

1 Connectionism

1.1 Perceptron

Threshold Unit $f[w, b](x) = \text{sign}(x \cdot w + b)$ with
Dec. Boundary $x \cdot w + b = 0 \Leftrightarrow \frac{x \cdot w}{\|w\|} + \frac{b}{\|w\|} = 0$.

Geometric Margin $\gamma[w, b](x, y) = \frac{y(x \cdot w + b)}{\|w\|}$.

Maximum Margin Classifier

$(w^*, b^*) \in \arg\max_{w, b} \gamma[w, b](\mathcal{S})$,
with $\gamma[w, b](\mathcal{S}) := \min_{(x, y) \in \mathcal{S}} \gamma[w, b](x, y)$.

Perception Learning

If $f[w, b](x) \neq y$: update $w += yx$, and $b += y$.

$w_t \in \text{span}(x_1, \dots, x_s) \Rightarrow w_t \in \text{span}(x_1, \dots, x_s) \forall t$.

Convergence

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

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 (general position).

$$C(s+1, n) = 2 \sum_{i=0}^{n-1} \binom{s}{i}, C(s, n) = 2^s \text{ for } s \leq n.$$

Phase transition at $s = 2n$. For $s < 2n$ empty version space is the exception, otherwise the rule.

1.1.1 Hopfield Networks

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

Hebbian Learning

Choose patterns $\{x\}_{t=1}^s \in \{\pm 1\}^n$, build 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: $s_{\max} \approx 0.138n$.

1.2 Feedforward Networks

1.2.1 Linear Models

Linear regression (MSE)
 $L[w](X, y) = \frac{\|Xw - y\|^2}{2n}$, $\nabla L = \frac{X^\top Xw - X^\top y}{n}$.

Moore-Penrose inverse solution

$w^* = X^*y \in \text{argmin}_w L[w](X, y)$, where $X^* = \lim_{\delta \rightarrow 0} (X^\top X + \delta I)^{-1} X^\top$ Moore-Penrose inverse.

Stochastic gradient descent update

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

Gaussian noise model

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

Ridge regression

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

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 CE loss: $L[w] = \frac{1}{n} \sum_{i=1}^n \ell_i(y_i, w^\top x_i), \nabla \ell_i = [\sigma(w^\top x_i) - y_i] x_i$.

1.2.2 Feedforward Networks

Generic feedforward layer definition

$$F : \mathbb{R}^{m(n+1)} \times \mathbb{R}^n \rightarrow \mathbb{R}^m,$$

$$F[\theta](x) := \varphi(Wx + b), \theta := \text{vec}(W, b)$$

Composition of layers

$$G = F^{L[\theta_L]} @ \dots @ F^1[\theta^1]$$

where $F^{l[W^l, b^l]}(x) := \varphi^{l(W^l x + B^l)}$

Layer activations

$$x^l := (F^l @ \dots @ F^1)(x) = F^{l(x^{l-1})}$$

identifying $x^0 = x$, $x^L = F(x)$

Softmax function

$$\text{softmax}(z)_i = \frac{e^{z_i}}{\sum_j e^{z_j}}$$

$$\text{softmax}(A)_{ij} = \frac{e^{A_{ij}}}{\sum_k e^{A_{ik}}}$$

$$\ell(y, z) = \frac{-z_y + \log \sum_j e^{z_j}}{\ln 2}$$

Residual layer definition

$$F[W, b](x) = x + (\varphi(Wx + b) - \varphi(0))$$

therefore $F[0, 0] = \text{id}$

Skip connection: Concatenate previous layer back in

1.2.3 Sigmoid Networks

Sigmoid activation

$$\varphi(z) := \sigma(z) = \frac{1}{1+e^{-z}}$$

Hyperbolic tangent activation

$$\tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}} = 2\sigma(2z) - 1$$

$$\tanh'(z) = 1 - \tanh^2(z)$$

Baron's Theorem: Approximation error

For f with finite $C_f := \int \|\omega\| |\hat{f}(\omega)| d\omega < \infty$ there exists MLP g with one hidden layer of width m that:
 $\int_B (f(x) - g_{m(x)})^2 \mu(dx) \leq O(\frac{1}{m})$

1.2.4 ReLU Networks

ReLU activation

$$\varphi(z) := (z)_+ := \max\{0, z\}$$

ReLU networks are universal function approximators

Zalabsky: Connected regions

$$R(H) \leq \sum_{i=0}^{\min\{n, m\}} \binom{m}{i} := R(m)$$

Montufar: Connected regions in ReLU network

$$R(m, L) \geq R(m) \left(\frac{m}{n}\right)^{n(L-1)}, L: \text{layers}, m: \text{width}$$

1.3 Gradient-Based Learning

1.3.1 Backpropagation

Parameter derivatives for ridge function layers

$$\begin{aligned} \frac{\partial x_i^l}{\partial w_{ij}^l} &= \dot{\varphi}_i^l x_j^{l-1}, \\ \dot{\varphi}_i^l &:= \dot{\varphi}^l \left((w_i^l)^\top x^{l-1} + b_i^l \right) \\ \frac{\partial x_i^l}{\partial b_i^l} &= \dot{\varphi}_i^l \end{aligned}$$

Loss derivatives

$$\begin{aligned} \frac{\partial h[\theta](x, y)}{\partial w_{ij}^l} &= \frac{\partial h^{l[\theta]}(x^l, y)}{\partial x_i^l} \frac{\partial x_i^l}{\partial w_{ij}^l} = \delta_i^l \dot{\varphi}_j^l x_j^{l-1}, \\ \frac{\partial h[\theta](x, y)}{\partial b_i^l} &= \frac{\partial h^{l[\theta]}(x^l, y)}{\partial x_i^l} \frac{\partial x_i^l}{\partial b_i^l} = \delta_i^l \dot{\varphi}_i^l \end{aligned}$$

with $\delta_i^l = \frac{\partial h}{\partial x_i^l} \dot{\varphi}_i^l$

1.3.2 Gradient Descent

Gradient descent update

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

Gradient flow ODE

$$d \frac{\theta}{dt} = -\nabla h(\theta)$$

L-smoothness

$$\|\nabla h(\theta_1) - \nabla h(\theta_2)\| \leq L \|\theta_1 - \theta_2\| \text{ (forall } \theta_1, \theta_2)$$

$$\lambda_{\max}(\nabla^2 h) \leq L$$

$$\ell(w) - \ell(w') \leq \nabla \ell(w')^\top (w - w') + \frac{L}{2} \|w - w'\|^2$$

$$\ell''(x) \leq L$$

Polyak-Lojasiewicz condition

$$\frac{1}{2} \|\nabla h(\theta)\|^2 \geq \mu(h(\theta) - \min h) \text{ (forall } \theta)$$

