

**Dict** BALD: Bayesian Active Learning by Disagreement; BLR: Bayesian Linear Reg.; BN: Bayesian Network; BNN: Bayesian NN; BO: Bayesian Opt.; BP: Belief Propagation; CPD: Cond Prob Dist; DAG: Directed Acyclic Graph; DBE: Detailed Balance Eq.; DDIM: Denoising Diffusion Implicit Models; DDPG: Deep Deterministic PG; DDPM: Denoising Diffusion Prob. Models; DQN: Deep Q-Nets; ECE: Expected Calibration Error; EI: Expected Improvement; ELBO: Evidence Lower Bound; GP: Gaussian Process; HMM: Hidden Markov Model; KF: Kalman Filter; KL: Kullback-Leibler; LDM: Latent Diffusion; LOTV: Law of Total Var.; MALA: Metropolis-Adjusted Langevin; MAP: Max A Posteriori; MCMC: Markov Chain MC; MDP: Markov Decision Process; MH: Metropolis-Hastings; MI: Mutual Info; MLE: Max Likelihood Est.; MPE: Most Probable Explanation; PF: Particle Filter; PI: Prob of Improvement; POMDP: Partially Observable MDP; RBF: Radial Basis Fnc; RFF: Random Fourier Features; SGLD: Stoch Grad Langevin Dyn; SWAG: Stoch Weight Avg Gaussian; TD: Temporal Diff.; UCB: Upper Confidence Bound; VE: Var Elimination; VI: Variational Inference;  $k_{XX'} := k(X, X')$ ;  $K_y := K_{XX} + \sigma_n^2 I$

## Probability Fundamentals

**Axioms:**  $\mathbb{P}(\Omega) = 1$ ;  $\mathbb{P}(A) \geq 0$ ; Disjoint:  $\mathbb{P}(\bigcup_i A_i) = \sum_i \mathbb{P}(A_i)$  **Product:**  $\mathbb{P}(X_{1:n}) = \mathbb{P}(X_1) \prod_{i=2}^n \mathbb{P}(X_i | X_{1:i-1})$  **Sum:**  $\mathbb{P}(X) = \sum_y \mathbb{P}(X, y)$

**Bayes:**  $\mathbb{P}(X|Y) = \frac{\mathbb{P}(Y|X)\mathbb{P}(X)}{\mathbb{P}(Y)}$  **Cond Indep:**  $X \perp Y | Z \leftrightarrow \mathbb{P}(X, Y | Z) = \mathbb{P}(X|Z)\mathbb{P}(Y|Z)$

**Gaussian**  $\mathcal{N}(\mu, \Sigma)$ :  $\mathcal{N}(x; \mu, \Sigma) = \frac{1}{\sqrt{(2\pi)^d \det(\Sigma)}} \exp(-\frac{1}{2}(x - \mu)^\top \Sigma^{-1}(x - \mu))$  **Marginal:**

$X_A \sim \mathcal{N}(\mu_A, \Sigma_{AA})$  **Conditional:**  $X_A | X_B \sim \mathcal{N}(\mu_{A|B}, \Sigma_{A|B})$   $\mu_{A|B} = \mu_A + \Sigma_{AB}\Sigma_{BB}^{-1}(x_B - \mu_B)$

$\Sigma_{A|B} = \Sigma_{AA} - \Sigma_{AB}\Sigma_{BB}^{-1}\Sigma_{BA}$  **Linear:**  $Y = MX \sim \mathcal{N}(M\mu, M\Sigma M^\top)$  **Sum:** indep  $X + X' \sim \mathcal{N}(\mu + \mu', \Sigma + \Sigma')$

**E, Var, Cov:**  $\mathbb{E}[AX + b] = A\mathbb{E}[X] + b$ ; **Tower:**  $\mathbb{E}_Y[\mathbb{E}_{X|X,Y}] = \mathbb{E}[X]$   $\text{Var}[X] = \mathbb{E}[(X - \mathbb{E}[X])^2]$ ;  $\text{Cov}[X, Y] = \mathbb{E}[XY] - \mathbb{E}[X]\mathbb{E}[Y]$   $\text{Var}[X + Y] = \text{Var}[X] + \text{Var}[Y] + 2\text{Cov}[X, Y]$  **LOTV:**  $\text{Var}[X] = \mathbb{E}[\text{Var}[X|Y]] + \text{Var}[\mathbb{E}[X|Y]]$

