

Deep Learning Cheat Sheet

Authors

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1 History

1.1 Perceptron

Threshold Unit

$$f[w, b](x) = \text{sign}(x^\top w + b)$$

Decision Boundary

$$x^\top w + b \neq 0 \Leftrightarrow \frac{x^\top w}{\|w\|} + \frac{b}{\|w\|} \neq 0$$

$$x^\top w - b = [x \cdot 1] \cdot \begin{bmatrix} w \\ b \end{bmatrix} =: \tilde{x}^\top \tilde{w}, \quad \tilde{x}, \tilde{w} \in \mathbb{R}^{n+1}.$$

Geometric Margin

$$\gamma[w, b](x, y) := y \frac{x^\top w + b}{\|w\|}$$

Maximum Margin Classifier

$$(w^*, b^*) \in \operatorname{argmax}_{w, b} \gamma[w, b](S), \text{ with } \gamma[w, b](S) := \min_{(x, y) \in S} \gamma[w, b](x, y)$$

Perceptron Learning

if $f[w, b](x) \neq y$: update $w \leftarrow w + yx$, and $b \leftarrow b + y$

$w_0 \in \text{span}(x_1, \dots, x_s) \Rightarrow w_t \in \text{span}(x_1, \dots, x_s)$ (forall t)

Convergence

If exists w , $\|w\| = 1$, such that $\gamma[w](S) = \gamma > 0$ then $w_t * w \geq t\gamma$.

$$R = \max_{x \in S} \|x\| \Rightarrow \|w_t\| \leq R\sqrt{\gamma} \quad \cos(u, w_t) = \frac{u^\top w_t}{\|w_t\|} \geq \frac{t\gamma}{\sqrt{t}R} = \sqrt{t}\frac{\gamma}{R} \leq 1 \Rightarrow t \leq \frac{R^2}{\gamma^2}$$

Cover's Theorem

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

$C(S, n)$: Number of ways to separate S with n dimensions

$$C(s, n) = 2^s \text{ for } s \leq n$$

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 $X_i \in \{-1, +1\}$

$w_{ij} = w_{ji}$ (forall i, j), $w_{ii} = 0$ (forall i): Interaction strengths

Hebbian Learning

$$x^t \in \{+1\}^n \quad (1 \leq t \leq s)$$

$$w_{ij} = \frac{1}{n} \sum_{t=1}^s x_i^t x_j^t$$

$$W = \frac{1}{n} \sum_{t=1}^s x^t (x^t)^\top$$

1.2 Feedforward Networks

1.2.1 Linear Models

Linear regression

$$h[w](S) = \frac{1}{2s} \|Xw - y\|^2$$

$$\nabla h = 2X^\top Xw - 2X^\top y$$

Moore-Penrose inverse solution

$$w^* = X^\top y \in \operatorname{argmin}_w h[w]$$

$$\text{where } X^* := \lim_{\delta \rightarrow 0} (X^\top X + \delta I)^{-1} X^\top$$

Stochastic gradient descent update

$$w_{t+1} := w_t + \eta(y_{i_t} - w_t^\top x_{i_t})x_{i_t}$$

$$\text{with } i_t \sim \text{Uniform}(1, \dots, s)$$

Gaussian noise model

$$y_i = w^\top x_i + \varepsilon_i, \quad \varepsilon_i \sim N(0, \sigma^2)$$

Least squares equivalent to negative log likelihood of gaussian noise model

Ridge regression

$$h_{\lambda[w]} := h[w] + \frac{\lambda}{2} \|w\|^2$$

$$w^* = (XX^\top + \lambda I)^{-1} X^\top y$$

Logistic function

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

$$\sigma(z) + \sigma(-z) = 1$$

$$\sigma' = \sigma(1 - \sigma), \quad \sigma'' = \sigma(1 - \sigma)(1 - 2\sigma)$$

Cross entropy loss

$$\ell(y, z) = -y \log \sigma(z) - (1 - y) \log(1 - \sigma(z))$$

$$= -\log \sigma((2y - 1)z)$$

Logistic regression with cross entropy loss

$$\nabla \ell_i = [\sigma(w^\top x_i) - y_i] x_i$$

1.2.2 Feedforward Networks

Generic feedforward layer definition

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

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

Composition of layers

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

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

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

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

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

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 $C_f := \int \|\omega\| |\dot{f}(\omega)| d\omega < \infty$ 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