Convergence rate

$$\eta = \frac{1}{L}$$

$$\Delta t = \frac{2L}{\varepsilon^2} (h(\theta_0) - \min h) \text{ for } \varepsilon\text{-critical point}$$

$$\Delta h(\theta_t) - \min h \leq (1 - \frac{\mu}{L})^t (h(\theta_0) - \min h)$$

1.3.3 Acceleration and Adaptivity

Heavy ball momentum update

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

Nesterov acceleration

$$\tilde{\theta}_{t+1} = \theta_t + \beta(\theta_t - \theta_{t-1})$$

$$\theta_{t+1} = \tilde{\theta}_{t+1} - \eta \nabla h(\tilde{\theta}_{t+1})$$

More theoretical grounding than heavy ball

AdaGrad updates

$$\theta_{i,t+1} = \theta_{i,t} - \eta_i^t \frac{\partial h}{\partial \theta_i}(\theta_t),$$

$$\gamma_i^t = \gamma_i^{t-1} + \left(\frac{\partial h}{\partial \theta_i}(\theta_t) \right)^2,$$

$$\eta_i^t = \frac{\eta}{\sqrt{\gamma_i^t + \delta}}$$

Adam updates

$$g_i^t = \beta g_i^{t-1} + (1 - \beta) \frac{\partial h}{\partial \theta_i}(\theta_t)$$

$$\gamma_i^t = \alpha \gamma_i^{t-1} + (1 - \alpha) \left(\frac{\partial h}{\partial \theta_i}(\theta_t) \right)^2$$

$$\theta_{i,t+1} = \theta_{i,t} - \eta_i^t g_i^t, \eta_i^t := \frac{\eta}{\sqrt{\gamma_i^t + \delta}}$$

RMSprop

Adam without momentum term

1.3.4 Stochastic Gradient Descent

Stochastic gradient descent update
 $\theta_{t+1} = \theta_t - \eta \nabla h(\theta_t)(x_{i_t}, y_{i_t})$

SGD variance

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

SGD convergence rate

$$E[h(|\theta_t|)] - \min h \leq O\left(\frac{1}{\sqrt{t}}\right) \text{ (general)}$$

$$E[h(|\theta_t|)] - \min h \leq O\left(\log \frac{t}{\epsilon}\right) \text{ (strongly convex)}$$

$$E[h(|\theta_t|)] - \min h \leq O\left(\frac{1}{t}\right) \text{ (additionally smooth)}$$

1.3.5 Function Properties

Convexity

$$\ell(\lambda w + (1-\lambda)w') \leq \lambda \ell(w) + (1-\lambda)\ell(w')$$

$$\ell''(x) \geq 0 \text{ forall } x$$

Convexity and differentiability

$$\ell(w) \geq \ell(w') + \nabla \ell(w')^\top (w - w')$$

Implies convexity for differentiable functions and vice versa

Strong convexity and differentiability

$$\ell(w) \geq \ell(w') + \nabla \ell(w')^\top (w - w') + \frac{\mu}{2} \|w - w'\|^2$$

$$\ell''(x) \geq \mu \text{ forall } x$$

1.4 Convolutional Networks

1.4.1 Convolutions

Convolution definition

$$(f * g)(u) := \int_{-\infty}^{\infty} g(u-t) f(t) dt = \int_{-\infty}^{\infty} f(u-t) g(t) dt$$

Fourier transform convolution property

$$F(f * g) = F(f) * F(g)$$

Discrete convolution

$$(f * g)[u] := \sum_{t=-\infty}^{\infty} f[t] g[u-t]$$

Cross-correlation

$$(g \star f)[u] := \sum_{t=-\infty}^{\infty} g[t] f[u+t]$$

Toepplitz matrices

$$(f * g) = \text{Toeplitz-Matrix}(g)f$$

1.4.2 Convolutional Networks

Conventions

Padding: Add zeros around input
Stride: Step size of convolution

Max-Pooling

Take maximum value in windows (size r)

ConvNets for Images

$$y[r][s, t] = \sum_u \sum_{\Delta s, \Delta t} w[r, u][\Delta s, \Delta t] * x[u][s + \Delta s, t + \Delta t]$$

$\Delta s, t + \Delta t]$ r : output channel, u : input channel**Number of parameters of a convolutional layer**

$D = (|r| * |u|) * (|\Delta s| * |\Delta t|)$

fully connected · window size

1.4.3 Natural Language Processing with ConvNets**Word embedding**

$\Omega : w \mapsto x_w \in \mathbb{R}^n$

Conditional log-bilinear modelPrediction of output word μ given word w in neighborhood

$P(\mu | w) = \frac{\exp(x_w^\top y_\mu)}{\sum_\mu} \exp(x_w^\top y_\mu)$

$$\begin{aligned} h(\{x_w\}, \{y_\mu\}) &= \sum_{(w,\mu)} \ell_{w\mu} \\ \ell_{w,\mu} &= -x_w^\top y_\mu + \ln \sum_\mu \exp(x_w^\top y_\mu) \end{aligned}$$

Negative sampling

$\tilde{\ell}_{w,\mu} = -\ln \sigma(x_w^\top y_\mu) - \beta E_{\mu \sim D} \ln(1 - \sigma(x_w^\top y_\mu))$

1.5 Recurrent Networks**1.5.1 Simple Recurrent Networks****Time evolution equation**

$z_t := F[\theta](z_{t-1}, x_t), z_0 := 0 \text{ (forall } t)$

Output map

$\hat{y}_t := G[\xi](z_t)$

RNN parameterization

$$\begin{aligned} F[U, V](z, x) &:= \varphi(Uz + Vx) \\ G[W](z) &:= \psi(Wz), W \in \mathbb{R}^{q \times m} \end{aligned}$$

Backpropagation through time

$$\begin{aligned} \frac{\partial h}{\partial z_i^s} &= \sum_{s=t}^T \delta_k^s \sum_{j=1}^m \frac{\partial \dot{y}_k^s}{\partial z_j^s} \frac{\partial z_j^s}{\partial z_i^t}, \\ \frac{\partial \dot{y}_k^s}{\partial z_i^t} &= \dot{\psi}_k^s w_{kj} \\ \frac{\partial h}{\partial v_{ij}} &= \sum_{t=1}^T \frac{\partial h}{\partial z_i^t} \dot{\varphi}_i^t x_j^t \\ \frac{\partial h}{\partial u_{ij}} &= \sum_{t=1}^T \frac{\partial h}{\partial z_i^t} \dot{\varphi}_i^t z_j^{t-1} \end{aligned}$$

Spectral norm

$\|A\|_2 = \max_{x: \|x\|=1} \|Ax\|_2 = \sigma_1(A)$

Gradient norms

$\frac{\partial z^T}{\partial z^0} = \Phi^T U * \dots * \Phi^1 U$

The norm of gradients either:

