^2)$, $p(y \mid X, w) = \mathcal{N}(X^\top w, \sigma^2 I)$. If $w \sim \mathcal{N}(0, \Sigma)$, $p(w \mid x, X) = \mathcal{N}(\sum_{\text{post}} \frac{1}{\sigma^2} Xy, \sum_{\text{post}})$, where $\Sigma_{\text{post}}^{-1} = \Sigma^{-1} + \frac{1}{\sigma^2} X X^\top$. Maximizing $\log p(w \mid x, X)$ is same as minimizing least-squares with ℓ_2 penalty $\frac{1}{2} w^\top \Sigma^{-1} w$, ridge when $\Sigma = \lambda^{-1} I$. **Predictive:** $f_* \mid x_*, y, X = x_*^\top w \sim \mathcal{N}(x_*^\top \mu_{\text{post}}, x_*^\top \Sigma_{\text{post}} x_*)$. $y_* \mid x_*, y, X$ adds σ^2 .
 $f = x^\top w$ with $w \sim \mathcal{N}(0, \Sigma)$ is GP w $k(x, x') = x^\top \Sigma x'$.

6.3.2 NNGPs

Setup: Random 1-hidden-layer NN with m units: $f(x) = v_0 + \frac{1}{\sqrt{m}} \sum_{j=1}^m v_j \varphi(\theta_j^\top x)$. Random init: $v_0 \sim \mathcal{N}(0, \sigma_0^2)$, $\mathbb{E}[v_j^2] = \sigma_v^2$, $\text{Cov}(\theta_j) = \Sigma_\theta$.

Result: As $m \rightarrow \infty$, $f(\cdot) \rightarrow \text{GP}(0, k)$ where $k(x, x') = \sigma_0^2 + \sigma_v^2 \mathbb{E}_\theta[\varphi(\theta^\top x) \varphi(\theta^\top x')]$

Monte Carlo approximation: Sample B random NNs $\{f_b\}_{b=1}^B$, define features:

• $\varphi(x) = \frac{1}{\sqrt{B}} (f_1(x), \dots, f_B(x))^\top$
• $\Phi = [f_1 \dots f_B] \in \mathbb{R}^{n \times B}$ (feature matrix)
• $\hat{K} = \Phi \Phi^\top$ (approximate kernel matrix)

GP regression: Posterior mean and variance: $\mathbb{E}[f(x) \mid \mathbf{y}] = \varphi(x)^\top (\Phi^\top \Phi + \sigma^2 I_B)^{-1} \Phi^\top \mathbf{y}$
 $\text{Var}[f(x) \mid \mathbf{y}] = \sigma^2 \varphi(x)^\top (\Phi^\top \Phi + \sigma^2 I_B)^{-1} \varphi(x)$

Key advantage: Inverts $B \times B$ matrix instead of $n \times n$ when $B \ll n$.

7 Generative Models

7.0.1 Linear Autoencoders

Setup. Encoder $C \in \mathbb{R}^{k \times d}$, decoder $D \in \mathbb{R}^{d \times k}$, data $\mathbf{X} \in \mathbb{R}^{d \times n}$ (centered cols): $\min_{C,D} \|\mathbf{X} - DC\mathbf{X}\|_F^2$.

Optimal Solution (PCA). Let $\mathbf{S} = \mathbf{X}\mathbf{X}^\top$ with eigendecomposition $\mathbf{S} = \mathbf{Q}\Lambda^2\mathbf{Q}^\top$, $\lambda_1 \geq \dots \geq \lambda_d \geq 0$. Optimal reconstruction via rank- k projection: $\hat{\mathbf{X}} = \mathbf{U}_k^* \mathbf{U}_k^{*\top} \mathbf{X}$ where $\mathbf{U}_k^* = \mathbf{Q}_{[:,1:k]}$ are top- k eigenvectors of \mathbf{S} (equiv, top- k left singular vectors of \mathbf{X}).

• Any $C = \mathbf{U}_k^{*\top} \mathbf{A}$, $D = \mathbf{A}^{-1} (\mathbf{U}_k^*)^\top$ is optimal ($\forall \mathbf{A}$)
• Reduces to truncated SVD: $\hat{\mathbf{X}} = \mathbf{U}^* \Lambda_k \mathbf{V}^\top$ with $\Lambda_k = \text{Diag}(\lambda_1, \dots, \lambda_k, 0, \dots, 0)$
• Convex objective with no spurious local minima (gradient descent finds global optimum)
• Singular vectors may not be uniquely identified

7.0.2 Factor analysis

Latent Variable Models are a generic way to describe generative models. Latent variable $z \sim p(z)$, conditional models for observables $x, p(x|z)$, observed data model: $p(x) = \int p(x|z)p(z)dz$.

Mixture models: simple discrete models: $z \in [K]$, $p(z)$ mixing proportions, $p(x|z)$ condit. densities.

$$x \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}):$$

$$p(x; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{\exp[-\frac{1}{2}(x-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(x-\boldsymbol{\mu})]}{\sqrt{(2\pi)^n} \det(\boldsymbol{\Sigma})}$$

7.0.3 Linear Factor Analysis

- Latent prior: $\boldsymbol{z} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I})$, $\boldsymbol{z} \in \mathbb{R}^m$
- Observation: $\boldsymbol{x} = \boldsymbol{\mu} + \boldsymbol{W}\boldsymbol{z} + \boldsymbol{\eta}$, $\boldsymbol{\eta} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma})$
- Independence: $\boldsymbol{\eta} \perp \boldsymbol{z}$
- Typically $m < n$ (fewer factors than features)

Marginal distribution: $x \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{W}\boldsymbol{W}^\top + \boldsymbol{\Sigma})$

- $\boldsymbol{W}\boldsymbol{W}^\top$: shared variance (low-rank, explained by latent factors)
- $\boldsymbol{\Sigma}$: unique variance (diagonal, observation-specific)

Non-identifiability: $(\boldsymbol{W}\boldsymbol{Q})(\boldsymbol{W}\boldsymbol{Q})^\top = \boldsymbol{W}\boldsymbol{Q}^\top \boldsymbol{W}^\top = \boldsymbol{W}\boldsymbol{W}^\top$ for any orthogonal \boldsymbol{Q} . Factors only identifiable up to rotations/reflections. \Rightarrow Use factor rotations (varimax, etc.) for interpretability.