**Info Theory:** **Entropy:**  $H[p] = -\mathbb{E}_{p|\log p(x)}$ ; **Gauss**  $H = \frac{1}{2} \log((2\pi e)^d \det \Sigma)$  **KL:**  $\text{KL}(p||q) = \mathbb{E}_{p|\log p_q} \geq 0$ ; need  $\text{supp}(q) \subseteq \text{supp}(p)$  **Forward KL**  $\text{KL}(p||q)$ : mean-seeking 覆盖; **Reverse KL**  $\text{KL}(q||p)$ : mode-seeking 过 confident MI:  $I(X; Y) = H[X] - H[X|Y] = H[Y] - H[Y|X] \geq 0$ , symmetric **Cond MI:**  $I(X; Y|Z) = H[X|Z] - H[X|Y, Z]$  **Gauss MI:**  $I[X; Y] = \frac{1}{2} \log \det(I + \sigma_n^{-2}\Sigma)$  for  $Y = X + \epsilon$

**MLE:**  $\hat{\theta}_{\text{MLE}} = \arg \max_{\theta} \sum_i \log p(y_i|x_i, \theta)$

**MAP:**  $\hat{\theta}_{\text{MAP}} = \arg \min_{\theta} \underbrace{-\log p(\theta)}_{\text{reg}} + \underbrace{\ell_{\text{null}}}_{\text{fit}}$  Gaussian prior  $\rightarrow$  L2; Laplace prior  $\rightarrow$  L1

## Bayesian Linear Regression

**Model:**  $y = w^\top x + \epsilon$ ,  $\epsilon \sim \mathcal{N}(0, \sigma_n^2)$ ; Prior:  $w \sim \mathcal{N}(0, \sigma_w^2 I)$

**Posterior:**  $w|X, y \sim \mathcal{N}(\mu, \Sigma)$  where  $\Sigma^{-1} = \sigma_n^{-2} X^\top X + \sigma_w^{-2} I$ ;  $\mu = \sigma_n^{-2} \Sigma X^\top y$  Note:  $\Sigma$  只依赖  $X$ , 不依赖  $y$

**Prediction:**  $y_*|x_*, X, y \sim \mathcal{N}(x_*^\top \mu, x_*^\top \Sigma x_* + \sigma_n^2)$

**Connection:** MAP=Ridge with  $\lambda = \frac{\sigma_w^2}{\sigma_n^2}$ ; Online update:  $O(nd^2)$

## Gaussian Processes

**Def:**  $f \sim \mathcal{GP}(\mu, k)$ : any finite subset jointly Gaussian.

$f_A \sim \mathcal{N}(\mu_A, K_{AA})$ ,  $[K_{AA}]_{ij} = k(x_i, x_j)$

**GP Regression:**  $y \sim \mathcal{N}(0, K_{XX} + \sigma_n^2 I) = \mathcal{N}(0, K_y)$  **Mean:**  $\mu_*(x) = k(x, X)K_y^{-1}y$  **Cov:**  $k_*(x, x') = k(x, x') - k(x, X)K_y^{-1}k(X, x')$  **Predictive:**  $y_* \sim \mathcal{N}(\mu_*, k_* + \sigma_n^2)$

**Kernels:** **Linear:**  $k(x, x') = x^\top x' + \sigma_0^2$  **RBF:**  $k = \exp(-\|x - x'\|^2_{2\ell^2})$  smooth 无限可微

**Exponential:**  $k = \exp(-\|x - x'\|_\ell)$  rough

**Matérn:**  $\nu = 0.5 \rightarrow \text{Exp}$ ,  $\nu \rightarrow \infty \rightarrow \text{RBF}$ ,  $\nu$  控制 smoothness

**Periodic:**  $k = \sigma^2 \exp(-\frac{1}{\ell^2} \sin^2(\pi|x - x'|_\ell))$  **Closure:**  $k_1 + k_2$ ,  $k_1 \cdot k_2$ ,  $c \cdot k$ ,  $\exp(k)$  仍 valid kernel