1. Vanishes exponentially if $\sigma_1(U) < \frac{1}{|\alpha|}$: $\left\| \frac{\partial z^t}{\partial z^0} \right\|_2 \leq ((|\alpha| \sigma_1(U))^t \rightarrow \infty$ 2. Explodes if $\sigma_1(U)$ is too large**Bidirectional RNNs**

$\hat{y}_t = \psi(Wz_t + \tilde{W}\tilde{z}_t)$

1.5.2 Gated Memory**LSTM**

$$\begin{aligned} z_t &:= \sigma(F\tilde{x}_t) * z_{t-1} + \sigma(G\tilde{x}_t) * \tanh(V\tilde{x}_t) \\ \tilde{x}_t &:= \text{mat}(x_t; h_t), h_{t+1} = \sigma(H\tilde{x}_t) * \tanh(Uz_t) \end{aligned}$$

GRU

$$\begin{aligned} z_t &= (1 - \sigma) * z_{t-1} + \sigma * \tilde{z}_t, \\ \sigma &:= \sigma(G[x_t, z_{t-1}]) \\ \tilde{z}_t &:= \tanh(V[r_t * z_{t-1}, x_t]) \\ r_t &:= \sigma(H[z_{t-1}, x_t]) \end{aligned}$$

1.5.3 Linear Recurrent Models**Linear state evolution**

$z_{t+1} = Az_t + Bx_t$

Diagonal form

$A = P\Lambda P^{-1}, \Lambda := \text{diag}(\lambda_1, \dots, \lambda_m), \lambda_i \in \mathbb{C}$

Stability condition

$\max_j |\lambda_j| \leq 1$

Initialization

$$\begin{aligned} \lambda_i &= \exp(-\exp(\kappa_i) + i\varphi_i), \\ e^{\kappa_i} &= -\ln r_i \\ \varphi_i &\sim \text{Uni}[0; 2\pi], r_i \sim \text{Uni}[I], I \subset [0; 1] \end{aligned}$$

Advantages

- (i) clear modeling of long/short range dependencies
- (ii) no channel mixing required
- (iii) parallelizable training

1.6 Attention and Transformers**1.6.1 Attention****Attention mixing**

$$\begin{aligned} \xi_s &:= \sum_t \alpha_{st} Wx_t, \alpha_{st} \geq 0, \sum_t \alpha_{st} = 1 \\ A &= (a_{st}) \in \mathbb{R}^{T \times T}, \text{s.t. } \Xi = WXA^\top \end{aligned}$$

Query-key matching

$$\begin{aligned} Q &= U_Q X, K = U_K X \\ (U_Q, U_K &\in \mathbb{R}^{q \times n}) \\ Q^\top K &= X^\top U_Q^\top U_K X \text{ rank } \leq q \\ (Q^\top K) &\in \mathbb{R}^{T \times T} \end{aligned}$$

Softmax attention

$$\begin{aligned} A &= \text{softmax}(\beta Q^\top K), \\ a_{st} &= \frac{e^{\beta [Q^\top K]_{st}}}{\sum_r e^{\beta [Q^\top K]_{sr}}} \text{ usually } \beta = \frac{1}{\sqrt{q}} \end{aligned}$$

Feature transformation

$$\begin{aligned} X &\mapsto \Xi \mapsto F(\Xi), \\ F(\theta)(\Xi) &= (F(\xi_1), \dots, F(\xi_T)) \end{aligned}$$

Positional encoding

$$\begin{aligned} p_{tk} &= \text{cases}(\sin(t\omega_k), k \text{ even}; \cos(t\omega_k), k \text{ odd}), \\ \omega_k &= C^k \end{aligned}$$

Transformer architecture

Self-attention: attend to its own values in the past

Cross-attention: E.g. decoder attends to encoder output (query from decoder, key and value from encoder)

Vision transformer patch embedding

$$\mathbb{R}^{p \times p \times q} \ni \text{patch}_t \mapsto x_t := V \text{ vec}(\text{patch}_t) \in \mathbb{R}^n \text{ with } V \in \mathbb{R}^{n \times (qp^2)}$$

GELU activation

$\varphi(z) = z \text{ Prob}(z \leq Z), Z \sim \mathcal{N}(0, 1)$

1.7 Geometric Deep Learning**1.7.1 Sets and Points****Function over sets**

$\{x_1, \dots, x_M\} \subset \mathbb{R}, f: 2^{\mathbb{R}} \rightarrow Y$

Order-invariance property

$f(x_1, \dots, x_M) = f(x_{\pi(1)}, \dots, x_{\pi(M)}) \text{ forall } \pi \in S_M$

Equivariance property

$$\begin{aligned} f(x_1, \dots, x_M) &= (y_1, \dots, y_M) \\ f(x_{\pi(1)}, \dots, x_{\pi(M)}) &= (y_{\pi(1)}, \dots, y_{\pi(M)}) \end{aligned}$$

Permutation invariant sum

$\sum_{m=1}^M x_m = \sum_{m=1}^M x_{\pi(m)}, \text{ forall } M, \text{ forall } \pi \in S_M$

Deep Sets model

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

Max pooling variant

$f(x_1, \dots, x_M) = \rho\left(\max_{m=1}^M \varphi(x_m)\right)$

Equivariant map construction

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

1.7.2 Graph Convolutional Networks**Feature and adjacency matrices**

$$X = \text{mat}(x_1^\top; \dots; x_M^\top), A = (a_{nm}) \text{ with } a_{nm} = \text{cases}(1, \text{if } \{v_n, v_m\} \in E; 0, \text{otherwise})$$

Permutation matrix constraints

$$\begin{aligned} P &\in \{0, 1\}^{M \times M} \text{ s.t.} \\ \sum_{n=1}^M p_{nm} &= \sum_{n=1}^M p_{mn} = 1 \text{ (forall } m) \end{aligned}$$

Graph invariance definition

$f(X, A) \neq f(PX, PAP^\top), \text{ forall } P \in \Pi_M$

Graph equivariance definition

$f(X, A) \neq Pf(PX, PAP^\top), \text{ forall } P \in \Pi_M$

Node neighborhood features

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

Message passing scheme

$\varphi(x_m, X_m) = \varphi(x_m, m_{X_m} \psi(x))$

 m is a permutation-invariant operation**Normalized adjacency matrix**

$|A| = D^{-\frac{1}{2}}(A + I)D^{-\frac{1}{2}}$

$D = \text{diag}(d_1, \dots, d_M), d_m = 1 + \sum_{n=1}^M a_{nm}$

GCN layer

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

Two-layer GCN

$Y = \text{softmax}(|(A)(|(A)XW^0|)W^1|)$

1.7.3 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

$L = D - A, (Lx)_n = \sum_{m=1}^M a_{nm}(x_n - x_m)$

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

$L = D - A = U\Lambda U^\top,$

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

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

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

Polynomial kernel network layer

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

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

1.7.4 Attention GNNs**Attention coupling matrix**

$Q = (q_{ij}),$

$q_{ij} = \text{softmax}(\rho(u^\top (Vx_i; Vx_j; x_{ij})))$

$\text{s.t. } \sum_j A_{ij} q_{ij} = 1$

Attention propagation

$X^+ = \sigma(QXW)$

Weisfeiler-Lehman test**1.8 Tricks of the Trade****1.8.1 Initialization****Random initialization**