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

1.3 Gradient-Based Learning

1.3.1 Backpropagation

Parameter derivatives for ridge function layers

$$\frac{\partial x_i^l}{\partial w_{ij}^l} = \dot{\varphi}_i^l x_j^{l-1},$$

$$\dot{\varphi}_i^l := \dot{\varphi}^l \left((w_i^l)^\top x^{l-1} + b_i^l \right)$$

$$\frac{\partial x_i^l}{\partial b_i^l} = \dot{\varphi}_i^l$$

Loss derivatives

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

$$\frac{\partial h[\theta](x, y)}{\partial b_i^l} = \frac{\partial h^{[l]\theta}(x^l, y)}{\partial x_i^l} \frac{\partial x_i^l}{\partial b_i^l} = \delta_i^l \dot{\varphi}_i^l$$

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

1.3.2 Gradient Descent

Gradient descent update

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

Gradient flow ODE

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

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

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

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

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

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

More theoretical grounding than heavy ball

AdaGrad updates

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

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

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

Adam updates

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

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

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

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

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

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

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

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

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

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 model

Prediction of output word μ given word w in neighborhood

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

$$h(\{x_w\}, \{y_\mu\}) = \sum_{(w,\mu)} \ell_{w\mu}$$

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

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

$$F[U, V](z, x) := \varphi(Uz + Vx)$$

$$G[W](z) := \psi(Wz), W \in \mathbb{R}^{q \times m}$$

Backpropagation through time

$$\frac{\partial h}{\partial z^t} = \sum_{s=t}^T \delta_k^s \sum_{j=1}^m \frac{\partial \hat{y}_j}{\partial z_j^s} \frac{\partial z_j^s}{\partial z_i^t},$$

$$\frac{\partial \hat{y}_k}{\partial z_j^t} = \psi_k^s w_{kj}$$

$$\frac{\partial h}{\partial v_{ij}} = \sum_{t=1}^T \frac{\partial h}{\partial z_i^t} \dot{\varphi}_i^t x_j^t$$

$$\frac{\partial h}{\partial u_{ij}} = \sum_{t=1}^T \frac{\partial h}{\partial z_i^t} \dot{\varphi}_i^t z_j^t$$

Spectral norm

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

Gradient norms

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

The norm of gradients either:

1. Vanishes exponentially if $\left\| \frac{\partial z^t}{\partial z^0} \right\|_2 \leq ((\alpha)\sigma_1(U))^t \rightarrow \infty$
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

$$z_t := \sigma(F\tilde{x}_t) * z_{t-1} + \sigma(G\tilde{x}_t) * \tanh(V\tilde{x}_t)$$

$$\tilde{x}_t := \text{mat}(x_t; h_t), h_{t+1} = \sigma(H\tilde{x}_t) * \tanh(Uz_t)$$

GRU

$$z_t = (1 - \sigma) * z_{t-1} + \sigma * \tilde{z}_t,$$

$$\sigma := \sigma(G[x_t, z_{t-1}])$$

$$\tilde{z}_t := \tanh(V[r_t * z_{t-1}, x_t])$$

$$r_t := \sigma(H[z_{t-1}, x_t])$$

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

$$\lambda_i = \exp(-\exp(\kappa_i) + i\varphi_i),$$

$$e^{\kappa_i} = -\ln r_i$$

$$\varphi_i \sim \text{Uni}[0; 2\pi], r_i \sim \text{Uni}[I], I \subset [0; 1]$$

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

$$\xi_s := \sum_t \alpha_{st} Wx_t, \alpha_{st} \geq 0, \sum_t \alpha_{st} = 1$$

$$A = (a_{st}) \in \mathbb{R}^{T \times T}, \text{s.t. } \Xi = WXA^\top$$

Query-key matching

$$Q = U_Q X, K = U_K X$$

$$(U_Q, U_K \in \mathbb{R}^{q \times n})$$

$$Q^\top K = X^\top U_Q^\top U_K X \text{ rank } \leq q$$

$$(Q^\top K \in \mathbb{R}^{T \times T})$$

Softmax attention

$$A = \text{softmax}(\beta Q^\top K),$$

$$a_{st} = \frac{e^{\beta [Q^\top K]_{st}}}{\sum_r e^{\beta [Q^\top K]_{sr}}}$$

$$\text{usually } \beta = \frac{1}{\sqrt{q}}$$

Feature transformation

$$X \mapsto \Xi \mapsto F(\Xi),$$

$$F(\theta)(\Xi) = (F(\xi_1), \dots, F(\xi_T))$$

Positional encoding

$$p_{tk} = \text{cases}(\sin(t\omega_k), k \text{ even}; \cos(t\omega_k), k \text{ odd}),$$