**Stationary:**  $k(x, x') = k(x - x')$ ; **Isotropic:**  $k = k(\|x - x'\|)$

**Marginal Lik:**  $\log p(y|X) = -\frac{1}{2}y^\top K_y^{-1}y - \frac{1}{2}\log \det(K_y) + C$  **Balance:** Datafit(前) vs Complexity(后)

**Approx**  $O(n^3) \rightarrow \text{lower}$ : **RFF:**  $k(x - x') \approx \varphi(x)^\top \varphi(x')$ ,  $O(nm^2 + m^3)$  Bochner: stationary kernel  $\leftrightarrow$  Fourier of non-neg measure

**Inducing Pts:** subset  $m \ll n$  points for approx

## Variational Inference

**Goal:** Approx  $p(\theta|D)$  with  $q(\theta|\lambda)$  by min  $\text{KL}(q||p)$

**ELBO:**  $\mathcal{L} = \mathbb{E}_{q|\log p(y|\theta)} - \text{KL}(q(\theta)||p(\theta))$   $\log p(y) = \mathcal{L} + \text{KL}(q||p(\cdot|D)) \geq \mathcal{L}$  Max ELBO  $\iff$  Min KL to posterior

**Derivation:** Jensen's log  $\mathbb{E}_q[\frac{p}{q}] \geq \mathbb{E}_q[\log \frac{p}{q}]$

**Gaussian KL:**  $\text{KL}(\mathcal{N}_p || \mathcal{N}_q) = \frac{1}{2} [\text{tr}(\Sigma_q^{-1} \Sigma_p) + (\mu_p - \mu_q)^\top \Sigma_q^{-1}(\mu_p - \mu_q) - d + \log(\frac{\det \Sigma_q}{\det \Sigma_p})]$

**Product:**  $\text{KL}(Q_X Q_Y || P_X P_Y) = \text{KL}(Q_X || P_X) + \text{KL}(Q_Y || P_Y)$

**Reparam Trick:**  $\theta = g(\varepsilon; \lambda)$ ,  $\varepsilon \sim \varphi$   $\mathbb{E}_{\theta \sim q}[f(\theta)] = \mathbb{E}_{\varepsilon \sim f(g(\varepsilon; \lambda))}[f(g(\varepsilon; \lambda))]$

**Gaussian:**  $\theta = \mu + \sigma \odot \varepsilon$ ,  $\varepsilon \sim \mathcal{N}(0, I)$  Enable gradient:  $\nabla_\lambda \mathbb{E}_q[f] = \mathbb{E}_{\varphi(\nabla_\lambda f(g(\varepsilon; \lambda)))}$

**Laplace Approx:**  $q(\theta) = \mathcal{N}(\hat{\theta}, \Lambda^{-1})$   $\hat{\theta} = \text{MAP}$ ;  $\Lambda = -\nabla^2 \log p(\theta|D)$  (Hessian) Good at mode, overconfident elsewhere

**Markov Chains & MCMC**

**MC basics:** **Markov:**  $X_{t+1} \perp X_{1:t-1}|X_t$

**Stationary**  $\pi$ :  $\pi = \pi P$  **Irreducible:** all states reachable from any state

**Aperiodic:**  $\gcd\{t : P^{t(x,x)} > 0\} = 1$  **Ergodic**=Irreducible+Aperiodic: unique  $\pi > 0$ ,  $\lim_{t \rightarrow \infty} q_t = \pi$

**DBE:**  $\pi(x)P(x'|x) = \pi(x')P(x|x')$  If satisfied  $\rightarrow \pi$  stationary, chain **reversible** Proof: sum over  $x'$ 得  $\pi(x) = \sum_{x'} \pi(x')P(x|x')$

**Ergodic Thrm:**  $\frac{1}{n} \sum_{i=1}^n f(X_i) \xrightarrow{\text{a.s.}} \mathbb{E}_{x \sim \pi}[f(x)]$  Hoeffding: error prob decays  $\exp(-n)$