$\theta_i^0 \sim \mathcal{N}(0, \sigma_i^2), \text{ or}$

$\theta_i^0 \sim \text{Uniform}(-\sqrt{3}\sigma_i; \sqrt{3}\sigma_i)$

LeCun initialization

$w_{ij} \sim \text{Uniform}[-a; a], a := \frac{1}{\sqrt{n}}, b_i = 0$

Stabilizes variance

Glorot initialization

$$w_{ij} \sim \text{Uniform}[-\sqrt{3}\gamma; \sqrt{3}\gamma],$$

$$\gamma := \frac{2}{n+m}$$

Stabilizes variance of gradients in backpropagation

He initialization

$$w_{ij} \sim N(0, \gamma) \text{ or } w_{ij} \sim \text{Uniform}[-\sqrt{3}\gamma; \sqrt{3}\gamma],$$

$$\gamma := \frac{2}{n}$$

In ReLU networks typically only $\frac{n}{2}$ units active

Orthogonal initialization

$$\frac{1}{\sqrt{m}} W \sim \text{Uniform}(O(m))$$

$$\text{s.t. } W^\top W = WW^\top = mI$$

1.8.2 Weight Decay

L2 regularization

$$\Omega_{\mu(\theta)} = \frac{\mu}{2} \|\theta\|^2, \mu \geq 0$$

Gradient descent with weight decay

$$\Delta \theta = -\eta \nabla E(\theta) - \eta \nabla \Omega_{\mu(\theta)} = -\eta \nabla E(\theta) - \eta \mu \theta$$

Weight decay for multiple layers

$$\theta = (\text{vec}(W^1), \text{vec}(W^2), \dots, \text{vec}(W^L)),$$

$$\Omega_{\mu(\theta)} = \sum_{l=1}^L \mu_l \|W^l\|_F^2$$

Local loss landscape

$$\theta^* = (H + \mu I)^{-1} H \theta^*, H = Q^\top \Lambda Q$$

$$(\Lambda + I)^{-1} \Lambda = \text{diag}\left(\frac{\lambda_i}{\lambda_i + \mu}\right)$$

The minimum θ^* is shrunk along directions with small eigenvalues

Generalization

$$\mu = \frac{\sigma^2}{u^2}, u: \text{teacher "sign"al}$$

Optimal weight decay inverse proportional to the "sign"al-to-noise ratio

1.8.3 Dropout

Probability φ_i of keeping a unit

Dropout as Ensembling

$$p(y | x) = \sum_{b \in \{0,1\}^R} p(b)p(y | x; b)$$

$$\text{with } p(b) = \prod_{i=1}^R \varphi_i^{b_i} (1 - \varphi_i)^{1-b_i}$$

Weight scaling for inference

$$\tilde{w}_{ij} \leftarrow \varphi_j w_{ij}$$

1.8.4 Normalization

Batch normalization

E and V from minibatches or population statistics

$$|(f) = \frac{f - E[f]}{\sqrt{V[f]}}, E[|(f)] = 0, V[|(f)] = 1$$

$$|(f)[\mu, \gamma] = \mu + \gamma |(f)$$

Weight normalization

$$f(v, \gamma)(x) = \varphi(w^\top x), w := \frac{\gamma}{\|v\|_2} v$$

Gradient descent with respect to decoupled γ and v :

$$\frac{\partial E}{\partial \gamma} = \nabla_w E * \frac{v}{\|v\|_2}$$

$$\nabla_v E = \frac{\gamma}{\|v\|} \left(I - \frac{ww^\top}{\|w\|^2} \right) \nabla_w E$$

Layer normalization

$$\tilde{f}_i = \frac{f_i - E[f]}{\sqrt{V[f]}},$$

$$E[f] = \frac{1}{m} \sum_{i=1}^m f_i$$

$$V[f] = \frac{1}{m} \sum_{i=1}^m (f_i - E[f])^2$$

Using population averages across units in a layer

1.8.5 Model Distillation

Tempered cross entropy loss for distillation

$$\ell(x) = \sum_{y=1}^K \frac{\exp\left[\frac{F_y(x)}{T}\right]}{\sum_{\mu=1}^K \exp\left[\frac{F_\mu(x)}{T}\right]} \left[\frac{1}{T} G_{y(x)} - \ln \sum_{\mu=1}^K \exp\left[\frac{G_\mu(x)}{T}\right] \right]$$

$T > 0$, F_y : teacher logits, G_y : student logits

Gradient of distillation loss

$$\frac{\partial \ell}{\partial G_y} = \frac{1}{T} \left[\frac{e^{\frac{F_y}{T}}}{\sum_\mu e^{\frac{F_\mu}{T}}} - \frac{e^{\frac{G_y}{T}}}{\sum_\mu e^{\frac{G_\mu}{T}}} \right]$$

1.9 Theory

1.9.1 Neural Tangent Kernel

Linearized DNN taylor approximation

$$h(\beta)(x) = f(x) + \beta * \nabla f(x)$$

with $\beta \approx \theta - \theta_0$, $f(x) := f(\theta_0)(x)$

Kernel of gradient feature maps

$$k(x, \xi) = \nabla f(x) * \nabla f(\xi), \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$$

Dual representation

$$h(\alpha)(x) = f(x) + \sum_{i=1}^s \alpha_i \nabla f(x_i) * \nabla f(x)$$

Squared loss

$$E(\alpha) = \frac{1}{2s} \sum_{i=1}^s \left(\sum_{j=1}^s \alpha_j \nabla f(x_j) * \nabla f(x_i) + f(x_i) - y_i \right)^2$$

Optimal solution of linearized DNN

$$K = [k(x_i, x_j)]_{i,j=1}^n \in \mathbb{R}^{n \times n}$$

$$\alpha^* = K^+(y - f),$$

$$h^{*(x)} = k(x)K^+(y - f)$$

Neural Tangent Kernel NTK

$$k(\theta)(x, \xi) := \nabla f(\theta)(x) * \nabla f(\theta)(\xi)$$

Quadratic loss

$$E(\theta) = \frac{1}{2} \|f(\theta) - y\|^2, y := (y_1, \dots, y_s)^\top$$

Gradient flow ODE

$$\dot{\theta} := d\frac{\theta}{dt} = \sum_{i=1}^s (y_i - f_{i(\theta)}) \nabla f_{i(\theta)}$$