$$\omega_k = C \frac{k}{K}$$

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

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

with $V \in \mathbb{R}^{n \times (qp^2)}$

GELU activation

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

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

$$f(x_1, \dots, x_M) = (y_1, \dots, y_M) \Rightarrow$$

$$f(x_{\pi(1)}, \dots, x_{\pi(M)}) = (y_{\pi(1)}, \dots, y_{\pi(M)})$$

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

$$\rho: \mathbb{R} \times \mathbb{R}^N \rightarrow Y,$$

$$(x_m, \sum_{k=1}^M \varphi(x_k)) \mapsto y_m$$

1.7.2 Graph Convolutional Networks

Feature and adjacency matrices

$$X = \text{mat}(x_1^\top; \dots; x_M^\top), A = (a_{nm})$$

with
 $a_{nm} = \text{cases}(1, \text{if } \{v_n, v_m\} \in E; 0, \text{otherwise})$

Permutation matrix constraints

$$P \in \{0, 1\}^{M \times M} \text{ s.t. }$$

$$\sum_{n=1}^M p_{nm} = \sum_{n=1}^M p_{mn} = 1 \text{ (forall } m)$$

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

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

$$\{\text{cdot}\} = \text{multiset}$$

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

$$L = D - A = UAU^\top, \\ \Lambda := \text{diag}(\lambda_1, \dots, \lambda_M), \lambda_i \geq \lambda_{i+1}$$

Convolution

$$x * y = U((U^\top x) \text{ odot } (U^\top y))$$

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

$$x_i^{l+1} = \sum_j p_{ij}(L)x_j^l + b_i, \\ p_{ij}(L) = \sum_{k=0}^K \alpha_{ijk} L^k$$

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

$$\theta_i^0 \sim N(0, \sigma_i^2), \text{ or} \\ \theta_i^0 \sim \text{Uniform}(-\sqrt{3}\sigma_i; \sqrt{3}\sigma_i)$$

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

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

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 :

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

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

Layer normalization

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

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

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

Using population averages across units in a layer

1.8.5 Model Distillation

Tempered cross entropy loss for distillation

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

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

$T > 0, F_y$: 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

$$E(\alpha) = \frac{1}{2s} \sum_{i=1}^s \left(\sum_{j=1}^s \alpha_j \nabla f(x_j) * \nabla f(x_i) + f(x_i) - \bar{y}_i \right)^2 = E(\theta) + \text{const}, \\ \bar{E}(\theta) = \frac{1}{2s} \|y - f\|^2 + \frac{1}{2s} \|\theta\|^2$$

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

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

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

Infinite width limit

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

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

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

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

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

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

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)

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

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

Posterior

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

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

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

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

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

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

Langevin dynamics

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

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

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

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

1.9.3 Gaussian Processes

Gaussian process

$$(f(x_1), \dots, f(x_s)) \sim N \\ \sum_{i=1}^s \alpha_i f(x_i) \sim N, \text{ forall } \alpha \in \mathbb{R}^s$$

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

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

GP 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

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

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

$$P(\sup_F |\hat{E}(f) - E(f)| > \varepsilon) \leq 8 |F(s)| e^{-s \frac{\varepsilon^2}{32}}$$

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

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

PAC-Bayesian theorem

For fixed E and any Q over s samples:

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

PAC-Bayesian bound

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

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

Favours minima robust to parameter perturbations

PAC-bayesian learning implementation

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

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

Gradient loss on perturbed parameters

Reparameterization trick

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

Backpropagation to θ and σ_i

1.10 Generative Models

1.10.1 Variational Autoencoders

Linear autoencoder

$$x \mapsto z = Cx, C \in \mathbb{R}^{m \times n} \\ z \mapsto \hat{x} = Dz, D \in \mathbb{R}^{n \times m} \\ E(C, D)(x) = \frac{1}{2} \|x - \hat{x}\|^2 = \frac{1}{2} \|x - DCx\|^2 \\ DCX = \hat{X} = U\Sigma_m V^\top$$