MLE estimation: $\boldsymbol{\theta} = (\boldsymbol{\mu}, \boldsymbol{W}) \stackrel{\text{max}}{\leftarrow} \log p(\boldsymbol{X}; \boldsymbol{\mu}, \boldsymbol{W})$

- $\hat{\boldsymbol{\mu}} = \frac{1}{s} \sum_{i=1}^s \boldsymbol{x}_i$ (closed form)
- No closed form for $\boldsymbol{W} \rightarrow$ use GD or EM algorithm

Posterior (encoder): $p(\boldsymbol{z} \mid \boldsymbol{x}) = \frac{p(\boldsymbol{x} \mid \boldsymbol{z})p(\boldsymbol{z})}{p(\boldsymbol{x})}$.

$\boldsymbol{\mu}_{\boldsymbol{z}|\boldsymbol{x}} = \boldsymbol{W}^\top (\boldsymbol{W}\boldsymbol{W}^\top + \boldsymbol{\Sigma})^{-1} (\boldsymbol{x} - \boldsymbol{\mu})$.

$\boldsymbol{\Sigma}_{\boldsymbol{z}|\boldsymbol{x}} = \boldsymbol{I} - \boldsymbol{W}^\top (\boldsymbol{W}\boldsymbol{W}^\top + \boldsymbol{\Sigma})^{-1} \boldsymbol{W}$.

Probabilistic PCA: Special case $\boldsymbol{\Sigma} = \sigma^2 \boldsymbol{I}$. Optimal i -th column: $\boldsymbol{w}_i = \rho_i \boldsymbol{u}_i$, $\rho_i^2 = \max\{0, \lambda_i - \sigma^2\}$. $\boldsymbol{W} = \boldsymbol{U}_m \boldsymbol{L}_m$ where $(\lambda_i, \boldsymbol{u}_i)$ is i -th eigenpair of data covariance.

As $\sigma \rightarrow 0$: $\boldsymbol{\mu}_{\boldsymbol{z}|\boldsymbol{x}} \rightarrow \boldsymbol{W}^\dagger (\boldsymbol{x} - \boldsymbol{\mu})$ (standard PCA). If \boldsymbol{W} has orthogonal columns, then $\boldsymbol{W}^\dagger = \boldsymbol{W}^\top$.

7.1 Variational Autoencoders

$\boldsymbol{z} \in \mathbb{R}^d$ is learned embedding of \boldsymbol{x} . For generation, $\boldsymbol{z} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I})$, decoder $p_\theta(\boldsymbol{x}|\boldsymbol{z})$ maps latent to data.

Problem: $p_\theta(\boldsymbol{x}) = \int p(\boldsymbol{z})p_\theta(\boldsymbol{x}|\boldsymbol{z}) \, \mathrm{d}\boldsymbol{z}$ intractable. **Solution:** Maximize ELBO instead: $\log p_\theta(\boldsymbol{x}) \geq \underbrace{\mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}[\log p_\theta(\boldsymbol{x}|\boldsymbol{z})]}_{\text{reconstruction}} - \underbrace{D_{\text{KL}}(q_\phi(\boldsymbol{z}|\boldsymbol{x}) \parallel p(\boldsymbol{z}))}_{\text{regularization}}$

- Reconstruction:** Encode $\boldsymbol{x} \rightarrow \boldsymbol{z}$, decode back
- KL term:** Keep encoder output close to prior $p(\boldsymbol{z}) \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I})$, ensures generation using latents

Encoder $q_\phi(\boldsymbol{z}|\boldsymbol{x}) = \mathcal{N}(\boldsymbol{\mu}_\phi(\boldsymbol{x}), \text{diag}(\boldsymbol{\sigma}_\phi^2(\boldsymbol{x})))$.

KL closed form: $D_{\text{KL}}(q_\phi(\boldsymbol{z}|\boldsymbol{x}) \parallel p(\boldsymbol{z})) = \frac{1}{2} \sum_{j=1}^d (\sigma_{\phi,j}^2 + \mu_{\phi,j}^2 - 1 - \log \sigma_{\phi,j}^2)$.

$$\text{KL}(\mathcal{N}(\mu_0, \sigma_0^2) \parallel \mathcal{N}(\mu_1, \sigma_1^2)) = \frac{1}{2} \left(\frac{\sigma_0^2}{\sigma_1^2} + \frac{(\mu_0 - \mu_1)^2}{\sigma_1^2} - 1 + \log \frac{\sigma_1^2}{\sigma_0^2} \right)$$

$$\text{KL}(p(\parallel q)) = \mathbb{E}_p \left[\log \frac{p(x)}{q(x)} \right]$$

- Fwd KL:** $q_1^* = \arg \min_{q \in \mathcal{Q}} \text{KL}(p \parallel q)$
- Rev KL:** $q_2^* = \arg \min_{q \in \mathcal{Q}} \text{KL}(q \parallel p)$

Rev KL: Mode-seeking ($p = 0 \Rightarrow q = 0$), FwdKL: Mean-seeking ($p \neq 0 \Rightarrow q \neq 0$). MLE minimizes fwd KL to empirical \mathcal{D} .

$$\log p_\theta(\boldsymbol{x}|\boldsymbol{z}) = -\frac{1}{2\sigma^2\boldsymbol{x}} \|\boldsymbol{x} - \boldsymbol{\mu}_\theta(\boldsymbol{z})\|_2^2 - \frac{d}{2} \log(2\pi\sigma^2).$$

Reparameterization trick: $\boldsymbol{z} = \boldsymbol{\mu}_\varphi(\boldsymbol{x}) + \boldsymbol{\sigma}_\varphi(\boldsymbol{x}) \odot \boldsymbol{\varepsilon}$, $\boldsymbol{\varepsilon} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I})$, enables backprop through sampling.