Functional gradient flow

$$\dot{f}_j = \nabla f_j * \theta = \sum_{i=1}^s (y_i - f_i) k(\theta)(x_i, x_j)$$

$$f = K(\theta)(y - f)$$

Infinite width limit

$$w_{ij}^l = \frac{\sigma_w}{\sqrt{m_l}} \varepsilon_{ij}^l,$$

$$b_i^l = \frac{\sigma_b}{\sqrt{m_l}} \beta_i^l,$$

$$\varepsilon_{ij}^l, \beta_i^l \sim N(0, 1)$$

$$k(\theta) \rightarrow k_\infty \text{ for } m_l \rightarrow \infty$$

Initial NTK converges to deterministic limit

NTK constancy

$$d\frac{k(\theta(t))}{dt} t = 0$$

$$f_{\infty(x)} = k(x)K^+(y - f), k = k_\infty$$

NTK remains constant when training in infinite width limit

Vanishing curvature

$$\frac{\|\nabla^2 f(\theta_0)\|_2}{\|\nabla f(\theta_0)\|_2} \ll 1$$

Near-constancy

$$\|k(\theta_0) - k(\theta_t)\|_F \in O\left(\frac{1}{m}\right), m = m_1 = \dots = m_L$$

1.9.2 Bayesian DNNs

Bayesian predictive distribution

$$f(x) = \int f(\theta)(x) p(\theta | S) d\theta$$

Bayes rule

$$p(\theta | S) = \frac{p(\theta)p(S | \theta)}{p(S)},$$

$$p(S) = \int p(\theta)p(S | \theta) d\theta$$

Parameter priors (Gaussian)

$$p(\theta) = \prod_{i=1}^d p(\theta_i), \theta_i \sim N(0, \sigma_i^2)$$

$$-\log p(\theta) = \frac{1}{2\sigma^2} \|\theta\|^2 + \text{const}$$

Essentially a weight decay term

Likelihood (Gaussian noise)

$$-\log p(S | \theta) = \frac{1}{2\sigma^2} \|y - f(\theta)\|^2 + \text{const.}$$

with $y_i = f^{*(x_i)} + \nu_i, \nu_i \sim N(0, \gamma^2)$

Posterior

$$-\log p(\theta | S) = E(\theta) + \text{const},$$

$$E(\theta) = \frac{1}{2\gamma^2} \|y - f\|^2 + \frac{1}{2\sigma^2} \|\theta\|^2$$

Bayesian ensembling (post hoc)

$$f(\Theta)(x) = \sum_{i=1}^n \frac{\exp[-E(\theta_i)]}{\sum_{j=1}^n \exp[-E(\theta_j)]} f(\theta_i)(x)$$

Relative posterior weighting

Markov chain monte carlo (MCMC)

$$\theta_0, \theta_1, \theta_2, \dots,$$

$$\theta_{t+1} | \theta_t \sim \Pi$$

$$p(\theta_1 | S) \Pi(\theta_2 | \theta_1) = p(\theta_2 | S) \Pi(\theta_1 | \theta_2)$$

Metropolis-Hastings

$$\Pi(\theta_1 | \theta_2) = \tilde{\Pi}(\theta_1 | \theta_2) A(\theta_1 | \theta_2)$$

$$A(\theta_1 | \theta_2) = \min\left\{1, \frac{p(\theta_1 | S) \tilde{\Pi}(\theta_2 | \theta_1)}{p(\theta_2 | S) \tilde{\Pi}(\theta_1 | \theta_2)}\right\}$$

Modified transition probability with acceptance step A

Hamiltonian monte carlo

$$E(\theta) = -\sum_{x,y} \log p(y | x; \theta) - \log p(\theta)$$

$$H(\theta, v) = E(\theta) + \frac{1}{2} v^\top M^{-1} v$$

with $p(\theta, v)$ propto $\exp[-H(\theta, v)]$

$$\dot{v} = -E(\theta), \dot{\theta} = v$$

$$\theta_{t+1} = \theta_t + \eta v_t$$

$$v_{t+1} = v_t - \eta \nabla E(\theta_t)$$

Langevin dynamics

$$\dot{\theta} = v$$

$$dv = -\nabla E(\theta) dt - Bv dt + N(0, 2B dt)$$

$$\theta_{t+1} = \theta_t + \eta v_t$$

$$v_{t+1} = (1 - \eta\gamma)v_t - \eta \int \nabla \tilde{E}(\theta) + \sqrt{2\gamma}N(0, I)$$

1.9.3 Gaussian Processes

Gaussian process

$$(f(x_1), \dots, f(x_s)) \sim N$$

$$\sum_{i=1}^s \alpha_i f(x_i) \sim N, \text{ for all } \alpha \in \mathbb{R}^s$$

Mean and covariance functions

GPs are completely defined by first and second order statistics

$$\mu(x) := E_{x,f(x)}$$

$$k(x, \xi) := E_{x,\xi}[f(x)f(\xi)] - \mu(x)\mu(\xi)$$

$$K_{\mu\nu} = k(x_\mu, x_\nu), K \in \mathbb{R}^{s \times s}$$

Example kernels

$$k(x, \xi) = x^\top \xi, k(x, \xi) = e^{-\gamma \|x - \xi\|^2}$$

GPs in DNN

Treating parameters as random variables. Each unit in a DNN becomes a random function.

Linear Layer

$$w \sim N(0, \frac{\sigma^2}{n} I_{n \times n})$$

$$E[y_i y_j] = \frac{\sigma^2}{n} x_i^\top x_j$$

Deep layers

$$W^{l+1} X^l, l \geq 1$$

No longer normal as products break normality, but near-normal for high dimensional inputs.