**MH Algorithm:** Propose  $x' \sim R(x'|x)$ . Accept w.p.:  $\alpha(x'|x) = \min\left\{1, \frac{q(x')R(x'|x')}{q(x)R(x'|x)}\right\}$  Stationary:  $p(x) \propto q(x)$  (unnormalized OK) Satisfies DBE  $\rightarrow$  correct stationary dist

**Gibbs Sampling:** Iterate:  $x_i^{(t+1)} \sim p(x_i|x_{-i}^{(t)})$  Special

MH with acceptance=1 **Practical:** 顺序 scan all vars, sample each from conditional

**Langevin & SGLD:** **Langevin:**  $R(x'|x) = \mathcal{N}(x'; x - \eta \nabla f(x), 2\eta I)$  where  $\eta \propto e^{-f}$  **MALA:** MH-corrected Langevin, poly-time for log-concave

**SGLD:**  $\theta_{t+1} = \theta_t + \varepsilon_t(\nabla \log p(\theta) + \nabla \log p(D|\theta)) + \sqrt{2\varepsilon_t \xi}$  Converge:  $\sum_t \varepsilon_t = \infty$ ,  $\sum_t \varepsilon_t^2 < \infty$ ; 常用  $\varepsilon_t \in \Theta(t^{-\frac{1}{3}})$

**Gibbs Distribution:**  $p(x) = \frac{1}{Z} \exp(-f(x))$ ,  $f$ =energy function

Posterior always interpretable as Gibbs

## Bayesian Neural Networks

**Model:** Prior:  $\theta \sim \mathcal{N}(0, \sigma_p^2 I)$  **Homoscedastic:**

$y|x, \theta \sim \mathcal{N}(f(x; \theta), \sigma^2)$  fixed noise

**Heteroscedastic:**  $y \sim \mathcal{N}(f_\mu(x; \theta), \exp(f_\sigma(x; \theta)))$  input-dependent noise

**Hetero NLL:**  $-\log p(y|x, \theta) = C + \frac{1}{2} [\log \sigma^2(x) + \frac{(y - f(x; \theta))^2}{\sigma^2(x)}]$  Model can “blame” noise but pays  $\log \sigma$  penalty  $\not\propto$  collapse

**MAP for BNN:**  $\hat{\theta}_{\text{MAP}} = \arg \min \frac{1}{2\sigma_p^2} \|\theta\|^2 + \frac{1}{2\sigma_n^2} \sum_{i=(y_i-f(x_i; \theta))}^2$  Weight decay = Gaussian prior

**Prediction:**  $p(y_*|x, D) \approx \frac{1}{m} \sum_{j=1}^m p(y_*|x, \theta^{(j)})$ ,  $\theta^{(j)} \sim q$  MC approx of posterior predictive

**Uncertainty Decomp:** **Total Var=Aleatoric+Epistemic** Aleatoric(data noise):  $\frac{1}{m} \sum_j \sigma^2(x_*, \theta^{(j)})$  Epistemic(model uncertainty):  $\frac{1}{m} \sum_j |\mu(x_*, \theta^{(j)}) - \mu|$  where  $|\mu| = \frac{1}{m} \sum_j \mu(x_*, \theta^{(j)})$

**MC Dropout:**  $q_j(\theta_j) = p\delta_0(\theta_j) + (1-p)\delta_{\lambda_j}(\theta_j)$  Test 时 keep dropout  $\rightarrow$  multiple forward passes  $\rightarrow$  uncertainty

**SWAG:** Store running avg of SGD iterates:  $\mu, \Sigma$  Space:  $O(d^2)$  covariance vs  $O(Td)$  all models

**Calibration:** Goal: Confidence  $\approx$  Accuracy ECE:  $\sum \frac{|B_m|}{n} |\text{acc}(B_m) - \text{conf}(B_m)|$  **Temp Scaling:**  $\frac{z}{T}$  on logits;  $T > 1$  less confident

## Active Learning

**Objective:**  $I(S) = I(f_S; y_S) = H[f_S] - H[f_S|y_S]$  NP-hard; Greedy gives  $(1 - \frac{1}{e})$ -approx (submodular, monotone)