$\log p_\theta(\boldsymbol{x}) - \text{ELBO} = D_{\text{KL}}(q_\phi(\boldsymbol{z}|\boldsymbol{x}) \parallel p_\theta(\boldsymbol{z}|\boldsymbol{x}))$, **tight when $q_\phi = \text{true posterior}$.**

Monte Carlo estimation: $E_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}[\log p_\theta(\boldsymbol{x}|\boldsymbol{z})] \approx -\frac{1}{2\sigma^2K} \sum_{k=1}^K \|\boldsymbol{x} - \boldsymbol{\mu}_\theta(\boldsymbol{z}_k)\|_2^2 - \frac{d}{2} \log(2\pi\sigma^2)$.

$$\begin{array}{llll} \textbf{Generative} & \textbf{Classifiers} & \text{Given} & y \in \\ & & \{0, 1\}, & p(y = 1) = p(y = 0) = \frac{1}{2}, \quad p(\boldsymbol{x} \mid y) = \\ & & \mathcal{N}(\boldsymbol{x}; \mu_y, I_d), & \text{where } \mu_0, \mu_1 \in \mathbb{R}^d, \quad p(y = 1 \mid \boldsymbol{x}) = \\ & & & \frac{p(y=1)p(\frac{\boldsymbol{x}}{2} \mid y=1)+p(y=0)p(\frac{\boldsymbol{x}}{2} \mid y=0)}{\frac{1}{2}(2\pi)^{-\frac{d}{2}} \exp(-\frac{1}{2}\|\boldsymbol{x}-\mu_1\|^2)} = \\ & & & \frac{\frac{1}{2}(2\pi)^{-\frac{d}{2}} \exp(-\frac{1}{2}\|\boldsymbol{x}-\mu_1\|^2) + \frac{1}{2}(2\pi)^{-\frac{d}{2}} \exp(-\frac{1}{2}\|\boldsymbol{x}-\mu_0\|^2)}{1 + \exp(\frac{1}{2}(\frac{1}{2}\|\boldsymbol{x}-\mu_1\|^2 - \frac{1}{2}\|\boldsymbol{x}-\mu_0\|^2))} = \\ & & & \frac{1}{(1 + \exp(-[(\mu_1 - \mu_0)^\top \boldsymbol{x} + \frac{1}{2}(\|\mu_0\|^2 - \|\mu_1\|^2)])})} \end{array}$$

equiv to logistic regression where $p(y = 1|\boldsymbol{x}) = \sigma(w^\top \boldsymbol{x} + b)$ with $w = \mu_1 - \mu_0$, $b = \frac{1}{2}(\|\mu_0\|^2 - \|\mu_1\|^2)$.

ELBO for Hierarchical VAEs: Model \boldsymbol{x} by decoding from latents $\boldsymbol{z} = (z_1, \dots, z_L)$. $p_\theta(\boldsymbol{x}, \boldsymbol{z}) = p_\theta(\boldsymbol{x}|\boldsymbol{z}_1) \prod_{i=1}^{L-1} p_\theta(z_i|z_{i+1})p(z_L)$. **Inference** top-down: $q_\phi(\boldsymbol{z}|\boldsymbol{x}) = q_\phi(z_L|\boldsymbol{x}) \prod_{i=1}^{L-1} q_\phi(z_i \mid z_{i+1})$. **ELBO** for HVAE: $\mathcal{L}(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{z}|\boldsymbol{x} \sim q_\phi} \left[\log \frac{p_\theta(\boldsymbol{x}, \boldsymbol{z})}{q_\phi(\boldsymbol{z}|\boldsymbol{x})} \right] = \mathbb{E}_{\boldsymbol{z}|\boldsymbol{x} \sim q_\phi} \left[\log p_\theta(\boldsymbol{x}|\boldsymbol{z}_1) + \log \frac{p_\theta(z_1|\boldsymbol{z}_2)}{q_\phi(z_1|\boldsymbol{x})} + \sum_{i=2}^{L-1} \log \frac{p_\theta(z_i|\boldsymbol{z}_{i+1})}{q_\phi(z_i|\boldsymbol{z}_{i-1})} + \log \frac{p_\theta(z_L|\boldsymbol{z}_{L-1})}{q_\phi(z_L|\boldsymbol{z}_{L-1})} \right]$.

Change of variables spherical to 3D euclidian $(x, y, z) \mapsto (r \cos \theta \cos \phi, r \cos \theta \sin \phi, r \sin \theta)$. Lengths of the three sides of an infinitesimal cuboid whose diagonally opposite vertices are at r, θ, ϕ and $(r + dr, \theta + d\theta, \phi + d\phi)$ are $(dr, r d\theta, r \cos \theta d\phi)$. Volume is $r^2 \cos \theta dr d\theta d\phi$. Determinant of jacobian $|\frac{\partial(x,y,z)}{\partial(r,\theta,\phi)}| = r^2 \cos \theta$.

Density on spherical coordinates $p(r, \theta, \phi) \rightarrow$ density on Euclidian coordinates is $p(\boldsymbol{x}, y, z) = p(r, \theta, \phi) |\frac{\partial(\boldsymbol{x}, y, z)}{\partial(r, \theta, \phi)}|^{-1}$. Infinitesimal probability mass of the cuboid above is equal to the mass of a Euclidian cuboid of size (dx, dy, dz) at (\boldsymbol{x}, y, z) .

7.2 Normalizing Flows

Transform simple distribution $\boldsymbol{z} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I})$ through invertible map T to get complex $\boldsymbol{x} = T(\boldsymbol{z})$. Exact likelihood (no ELBO like VAEs), easy sampling.

Change of Variables Formula:

$$p_{\boldsymbol{x}}(\boldsymbol{x}) = p_{\boldsymbol{z}}(T^{-1}(\boldsymbol{x})) \cdot |\det J_{T^{-1}}(\boldsymbol{x})|, \quad |\det J_{T^{-1}}(\boldsymbol{x})| = \frac{1}{|\det J_T(T^{-1}(\boldsymbol{x}))|}.$$

Diffeomorphism: T is bijective, differentiable, with differentiable inverse. Guarantees $\det J_T \neq 0$.

Computational problem: Computing $\det J$ is $O(d^3)$ for dense Jacobian. **Solution:** Design T s.t. Jacobian is **triangular**, then only $O(d)!$

Two architectures with triangular Jacobians:

	MAF	IAF
Fast / parallel	Density eval	Sampling
Slow / sequential	Sampling	Density

Coupling layers: Trick that makes both directions fast, at the cost of being less expressive per layer.

7.3 Autoregressive Models

$$p(\boldsymbol{x}) = \prod_{i=1}^d p(\boldsymbol{x}_i \mid \boldsymbol{x}_{<i}).$$

7.4 Generative Adversarial Networks

Likelihood-free generative model: train via adversarial game between two networks: **Generator** G_θ maps latent $\boldsymbol{z} \sim p_z$ (typically Gaussian) to fake samples; **Discriminator** D_φ : outputs prob that input is **real**.