Non-linear activations

$$\mu(x^{l+1}) = E[\varphi(W^l x^l)]$$

Kernel recursion

$$K_{\mu\nu}^l = E[\varphi(x_{i\mu}^{l-1}) \varphi(x_{i\nu}^{l-1})]$$

$$= \sigma^2 E[\varphi(f_\mu) \varphi(f_\nu)]$$

$$f \sim GP(0, K^{l-1})$$

Kernel regression

Mean of bayesian predictive distribution

$$f^{*(x)} = k(x)^\top K^+ y$$

$$E\left[(f(x) - f^{*(x)})^2\right] = K(x, x) - k(x)^\top K^+ k(x)$$

1.9.4 Statistical Learning Theory

VC learning theory

$$L_t = -\frac{\|m(x_t, x_0, t) - m_{\theta(x_t, t)}\|^2}{2\sigma_t^2} + \text{const.}$$

$$\text{VC-dim}(F) := \max_s \sup_{|S|=s} 1\|F(S)\| = 2^s$$

VC inequality

$$P(\sup_F |\hat{E}(f) - E(f)| > \varepsilon) \leq 8 |F(s)| e^{-s \frac{\varepsilon^2}{3}}$$

Double descent

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

Generalization gap

$$\Delta := \max(0, E - \hat{E})$$

E : expected population error, \hat{E} : empirical error

KL divergence

$$D_{\text{KL}}(p \parallel q) = \int p(x) \log\left(\frac{p(x)}{q(x)}\right) dx = E_{x \sim p} [\ln\left(\frac{p(x)}{q(x)}\right)]$$

PAC-Bayesian theorem

For fixed E and any Q over s samples:

$$E_{Q[E(f)]} - E_{Q[\hat{E}(f)]} \leq \sqrt{\frac{2}{s} [\text{KL}(Q \parallel P) + \ln\left(\frac{1}{2\sqrt{s}\varepsilon}\right)]}$$

Ensures general rate $\tilde{O}\left(\frac{1}{\sqrt{s}}\right)$

PAC-Bayesian bound

$$Q := N(\theta, \text{diag}(\sigma_i^2))$$

$$\text{KL}(Q \parallel P) = \sum_i \log\left(\frac{\lambda_i}{\sigma_i} + \frac{\sigma_i^2 + \theta_i^2}{2\lambda_i^2} - \frac{1}{2}\right)$$

$$E_{\text{PAC}}(Q) :=$$

$$E_{Q[\hat{E}]} + \sqrt{\frac{2}{s} [\text{KL}(Q \parallel P) + \ln\left(\frac{1}{2\sqrt{s}\varepsilon}\right)]}$$

Favours minima robust to parameter perturbations

PAC-bayesian learning implementation

$$\theta_{t+1} = \theta_t - \eta \nabla E_{Q[\hat{E}]} = \theta_t - \eta \nabla \hat{E}(\hat{\theta}),$$

with $\hat{\theta} \sim Q(\theta, \sigma)$

Gradient loss on perturbed parameters

Reparameterization trick

$$\hat{\theta} = \theta + \text{diag}(\sigma_i)\varepsilon, \varepsilon \sim N(0, I)$$

Backpropagation to θ and σ_i

1.10 Generative Models

1.10.1 Variational Autoencoders

Linear autoencoder

$$x \mapsto z = Cx, C \in \mathbb{R}^{m \times n}$$

$$z \mapsto \hat{x} = Dz, D \in \mathbb{R}^{n \times m}$$

$$E(C, D)(x) = \frac{1}{2}\|x - \hat{x}\|^2 = \frac{1}{2}\|x - DCx\|^2$$

$$DCX = \hat{X} = \bar{U}\Sigma_m V^\top$$

$$\Sigma_m = \text{diag}(\sigma_1, \dots, \sigma_m, 0, \dots, 0)$$

For centered data equivalent to PCA, but generally has non-global minima

Linear factor analysis

Probability Model

$$p_{X(z)} = \int p_{Z(z)} p_{X|Z}(x \mid z) dz$$

Z : latent variables, X : observed variables

Linear observation model

$$x = \mu + Wz + \nu \text{ with } \nu \sim N(0, \Sigma)$$

$$x \sim N(\mu, WW^\top + \Sigma) \text{ for } z \sim N(0, I)$$

Posterior mean and covariance

$$\mu_{z|x} = W^\top(WW^\top + \Sigma)^{-1}(x - \mu)$$

$$\Sigma_{z|x} = I - W^\top(WW^\top + \Sigma)^{-1}W$$

Pseudoinverse limit

$$W^\top(WW^\top + \sigma^2 I)^{-1} \rightarrow W^+ \in \mathbb{R}^{m \times n}$$

$$\mu_{z|x} \rightarrow W^+(x - \mu), \Sigma_{z|x} \rightarrow 0$$

Maximum likelihood estimation

$$\mu, W \text{ max} \rightarrow \log p_{\mu, W}(S)$$

Optimality condition for W

$$w_i = \rho_i u_i, \rho_i = \max\{0, \sqrt{\lambda_i - \sigma^2}\}$$

With (λ_i, u_i) eigenvalues and eigenvectors of covariance matrix.

For $\sigma = 0$ equivalent to PCA.

Variational autoencoder (VAE)

$$z \sim N(0, I)$$

$$x = F(\theta)(z) = (F^L @ \dots @ F^1)(z)$$

Evidence lower bound (ELBO)

$$\begin{aligned} \log p_\theta(x) &= \log \int p_\theta(x \mid z)p(z) dz \\ &= \log \int q(z) \left[\frac{p_\theta(x \mid z)p(z)}{q(z)} \right] dz \\ &\geq \int q(z) \log p_\theta(x \mid z) dz - \int q(z) \log\left(\frac{q(z)}{p(z)}\right) dz \\ &=: L(\theta, q)(x) \\ \theta \text{ max} \rightarrow L(\theta, q)(S) &= \sum_{i=1}^s L(\theta, q)(x_i) \end{aligned}$$

Inference network

$$z \sim N(\mu(x), \Sigma(x))$$

$$z = \mu + \Sigma^{\frac{1}{2}}\varepsilon, \varepsilon \sim N(0, I)$$

$$\nabla_\mu E[f(z)] = E[\nabla_z f(z)]$$

$$\nabla_\Sigma E[f(z)] = \frac{1}{2}E[\nabla_z^2 f(z)]$$

Integration by parts derivation

1.10.2 Generative Adversarial Networks

GAN objective

$$V(G, D) = E_{x_r \sim p_{\text{data}}} D(x_r) + E_{z \sim p_z} (1 - D(G(z)))$$

Discriminator Mixture Model

$$\tilde{p}_{\theta(x,y)} = \frac{1}{2}(yp(x) + (1-y)p_{\theta(x)}),$$

$$y \in \{0, 1\},$$

p : true probability, p_θ : model probability

Bayes-optimal classifier

$$q_{\theta(x)} := P\{y = 1 \mid x\} = \frac{p(x)}{p(x) + p_{\theta(x)}}$$

To detect fake samples, $y = 1$ for real samples, $y = 0$ for fake samples

Logistic likelihood

$$\theta \text{ min} \rightarrow \ell^*(\theta) := E_{\tilde{p}_\theta} [y \ln q_{\theta(x)} + (1-y) \ln(1 - q_{\theta(x)})]$$