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

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

Linear factor analysis

Probability Model

$$p_{X|Z}(x) = \int p_{Z|Z}(x|z) dz \\ Z: \text{latent variables}, X: \text{observed variables}$$

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

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

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)

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

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

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

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

p : true probability, p_θ : model probability

Bayes-optimal classifier

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

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

Logistic likelihood

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

Jensen-Shannon as effective objective

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

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

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

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

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

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

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

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

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

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

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

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

Forward SDE

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

Backward SDE

$$dx_t = \left[-\frac{1}{2} \beta_t x_t - \beta_t \nabla_{x_t} \log q_{t(x_t)} \right] dt + \sqrt{\beta_t} d\langle \omega_t \rangle_t$$

score · wiener process

ELBO bound

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

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

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

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

$$L_t := \text{cases} \left(E \left[\ln p_{\theta(x_0 | x_1)} \right], t = \right.$$

$$0; -D(q(x_T | x_0) \| \pi), t =$$

$$T; -D(q(x_{t-1} | x_t, x_0) \| p_{\theta(x_{t-1} | x_t)}), \text{else} \right)$$

Backward model assumption

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

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

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

Forward trajectory target

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

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

$$x_t = \sqrt{|(\alpha)_t}x_0 + \sqrt{1 - |(\alpha)_t}\varepsilon \Rightarrow x_0 = \frac{1}{\sqrt{|(\alpha)_t}}x_t - \frac{\sqrt{1 - |(\alpha)_t}}{\sqrt{|(\alpha)_t}}\varepsilon \\ m(x_t, x_0, t) = \frac{1}{\sqrt{\alpha_t}} \left[x_t - \frac{\beta_t}{\sqrt{1 - |(\alpha)_t}}\varepsilon \right] \\ \text{with } \varepsilon \sim N(0, I)$$

Expected squared error

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

Final simplified criterion

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

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)

$$\nu \propto \text{sign}(f_1(x) - f_2(x))(w_2 - w_1) \\ \text{for } f_i = w_i^\top x + b_i$$

Optimal perturbation (multiclass)

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

DeepFool iterative optimization

$$\text{Iterate: } \underset{\Delta\nu}{\operatorname{argmin}} \|\Delta\nu\|_2 \text{ s.t.} \\ (\nabla f_1(x) - \nabla f_2(x))^\top \Delta\nu < f_1(x) - f_2(x)$$

Robust training

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

Projected gradient ascent ($p = 2$)

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

Projected gradient ascent ($p = \infty$)

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

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/ Mean	/	High-pass Box
Laplacian	Prewitt _x			
Gaussian	Sobel _x	Diff _x		Diff _y

$\frac{1}{2\pi\sigma^2} e^{-\frac{x^2+y^2}{2\sigma^2}}$

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

$$\begin{array}{ll} f(x) & F(u) \\ \text{Linearity} & \alpha f_1(x) + \beta f_2(x) \\ \text{Duality} & F(x) \end{array} \quad \begin{array}{ll} & \alpha F_1(u) + \beta F_2(u) \\ & f(-u) \end{array}$$

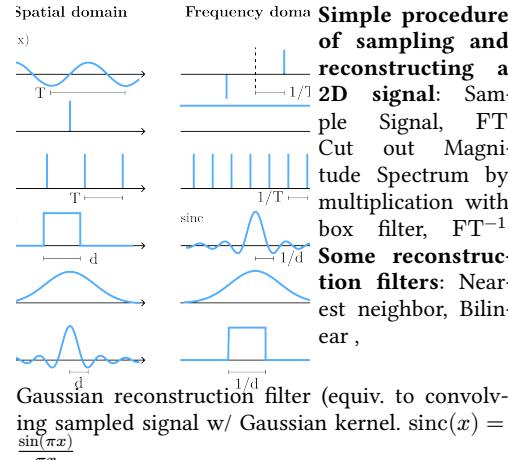


Image restoration

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 \rightarrow Regularize using $\tilde{\mathcal{F}}[\tilde{h}](u, v) = \mathcal{F}[h] / (|\mathcal{F}[h]|^2 + \varepsilon)$.

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