GAN

Objective: $\min_\theta \max_\varphi \mathbb{E}_{\boldsymbol{x} \sim p_r} [\log D_\varphi(\boldsymbol{x})] + \underbrace{\mathbb{E}_{\boldsymbol{z} \sim p_z} [\log (1 - D_\varphi(G_\theta(\boldsymbol{z})))]}_{\text{fake samples}}$

- Discriminator** maximizes: correctly classify real (high D) and fake (low D)
- Generator** minimizes: fool discriminator (make $D(G(\boldsymbol{z}))$ high)

Common alternative objective for the generator is to maximize $\mathbb{E}_{\boldsymbol{z} \sim p(\boldsymbol{z})} [\log D(G(\boldsymbol{z}))]$ instead of minimizing $\mathbb{E}_{\boldsymbol{z} \sim p(\boldsymbol{z})} [\log (1 - D(G(\boldsymbol{z})))]$ to help mitigate vanishing gradient problem when discriminator becomes to good, i.e. $D(G(\boldsymbol{z})) \rightarrow 0$. For a fixed generator G , **optimal discriminator** D^* is given by $D^*(\boldsymbol{x}) = \frac{p_{\text{data}}(\boldsymbol{x})}{p_{\text{data}}(\boldsymbol{x}) + p_G(\boldsymbol{x})}$. If **discriminator optimal**, GAN objective reduces to $V(D^*, G) = 2D_{\text{JS}}(p_{\text{data}} \parallel p_G) - \log 4$.

7.4.1 Theoretical Foundation

Binary classification with $p(y = 1) = p(y = 0) = \frac{1}{2}$:

- $y = 1$: sample from real $p_{r(x)}$
- $y = 0$: sample from generator $p_{\theta(x)}$

Bayes Optimal Classifier (prob that \boldsymbol{x} is real):

$$q_\theta(\boldsymbol{x}) = P(y = 1|\boldsymbol{x}) = \frac{p_r(\boldsymbol{x})}{p_r(\boldsymbol{x}) + p_\theta(\boldsymbol{x})}.$$

Generator Logistic Objective = JS Divergence:

$\ell^*(\theta) = \mathbb{E}_{\tilde{p}_\theta(\boldsymbol{x}, y)}[y \ln q_\theta(\boldsymbol{x}) + (1 - y) \ln(1 - q_\theta(\boldsymbol{x}))]$

$= \text{JS}(p_r \parallel p_\theta) - \ln 2$.

Jensen-Shannon Divergence: $\text{JS}(p_r \parallel p_\theta) = \frac{1}{2} D_{\text{KL}}(p_r \parallel p_m) + \frac{1}{2} D_{\text{KL}}(p_\theta \parallel p_m), \quad p_m = \frac{p_r + p_\theta}{2}$.

Bounded: $0 \leq \text{JS}(p_r \parallel p_\theta) \leq \log 2$.

Jensen Inequality

If φ convex: $\varphi(\mathbb{E}[X]) \leq \mathbb{E}[\varphi(X)]$. If concave, other way around.

7.4.2 Training

Alternating SGD (heuristic, may diverge!). Training is **Saddle-point problem**, notoriously unstable!

JS Divergence Saturates when distributions don't overlap. If p_r and p_θ have disjoint supports: discriminator perfect, no gradient for generator!

Wasserstein Distance (Earth Mover's Distance):

$W(p_r, p_\theta) = \inf_{\gamma \in \Pi(p_r, p_\theta)} \mathbb{E}_{(\boldsymbol{x}, y) \sim \gamma} [\|\boldsymbol{x} - \boldsymbol{y}\|]$

Minimum total “work” to transport mass from p_r to p_θ . Provides meaningful gradients even without overlap.

Dual (Kantorovich-Rubinstein):

$$W(p_r, p_\theta) = \sup_{\|f\|_L \leq 1} \mathbb{E}_{\boldsymbol{x} \sim p_r} [f(\boldsymbol{x})] - \mathbb{E}_{\boldsymbol{x} \sim p_\theta} [f(\boldsymbol{x})].$$

Maximize gap between avg score of real vs fake samples w.r.t. Lipschitz constraint. Max achievable gap = Wasserstein distance.

WGAN uses critic f_w (not classical discriminator!):

$$\min_g \max_w \mathbb{E}_{\boldsymbol{x} \sim p_r} [f_w(\boldsymbol{x})] - \mathbb{E}_{\boldsymbol{z} \sim p_z} [f_w(G_\theta(\boldsymbol{z}))].$$

Enforcing Lipschitz:

- Weight clipping** (original): crude, problematic
- Gradient penalty:** add $\mathbb{E}_{\hat{\boldsymbol{x}}} [(\|\nabla_{\hat{\boldsymbol{x}}} f_w(\hat{\boldsymbol{x}})\|_2 - 1)^2]$

Mode Collapse: Generator produces only few samples that fool discriminator, ignoring full distribution diversity.

7.5 Diffusion Models

Forward process (fixed): Gradually add Gaussian noise over T steps until data becomes pure noise.

$$\text{Fwd step:} \quad q(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}) = \mathcal{N}(\boldsymbol{x}_t; \sqrt{1 - \beta_t} \boldsymbol{x}_{t-1}, \beta_t \boldsymbol{I}). \quad \text{Full fwd proces:} \quad q(\boldsymbol{x}_{1:T} \mid \boldsymbol{x}_0) = \prod_{t=1}^T q(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}).$$

Noise schedule: $\{\beta_t \in (0, 1)\}_{t=1}^T$ noise added at each step. **Define:** $\alpha_t = 1 - \beta_t$ and $\bar{\alpha}_t = \prod_{i=1}^t \alpha_i$.

Direct sampling (reparameterization trick):

$$q(\boldsymbol{x}_t \mid \boldsymbol{x}_0) = \mathcal{N}(\boldsymbol{x}_t; \sqrt{\bar{\alpha}_t} \boldsymbol{x}_0, (1 - \bar{\alpha}_t) \boldsymbol{I}). \quad \boldsymbol{x}_t = \sqrt{\bar{\alpha}_t} \boldsymbol{x}_0 + \sqrt{1 - \bar{\alpha}_t} \boldsymbol{\varepsilon}_0, \quad \boldsymbol{\varepsilon}_0 \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I}).$$

Reverse process (learned): Train NN to denoise step by step: $p_\theta(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t) = \mathcal{N}(\boldsymbol{x}_{t-1}; \mu_\theta(\boldsymbol{x}_t, t), \sigma_t^2 \boldsymbol{I})$.