Jensen-Shannon as effective objective

$$\begin{aligned} \ell^* &= E_{\tilde{p}_\theta} [y \ln q_{\theta(x)} + (1-y) \ln(1 - q_{\theta(x)})] \\ &= -\frac{1}{2}H(p) - \frac{1}{2}H(p_\theta) + H\left(\frac{1}{2}(p + p_\theta)\right) - \ln 2 \\ &= \text{JS}(p, p_\theta) - \ln 2. \end{aligned}$$

Discriminator model

$$q_\varphi : x \mapsto [0; 1], \varphi \in \Phi$$

Objective bounds

$$\ell^*(\theta) \geq \sup_{\varphi \in \Phi} \ell(\theta, \varphi)$$

$$\ell(\theta, \varphi) := E_{\tilde{p}_\theta} [y \ln q_{\varphi(x)} + (1-y) \ln(1 - q_{\varphi(x)})]$$

Saddle point optimization

$$\theta^* := \operatorname{argmin}_{\theta \in \Theta} \left(\sup_{\varphi \in \Phi} \ell(\theta, \varphi) \right)$$

φ : Generator, θ : Discriminator

Alternating gradient descent/ascent

$$\theta_{t+1} = \theta_t - \eta \nabla_\theta \ell(\theta_t, \varphi_t)$$

$$\varphi_{t+1} = \varphi_t + \eta \nabla_\varphi \ell(\theta_{t+1}, \varphi_t)$$

Extra-gradient steps

$$\theta_{t+1} = \theta_t - \eta \nabla_\theta \ell(\theta_{t+0.5}, \varphi_t)$$

with $\theta_{t+0.5} := \theta_t - \eta \nabla_\theta \ell(\theta_t, \varphi_t)$

$$\varphi_{t+1} = \varphi_t + \eta \nabla_\varphi \ell(\theta_t, \varphi_{t+0.5})$$

with $\varphi_{t+0.5} := \varphi_t + \eta \nabla_\varphi \ell(\theta_t, \varphi_t)$

Deconvolutional DNN

Upside-down ConvNet for image generation

1.10.3 Denoising Diffusion

Markov chains

$$x_{0:t-1} \perp x_{t+1:\infty} \mid x_t \text{ (forall } t)$$

$$p(x_t \mid x_{t-1}) = p(x_1 \mid x_0) \text{ (forall } t),$$

$$p(x_{s:t}) = p(x_t) \prod_{\tau=s+1}^t p(x_{\tau-1} \mid x_\tau)$$

$$p(x_{s:t}) = p(x_s) \prod_{\tau=s+1}^t p(x_\tau \mid x_{\tau-1}),$$

$$\pi(x_{t+1}) = \int \pi(x_t) p(x_{t+1} \mid x_t) dx_t$$

Denoising diffusion

Forward (noise generation)

$$\pi^* = \nu_0 \mapsto \nu_1 \mapsto \dots \mapsto \nu_{T-1} \mapsto \nu_T = \pi$$

Backward (denoising)

$$\pi = \mu_T^0 \mapsto \mu_{T-1}^0 \mapsto \dots \mapsto \mu_1^0 \mapsto \mu_0^0 \approx \pi^*$$

Gaussian example

$$\pi \approx N(0, I),$$

$$x_t \mid x_{t-1} \sim N(\sqrt{1 - \beta_t}x_{t-1}, \beta_t I)$$

Forward SDE

$$dx_t = -\frac{1}{2}\beta_t x_t dt + \sqrt{\beta_t} d\omega_t$$

Backward SDE

$$\begin{aligned} dx_t &= -\frac{1}{2}\beta_t x_t - \\ &\quad \beta_t \nabla_{x_t} \log q_{t(x_t)} dt + \sqrt{\beta_t} d|\omega_t| \end{aligned}$$

score · wiener process

ELBO bound

$$x_t = \sqrt{1 - \beta_t}x_{t-1} + \sqrt{\beta_t}\varepsilon_t, \varepsilon_t \sim N(0, I)$$

$$\ln p_{\theta(x_0)} = \ln \int q(x_{1:T} \mid x_0) \left(\frac{p_{\theta(x_0:T)}}{q(x_{1:T} \mid x_0)} \right) dx_{1:T}$$

$$\geq E \left[\ln \left(\frac{p_{\theta(x_0:T)}}{q(x_{1:T} \mid x_0)} \right) \mid x_0 \right]$$

$$= \sum_{t=0}^T L_t$$

$$L_t := \text{cases}\left(E\left[\ln p_{\theta(x_0 \mid x_1)}\right], t = 0; -D(q(x_T \mid x_0) \parallel \pi), t = T; -D(q(x_{t-1} \mid x_t, x_0) \parallel p_{\theta(x_{t-1} \mid x_t)}), \text{else}\right)$$

Backward model assumption

$$x_{t-1} \mid x_t \sim N(m(x_t, t), \Sigma(x_t, t))$$

Entropy bounds

$$H(x_t) \geq H(x_{t-1}) \Rightarrow H(x_t \mid x_{t-1}) \geq H(x_{t-1} \mid x_t)$$

Noise schedules

$$\begin{aligned} |(\alpha)_t &= \prod_{\tau=1}^t (1 - \beta_\tau), |(\beta)_t = 1 - |(\alpha)_t \\ x_t &\approx N\left(\sqrt{|(\alpha)_t}x_0, |(\beta)_t I\right) t \rightarrow \infty \rightarrow N(0, I) \end{aligned}$$

Forward trajectory target

$$\begin{aligned} x_{t-1} \mid x_t, x_0 &= N\left(m(x_t, x_0, t), \beta_t I\right) \\ m(x_t, x_0, t) &= \left(\frac{\sqrt{|(\alpha)_{t-1}\beta_t}}{1 - |(\alpha)_t}\right)x_0 + \left(\frac{1 - |(\alpha)_{t-1}\sqrt{1 - \beta_t}}{1 - |(\alpha)_t}\right)x_t \\ \text{with } \tilde{\beta}_t &= \frac{1 - |(\alpha)_{t-1}}{1 - |(\alpha)_t} \beta_t \end{aligned}$$

Fixed isotropic covariance

$$\Sigma(x_t, t) = \sigma_t^2 I, \text{ where } \sigma_t^2 \in \{\beta_t, \tilde{\beta}_t\}$$

Simplified ELBO

$$L_t = -\frac{\|m(x_t, x_0, t) - m_{\theta(x_t, t)}\|^2}{2\sigma_t^2} + \text{const.}$$

Reparameterization

$$x_t = \sqrt{|(\alpha)_t}x_0 + \sqrt{1 - |(\alpha)_t}\varepsilon \Rightarrow x_0 = \frac{1}{\sqrt{|(\alpha)_t}}x_t - \frac{\sqrt{1 - |(\alpha)_t}}{\sqrt{|(\alpha)_t}}\varepsilon$$

$$m(x_t, x_0, t) = \frac{1}{\sqrt{\alpha_t}} \left[x_{t(x_0, \varepsilon)} - \frac{\beta_t}{\sqrt{1 - |(\alpha)_t}}\varepsilon \right]$$

with $\varepsilon \sim N(0, I)$

Expected squared error

$$\begin{aligned} E_{q[L_t \mid x_0]} &= E \left[\varepsilon \mid \rho_t \left\| \varepsilon - \varepsilon_{\theta(\sqrt{|(\alpha)_t}x_0 + \sqrt{1 - |(\alpha)_t}\varepsilon, t)} \right\|^2 \mid x_0 \right] \\ \text{with } \rho_t &= \frac{\beta_t^2}{2\sigma_t^2 \alpha_t (1 - |(\alpha)_t)} \end{aligned}$$

Final simplified criterion

$$\begin{aligned} h(\theta)(x) &= \frac{1}{T} \sum_{t=1}^T E \left[\left\| \varepsilon - \varepsilon_{\theta(\sqrt{|(\alpha)_t}x + \sqrt{1 - |(\alpha)_t}\varepsilon, t)} \right\|^2 \right] \end{aligned}$$

1.11 Ethics

1.11.1 Adversarial Examples

Adversarial perturbation

$$f(x + \nu) \neq f(x) \text{ s.t. } \|\nu\|_p \leq \varepsilon$$

p-norm definitions

$$\|x\|_p = \left(\sum_i |x_i|^p \right)^{\frac{1}{p}}$$

$$\|x\|_\infty = \max_i |x_i|, \|x\|_0 = |\{i : x_i \neq 0\}|$$

Optimal perturbation (linear binary classification)

$$\nu \propto \text{sign}(f_1(x) - f_2(x))(w_2 - w_1)$$

for $f_i = w_i^\top x + b_i$

Optimal perturbation (multiclass)

$$\nu = \operatorname{argmin}_{i>1} \frac{f_1(x) - f_i(x)}{\|w_1 - w_i\|_2^2} (w_i - w_1)$$

DeepFool iterative optimization

Iterate: $\operatorname{argmin}_{\Delta\nu} \|\Delta\nu\|_2$ s.t.

$$(\nabla f_1(x) - \nabla f_2(x))^\top \Delta\nu < f_1(x) - f_2(x)$$

Robust training

$$\ell(f(x), y) \rightarrow \max_{\nu: \|\nu\|_p \leq \varepsilon} \ell(f(x + \nu), y)$$

Projected gradient ascent ($p = 2$)

$$\begin{aligned}\nu_{t+1} &= \varepsilon \Pi[\nu_t + \alpha \nabla_x \ell(f(x + \nu_t), y)] \\ \Pi[z] &:= \frac{z}{\|z\|_2}\end{aligned}$$

Projected gradient ascent ($p = \infty$)

$$\begin{aligned}\nu_{t+1} &= \varepsilon \Pi[\nu_t + \alpha \operatorname{sign}(\nabla_x \ell(f(x + \nu_t), y))] \\ \Pi[z] &:= \frac{z}{\|z\|_\infty}\end{aligned}$$

Fast Gradient Sign Method (FGSM)

$$\nu = \varepsilon \operatorname{sign}(\nabla_x \ell(f(x), y))$$

2 Computer Vision

2.1 The Digital Image & Sensors

Charge Coupled Device (CCD)

Photons

- Blooming:** Oversaturated photosites cause vertical channels to "flood" (bright vertical line)

Image Noise

Additive Gaussian noise:

Color camera concepts:

- Prism (split light, 3 sensors, needs good alignment, good color separation)

2.2 Image Segmentation

Pixel-wise classification problem, to group pixels in an image that share common properties.

Segmentation of I : Find R_1, \dots, R_n such that
 $I = \bigcup_{i=1}^N R_i$ with $R_i \cap R_j = \emptyset \quad \forall i \neq j$.

Thresholding

Segment image into 2 classes.
 $B(x, y) = 1$ if $I(x, y) \geq T$ else 0, finding T with trial and error, compare results with ground truth.

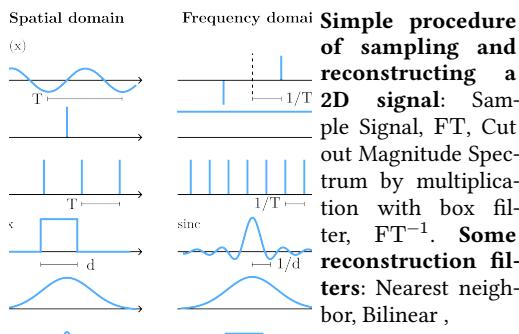
Important Kernels

	Low-pass/ High-pass		
Laplacian	Prewitt _x	Mean / Box	High-pass
Gaussian	Sobel _x	Diff _x	Diff _y
$\frac{1}{2\pi\sigma^2} e^{-\frac{x^2+y^2}{2\sigma^2}}$	mat(-1, 0, 1; mat([0, -2], 1), mat([-1], 1)) ^T		

Dirac delta: $\delta(x) = \text{cases}(0 \text{ if } x \neq 0, \text{undefined else})$ with $\int_{-\infty}^{\infty} \delta(x) dx = 1$. $\mathcal{F}[\delta(x - x_0)](u) = e^{-i2\pi u x_0}$. $\delta(u) = \int_{\mathbb{R}} e^{-i2\pi x u} dx$.

Sampling f at points x_n : $f_s(x) = \sum_n f(x_n) \delta(x - x_n)$.

Property $f(x)$ $F(u)$
 Linearity $\alpha f_1(x) + \beta f_2(x)$ $\alpha F_1(u) + \beta F_2(u)$
 Duality $F(x)$ $f(-u)$



Gaussian reconstruction filter (equiv. to convolving sampled signal w/ Gaussian kernel. $\text{sinc}(x) = \frac{\sin(\pi x)}{\pi x}$

Image restoration

Image degradation is applying kernel h to some image I . The inverse \tilde{h} should compensate: $I \xrightarrow{h(x)} J \xrightarrow{\tilde{h}(x)} I$.

Determine with $\mathcal{F}[\tilde{h}](u, v) \cdot \mathcal{F}[h](u, v) = 1$. Or $\tilde{h} = \mathcal{F}^{-1}\left[\frac{1}{\mathcal{F}[h]}\right]$

Cancellation of frequencies & noise amplification → Regularize using $\tilde{\mathcal{F}}[\tilde{h}](u, v) = \mathcal{F}[h] / (\|\mathcal{F}[h]\|^2 + \varepsilon)$.

Motion blur: $h(x, y) = \frac{1}{2l} [\theta(x + l) - \theta(x - l)] \delta(y)$