For small β_t , the reverse $q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)$ is also Gaussian.

$\log p_\theta(\boldsymbol{x}_0)$ intractable, so derive **Variational Lower Bound (VLB)**: $-\log p_\theta(\boldsymbol{x}_0) \leq \mathcal{L}_{\text{VLB}} = \mathbb{E}_q \left[\log \frac{q(\boldsymbol{x}_{1:T} \mid \boldsymbol{x}_0)}{p_\theta(\boldsymbol{x}_{0:T})} \right]$. **Decomposition into 3 terms:** $\mathcal{L}_{\text{VLB}} = \underbrace{D_{\text{KL}}(q(\boldsymbol{x}_T|\boldsymbol{x}_0) \parallel p(\boldsymbol{x}_T))}_{L_T} +$

$$\sum_{t=2}^T \underbrace{\mathbb{E}_{q(\boldsymbol{x}_t|\boldsymbol{x}_0)} [D_{\text{KL}}(q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0) \parallel p_\theta(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t))]}_{L_{t-1}} - \underbrace{\mathbb{E}_{q(\boldsymbol{x}_1|\boldsymbol{x}_0)} [\log p_\theta(\boldsymbol{x}_0 \mid \boldsymbol{x}_1)]}_{L_0}$$

- L_T : Is $q(\boldsymbol{x}_T \mid \boldsymbol{x}_0) \approx \mathcal{N}(\mathbf{0}, \boldsymbol{I})$? Not optimized.
- L_{t-1} : Match learned reverse to true reverse
- L_0 : Reconstruction term

Tractable Reverse Posterior $q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0)$ is Gaussian with closed form (product of Gaussians): $q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0) = \mathcal{N}(\boldsymbol{x}_{t-1}; \mu_{q,t}(\boldsymbol{x}_t, \boldsymbol{x}_0), \sigma_t^2 \boldsymbol{I})$, with:

$$\mu_{q,t}(\boldsymbol{x}_t, \boldsymbol{x}_0) = \frac{1}{\sqrt{\bar{\alpha}_t}} \left(\boldsymbol{x}_t - \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t}} \boldsymbol{\varepsilon}_0 \right), \quad \sigma_t^2 = \frac{1 - \bar{\alpha}_{t-1}}{1 - \bar{\alpha}_t} \beta_t.$$

7.6 Noise Prediction Parameterization

Predict the **noise** $\boldsymbol{\varepsilon}_\theta(\boldsymbol{x}_t, t)$ instead of mean directly. Parameterize learned mean to mirror true posterior: $\mu_\theta(\boldsymbol{x}_t, t) = \frac{1}{\sqrt{\bar{\alpha}_t}} \left(\boldsymbol{x}_t - \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t}} \boldsymbol{\varepsilon}_\theta(\boldsymbol{x}_t, t) \right)$. Since both distributions are Gaussian with same variance: $D_{\text{KL}}(\mathcal{N}(\mu_q, \sigma^2 \boldsymbol{I}) \parallel \mathcal{N}(\mu_p, \sigma^2 \boldsymbol{I})) = \frac{1}{2\sigma^2} \|\mu_q - \mu_p\|^2$. This simplifies L_{t-1} to comparing noise: $L_{t-1} = \mathbb{E}_{\boldsymbol{x}_0, \boldsymbol{\varepsilon}_0} \left[\frac{(1 - \alpha_t)^2}{2\alpha_t(1 - \bar{\alpha}_t)^2} \|\boldsymbol{\varepsilon}_0 - \boldsymbol{\varepsilon}_\theta(\boldsymbol{x}_t, t)\|^2 \right]$.

$$\mathcal{L}_{\text{simple}} = \mathbb{E}_{t \sim [1, T], \boldsymbol{x}_0, \boldsymbol{\varepsilon}_0} [\|\boldsymbol{\varepsilon}_0 - \boldsymbol{\varepsilon}_\theta(\boldsymbol{x}_t, t)\|^2].$$

Training	Sampling
<ol style="list-style-type: none">Sample real image $\boldsymbol{x}_0 \sim q(\boldsymbol{x}_0)$ Sample random timestep $t \sim \text{Uniform}(\{1, \dots, T\})$ Sample noise $\boldsymbol{\varepsilon} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I})$ Compute noisy image: $\boldsymbol{x}_t = \frac{1}{\sqrt{\bar{\alpha}_t}} \boldsymbol{x}_0 + \sqrt{1 - \bar{\alpha}_t} \boldsymbol{\varepsilon}$ Grad step on $\nabla_\theta \ \boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_\theta(\boldsymbol{x}_t, t)\ ^2$	<ol style="list-style-type: none">Sample $\boldsymbol{x}_T \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I})$ For $t = T, \dots, 1$: $\boldsymbol{z} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I})$ if $t > 1$, else $\boldsymbol{z} = \mathbf{0}$ $\boldsymbol{x}_{t-1} = \frac{1}{\sqrt{\bar{\alpha}_t}} (\boldsymbol{x}_t - \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t}} \boldsymbol{\varepsilon}_\theta(\boldsymbol{x}_t, t)) + \sigma_t \boldsymbol{z}$ Return \boldsymbol{x}_0

Cosine noise schedule performs better than linear.

Used architecture is U-Net. **Input:** Noisy image \boldsymbol{x}_t + timestep t ; **Output:** Predicted noise $\boldsymbol{\varepsilon}_\theta(\boldsymbol{x}_t, t)$.

Model **conditional distribution** $p_\theta(\boldsymbol{x}_{0:T} \mid \boldsymbol{y})$ where \boldsymbol{y} is condition (class, text, image). Extend denoiser to take \boldsymbol{y} as input.

Latent Diffusion Models (LDM) run diffusion in **compressed latent space** instead of pixel space.

8 Tricks

Short Connections in DNs: Add less deep paths to a very deep network. **Residual** connections:

shortcut and add back in. **Skip** connections: concatenate.

For $y_1 = \alpha f(x, \Theta_1) + x$, $x \in \mathbb{R}^d$, $y_i \in \mathbb{R}^d$, $\Theta_i \in \mathbb{R}^{d \times d}$ and $y_{i \geq 2} = \alpha f(y_{i-1}, \Theta_i) + y_{i-1}$, $l = L(y_n)$ it holds that $\frac{\partial y_k}{\partial \Theta_k} = \alpha \frac{\partial f(y_{k-1}, \Theta_k)}{\partial y_{k-1}} + I_d$ and $\frac{\partial y_k}{\partial \Theta_k} = \alpha \frac{\partial f(y_{k-1}, \Theta_k)}{\partial \Theta_k}$. By applying the chain rule we have $\frac{\partial l}{\partial \Theta_k} = \frac{\partial L(y_n)}{\partial y_n} \frac{\partial y_n}{\partial y_{k-1}} \dots \frac{\partial y_{k+1}}{\partial y_k} \alpha \frac{\partial f(y_{k-1}, \Theta_k)}{\partial \Theta_k}$. Set $\alpha^2 = \frac{a}{n}$ for $a > 0$ s.t. $\lim_{n \rightarrow \infty} \mathbb{E}[\|y\|^2] < \infty$.

8.1 Weight Decay & Early Stopping

L2 regularization
 $\mathcal{R}_\Omega(\theta; \mathcal{S}) = \mathcal{R}(\theta; \mathcal{S}) + \Omega(\theta)$, $\Omega_\mu(\theta) = \frac{\mu}{2} \|\theta\|^2$, $\mu \geq 0$.
Only penalize weights, not biases. **GD upd w/ WD**: $\Delta \theta = -\eta \nabla \mathcal{R}(\theta) - \eta \nabla \Omega_\mu(\theta) = -\eta \nabla \mathcal{R}(\theta) - \eta \mu \theta$.

Geometric interpration (local quadratic approx): Regularized optimum: $\theta_\mu^* = (H + \mu I)^{-1} H \theta^*$, where $H = Q^\top \Lambda Q$ gives $\theta_\mu^* = Q \text{diag}\left(\frac{\lambda_i}{\lambda_i + \mu}\right) Q^\top \theta^*$.

$\lambda_i \gg \mu$: $\frac{\lambda_i}{\lambda_i + \mu} \approx 1 \rightarrow$ weak shrinkage (important dirs).
 $\lambda_i \ll \mu$: $\frac{\lambda_i}{\lambda_i + \mu} \approx 0 \rightarrow$ strong shrinkage (flat dirs).

Adaptively shrinks based on loss geometry, preserves important dirs, removes unnecessary complexity.

Early stopping: Rather than training to convergence, stop when validation performance plateaus. Analysis shows that this is approximately equivalent to L2 regularization. GD trajectories can be approximated as $\theta(k) = [I - (I - \eta \Lambda)^k] \theta^*$. For small step sizes, behaves like weight decay when $k = \frac{1}{\eta \mu}$.

L^1 regularized second-order approximation of an arbitrary loss function around optimal θ^* is $R_{L^1}(\theta) \approx R(\theta^*) + \frac{1}{2}(\theta - \theta^*)^\top H(\theta - \theta^*) + \lambda \|\theta\|_1$. Assuming $H = \text{diag}(h_1, \dots, h_d)$, we get $R_{L^1}(\theta) \approx \sum_{i=1}^d \left[\frac{h_i}{2} (\theta_i - \theta_i^*)^2 + \lambda |\theta_i| \right] + \text{const}$ so we need to minize $f(a) = \frac{1}{2}(a - b)^2 + \beta |a|$ and this gives $a^* = \text{sgn}(b) \max\{0, |b| - \beta\}$, so $\theta_i = \text{sgn}(\theta_i^*) \max\{0, |\theta_i^*| - \frac{\lambda}{h_i}\}$. For L^2 regularization we get $\theta_i = \frac{h_i}{h_i + \lambda} \theta_i^*$. **Connecting L^2 w early stopping**: $R(w) \approx R(w^*) + \frac{1}{2}(w - w^*)^\top H(w - w^*)$. $\nabla R(w) = H(w - w^*)$. GD update: $w^t = w^{t-1} - \eta H(w^{t-1} - w^*)$ gives $w^t - w^* = (I_d - \eta H)(w^{t-1} - w^*)$. Using $H = Q \Lambda Q^\top$: $Q^\top(w^t - w^*) = (I_d - \eta \Lambda) Q^\top(w^{t-1} - w^*)$. If $w^0 = 0$, $Q^\top(w^t - w^*) = (I_d - \eta \Lambda)^t Q^\top(0 - w^*) \Rightarrow Q^\top w^t = [I_d - (I_d - \eta \Lambda)^t] Q^\top w^*$. Optimal w under L^2 reg gives $Q^\top w = [I_d - \lambda(\Lambda + \lambda I_d)^{-1}] Q^\top w^*$. Matching both gives $t \approx \frac{1}{\eta \lambda}$. **Weight normalization** is like Batch-Norm, with the covariance matrix replaced by the identity matrix.

8.2 Ensemble Methods

Bagging: Create K bootstrap samples of Data (sampling with replacement), train separate models, and average predictions: $p(y|x) = \frac{1}{K} \sum_{k=1}^K p(y|x; \theta_k)$.

Dropout: Randomly drop units during training with probability $1 - \pi$. Creates an exponential ensemble of sub-networks sharing weights. Test time: Scale weights by π to approximate the ensemble average.

8.3 Normalization

Batch Norm: Normalize activations across mini-batch: $\tilde{z} = \frac{z - \mu_{\text{batch}}}{\sigma_{\text{batch}}}$, $\hat{z} = \alpha \tilde{z} + \beta$, $\mu_{\text{batch}} = \frac{1}{b} \sum_{i=1}^b z_i$, $\sigma_{\text{batch}} = \sqrt{\frac{1}{b} \sum_{i=1}^b (z_i - \mu_{\text{batch}})^2}$.
Layer Norm: Normalize features in a layer instead; particularly effective for RNNs (batch statistics are less stable).

8.4 Data / Task Augmentation

Augment Data by applying valid transformations. Semi-supervised Learning: Train jointly on labeled and unlabeled data w combined loss. Pre-training & Fine-tuning. Multi-task Learning. Self-supervised Learning: Create free supervision from data.

9 Recurrent Neural Networks

Evolution: $z_t = F[\theta](z_{t-1}, x_t)$, with $z_0 = 0$.
Optional output: $y_t = G[\theta](z_t)$.

Simple RNN: $z_t = \phi(W z_{t-1} + U x_t)$ where $W \in \mathbb{R}^{m \times m}$, $U \in \mathbb{R}^{m \times n}$

Backpropagation Through Time (param sharing): $\frac{\partial R}{\partial w_{ij}} = \sum_t \frac{\partial R}{\partial z_i^t} \cdot \dot{\phi}_i^t \cdot z_j^{t-1}$.
 $\frac{\partial R}{\partial u_{ik}} = \sum_t \frac{\partial R}{\partial z_i^t} \cdot \dot{\phi}_i^t \cdot x_k^t$; $\dot{\phi}_i^t = \phi'(F_i(z^{t-1}, x^t))$.

Gradient flow backward through time: $\nabla_{x_t} \mathcal{R} = \left[\prod_{\tau=t+1}^T W^\top S(z^\tau) \right] \cdot J_G \cdot \nabla_y \mathcal{R}$
Spectral analysis: $\|\prod W^\top S(z^\tau)\|_2 \leq [\sigma_{\max}(W)]^{s-t}$ **Root cause**: Repeated matmul through time.
 \Rightarrow Simple RNNs cannot learn long dependencies.

Deep RNNs stack layers vertically:
 $z^{t,\ell} = \varphi(W_\ell z^{t-1,\ell} + U_\ell z^{t,\ell-1})$ where $z^{t,0} = x_t$.

For RNN with $z_{t+1} = \varphi(U z_t + V x_{t+1})$, $L = \sum_{t=1}^T \ell(\hat{y}_t, y_t)$, where \hat{y}_t depends on z_t . Then $\frac{\partial L}{\partial U} = \sum_{t=1}^T \frac{\partial \ell}{\partial z_t} \cdot (\varphi'_t \cdot z_t)$, $\frac{\partial L}{\partial V} = \sum_{t=1}^T \frac{\partial \ell}{\partial z_t} \cdot (\varphi'_t \cdot x_{t+1})$.
Weight Sharing in RNNs (LSTM): $\frac{\partial L}{\partial W} = \sum_{t=1}^T \frac{\partial L}{\partial W_t}$.
Proof idea: Introduce dummy parameters $\tilde{W}_i = f(W)$ for each time step. By chain rule: $\frac{\partial L}{\partial W} = \sum_i \frac{\partial L}{\partial \tilde{W}_i} \frac{\partial \tilde{W}_i}{\partial W}$. With constraint $\tilde{W}_i = W$, we have $\frac{\partial \tilde{W}_i}{\partial W} = I$, giving the sum.
Initialization of bias in RNNs: Use 1.

9.1 Long Short-Term Memory (LSTM)

- C_t : cell state (internal memory, protected highway)
- z_t : hidden state (external output, filtered view)

$$C_t = \underbrace{\sigma(F \tilde{x}^t) \odot C_{t-1}}_{\text{forget}} + \underbrace{\sigma(G \tilde{x}^t) \odot \tanh(V \tilde{x}^t)}_{\text{input}}$$
$$z_t = \underbrace{\sigma(H \tilde{x}^t) \odot \tanh(C_t)}_{\text{output}}, \text{ where } \tilde{x}^t = [x_t, z_{t-1}].$$

9.2 Gated Recurrent Unit (GRU)

Single state z_t . Input: $\tilde{x}^t = [x_t, z_{t-1}]$.
 $u_t = \sigma(U \tilde{x}^t)$, $r_t = \sigma(R \tilde{x}^t)$,
 $z_t = u_t \odot z_{t-1} + (1 - u_t) \odot \tanh(W[r_t \odot z_{t-1}, x_t])$

Often comparable to LSTM with fewer resources. Gating creates identity paths \rightarrow better gradient flow.

9.3 Linear Recurrent Models

RNNs not parallelizable during training. LRU has linear dynamics: $z_{t+1} = A z_t + B x_t$. Diagonalize to $A = P \Lambda P^{-1}$, $\lambda_i \in \mathbb{C}$, change basis $\zeta_t = P^{-1} z_t$. Then: $\zeta_{t+1} = \Lambda \zeta_t + C x_t$. Each dimension evolves independently (no channel mixing). Compensate with expressive output: $y_t = \text{MLP}(\text{Re}(G z_t))$.

Stability: Require $\max |\lambda_j| \leq 1$ (spectral radius ≤ 1).

Parameterization: $\lambda_i = \exp(-\exp(\nu_i) + i \varphi_i)$ ensures $|\lambda_i| \in (0, 1)$ automatically, $|\lambda_i| \approx 1$: Long-term memory, $|\lambda_i| \approx 0$: Short-term patterns.
Provably universal as sequence-to-sequence map.

9.3.1 Connectionist Temporal Classification

Problem: Unsegmented sequences (e.g., speech).
Solution: RNN outputs prob distribution over vocabulary at each time step. Model all alignments with blank symbol ϵ . $p(\ell|x) = \sum_{\pi \in \mathcal{B}^{-1}(\ell)} \prod_t y_{\pi_t}$.
 \mathcal{B} removes blanks and repeated symbols.

9.4 Sequence Learning

Teacher Forcing: $p(y^t)$ depends on $y^{1:t-1}$ only through z^t , means during autoregressive generation, model doesn't see its own predictions.
Solution: Add feedback connections from y^{t-1} to z^t : $z^t = \text{RNN}(z^{t-1}, x^t, y^{t-1})$, now model conditions on its own previous predictions \rightarrow more coherent gen.

Professor Forcing: Train two networks (teacher-forced + free-running), discriminator matches hidden states \rightarrow improved generalization.

Exposure bias: Model relies on itself where inputs come from the previous output because of the non-availability of the ground truth.

Seq2Seq: Input and output sequences have different lengths: Use encoder-decoder framework.

Gradients in bi-directional RNNs are computed by making a forward and backward run, then at timestep t we combine (concatenate/add) and continue with the backpropagation. This happens at every bidirectional layer.

To initialize points uniformly on the unit ring in \mathbb{C} between circles of radii $r_2 > r_1$, sample from $\exp(\frac{1}{2} \log(u_1(r_2^2 - r_1^2) + r_1^2) + i 2\pi u_2)$ w $u_1, u_2 \sim \mathcal{U}(0, 1)$.

10 Attention and Transformers

Seq2Seq with Attention: Encoder generates hidden state sequence. Decoding RNNs output attends to encoder states and gets used as input in next step.

Attention: Learn to index, multiplicative gating to combine bottom-up and top-down information.
KV - attention map:
 $F(\xi, ((x_1, z_1), \dots, (x_s, z_s))) = [z_1, \dots, z_s]$.
 $f(\xi, (x_1, \dots, x_s))$ consisting of a query ξ (what to look for?), keys x_i (index) and values z_i .

Scaled Dot-Product Attention: $f(\xi, x) = \frac{\xi \cdot x}{\sqrt{n}}$

Multi-headed attention:
 $G(\xi, (x^t, z^t)_{t=1}^s) = W \begin{bmatrix} F_1(\xi, (x^t, z^t)) \\ \vdots \\ F_h(\xi, (x^t, z^t)) \end{bmatrix}$,

where
 $F_j(\xi, (x^t, z^t)) = F(W_j^q \xi, (W_j^k x^t, W_j^v z^t))$.

Attention(Q, K, V) = $\text{softmax}\left(\frac{QK^\top}{\sqrt{d_k}}\right)V$,
where
 $Q = XW_Q$, $K = XW_K$, $V = XW_V$ and
 $X \in \mathbb{R}^{T \times d_{\text{model}}}$, $W_Q, W_K \in \mathbb{R}^{d_{\text{model}} \times d_k}$, $W_V \in \mathbb{R}^{d_{\text{model}} \times d_v}$, $Q, K \in \mathbb{R}^{T \times d_k}$, $V \in \mathbb{R}^{T \times d_v}$.

Positional encodings necessary since no use of recurrence. Can use predefined approaches, or learned.

Self attention used in encoder, masked self-attention in decoder. Can also add cross-attention to decoder.

ELMo consists of multiple layers of 2 LSTMs working in opposite directions. Can then be used to collapse all layers $2L + 1$ and train in task-specific manner.

BERT is trained on two simultaneous tasks (Masked Language Modeling and Binary Prediction whether sentence B follows A). Has bidirectional encoder, and task-specific heads. Can do FT for various tasks.

Vision Transformers split images into patches, add pos embeddings and a [CLS] token, then process with a standard transformer encoder.

Complexity metrics for different layer types in terms of input sequence length n .

Key Metrics:
• **Complexity per Layer**: Total computational operations per layer
• **Sequential Operations**: Number of operations needed to connect any two input positions
• **Maximum Path Length**: Longest path between any two input positions in the network

Self-Attention:
• Complexity per Layer: $\mathcal{O}(n^2 d)$ — quadratic in sequence length due to all-pairs attention
• Sequential Operations: $\mathcal{O}(1)$ — fully parallelizable
• Maximum Path Length: $\mathcal{O}(1)$ — direct connections between all positions

RNN:
• Complexity per Layer: $\mathcal{O}(nd^2)$ — linear in sequence length
• Sequential Operations: $\mathcal{O}(n)$ — must process sequentially
• Maximum Path Length: $\mathcal{O}(n)$ — information flows through entire sequence

Trade-off: Self-attention enables parallel processing and direct long-range connections but has quadratic complexity, while RNNs have linear complexity but require sequential processing.

11 Ethics

Adversarial examples (given $f(x) = y$ correctly):
• Untargeted: $|\delta| \leq \epsilon$ s.t. $f(x + \delta) \neq y$.
• Optimize $\max_{|\delta| \leq \epsilon} L(f(x + \delta), y)$.
• Targeted: $|\delta| \leq \epsilon$ s.t. $f(x + \delta) = t \neq y$.
• Optimize $\min_{|\delta| \leq \epsilon} L(f(x + \delta), t)$.

Linear Binary ($y \in \{-1, 1\}$, $f(x) = w^\top x + b$):
Correct: $y(w^\top x + b) > 0$.
Adv. flips when $yw^\top \delta \leq -y(w^\top x + b)$ cross hyperplane. **L2 optimal**: $\delta^* = \frac{-w^\top x + b}{\|w\|_2^2} w$, $\|\delta^*\|_2 = \frac{|w^\top x + b|}{\|w\|_2}$.
Multi-class: $f_k(x) = w_k^\top x + b_k$, use $\text{argmax}_k f_k(x)$.
Margin to class j : $m_j(x) = (w_j - w_{j'})^\top x + (b_j - b_{j'})$.
 $f_{y_j}(x) = f_j(x) \Leftrightarrow m_j(x) = 0$. **Correct** if $f_{y_j}(x) > f_j(x) \forall j \neq y$, **adversarial** if $\exists j \neq y$ s.t. $f_{y_j}(x + \delta) < f_j(x + \delta)$. Distance to boundary: $\frac{m_{j^*}(x)}{\|w_{j^*} - w_{j^*'}\|_2}$.
Adversarial attacks for NNs: Approximate boundary by $f(x + \delta) \approx f(x) + \nabla f(x)^\top \delta$. **FGSM** is a one-step L_∞ attack: $\delta = \epsilon \text{sign}(\nabla_x L(f(x), y))$. **PGD** is multi-step $\delta_{t+1} = \text{Proj}_{|\delta| \leq \epsilon}(\delta_t + \alpha \text{sign}(g_t))$.
Distributionally Robust Optimization:
 $\min_y \sup_{Q \in \mathcal{U}(P)} E_Q[L(f(x))]$, where U means close. Can use upper bound on Wasserstein distance e.g.
Robust training $\min_y \mathbb{E}[\max_{k \in S} L(f(x + \delta), y)]$.
Adversarial training can be viewed as robustness to distribution shift measured by Wasserstein distance.
Interpretability: Local - explain pred for specific x , Global - explain model behaviour on avg over data.

Local: Ceteris paribus (vary x_j , fix x_{-j}). Sensitivity ($\partial_{x_j} f(x)$), missing info ($f(x) - \mathbb{E}[f(X) | X_{-j} = x_{-j}]$). **Global**: Mutual info ($I(X_j; Y | \{X_{-j}\})$). Predictive util (train f w/ and w/o x_j). For log-loss predictive util \approx conditional mutual information.

SHAP attributes predictions, while SAGE attributes risk reduction.
A protected attribute, Y target outcome, \hat{Y} prediction. Demographic Parity: $\hat{Y} \perp A$; Equalized Odds: $\hat{Y} \perp A | Y$, Equality of Opportunity: $\hat{Y} \perp A | Y = 1$.