**Strategies:** **Uncertainty Sampling:**  $x = \arg \max H[y_x|D]$  Cannot distinguish aleatoric vs epistemic

**BALD:**  $x = \arg \max I(\hat{\theta}; y_x|D) = H[y_x|D] - \mathbb{E}_{\theta|H[y_x|D]}$  Finds where models disagree about  $y_x$

**Hetero:**  $x = \arg \max \frac{\sigma_{\text{epistemic}}^2}{\sigma_{\text{aleatoric}}^2}$

**Submodular:**  $F(A \cup \{x\}) - F(A) \geq F(B \cup \{x\}) - F(B)$  for  $A \subseteq B$  Diminishing returns; MI is submodular

## Bayesian Optimization

**Regret:**  $R_T = \sum_{t=1}^T (f^* - f(x_t))$  Goal: sublinear  $\frac{R_T}{T} \rightarrow 0$

**Acquisition Fns:** **UCB:**  $x_{t+1} = \arg \max [\mu_{t(x)} + \beta_t \sigma_{t(x)}]$   $\beta_t = 0$ : pure exploit;  $\beta_t \rightarrow \infty$ : uncertainty sampling

**Regret:**  $R_T = O(\sqrt{T\gamma_T})$  **PI:**  $\text{PI}(x) = \Phi\left(\frac{\mu(x) - f(x^+)}{\sigma(x)}\right)$  **EI:**  $\text{EI}(x) = (\mu - f^+) \Phi(Z) + \sigma \varphi(Z)$ ,  $Z = \frac{\mu(x) - f^+}{\sigma(x)}$

**Thompson:** Sample  $\tilde{f} \sim p(f|D_t)$ , pick  $\arg \max \tilde{f}$

**Info Gain**  $\gamma_T$ : Linear:  $\gamma_T = O(d \log T)$  RBF:  $\gamma_T = O((\log T)^{d+1})$  Matérn( $\nu > \frac{1}{2}$ ):  $\gamma_T = O(T^{\frac{d}{2\nu+d}} (\log T)^{\frac{2\nu}{2\nu+d}})$

## MDP & RL Foundations

**MDP:**  $(\mathcal{S}, \mathcal{A}, P, R, \gamma)$ : states, actions,  $P(s'|s, a)$ , reward, discount **Value:**  $V^{\pi(s)} = \mathbb{E} \left[ \sum_{t \geq 0} \gamma^t R_t | s_0 = s, \pi \right]$  **Q-fnc:**  $Q^{\pi(s,a)} = R(s, a) + \gamma \sum_{s'} P(s'|s, a) V^{\pi(s')}$

**Bellman Eqs:** **Expectation:**  $V^{\pi(s)} = R(s, \pi(s)) + \gamma \sum_{s'} P(s'|s, \pi(s)) V^{\pi(s')}$  **Optimality:**  $V^*(s) = \max_a [R(s, a) + \gamma \sum_{s'} P(s'|s, a) V^*(s')]$  **Q\*(s, a) =**  $R(s, a) + \gamma \sum_{s'} P(s'|s, a) \max_{a'} Q^*(s', a')$  **Matrix:**  $v^\pi = (I - \gamma P^\pi)^{-1} r^\pi$

**Bellman's Thrm:**  $\pi^*$  optimal iff greedy w.r.t. own  $V^*$ :  $\pi^*(s) = \arg \max_a Q^*(s, a)$

**PI & VI: Policy Iter:** (1) Eval  $V^\pi$  exactly(solve LSE), (2)  $\pi \rightarrow$  greedy. Fewer iters,  $O(n^3)/\text{iter}$ . **Value Iter:**  $V \rightarrow \max_{a[r+\gamma PV]}$ . More iters,  $O(n^2m)/\text{iter}$ . Both converge to optimal; VI gives  $\varepsilon$ -optimal

**POMDP:** **Belief:**  $b_{t(x)} = P(X_t = x|y_{1:t}, a_{1:t-1})$  **Bayes Filter:**  $b_{t+1}(x) \propto o(y_{t+1}|x) \sum_{x'} P(x'|x, a_t) b_{t(x)}$  Belief-state MDP: reward  $p(b, a) = \mathbb{E}_{x \sim b}[r(x, a)]$

## Tabular RL

**Model-based:**  $\hat{P}(x'|x, a) = \frac{N(x'|x, a)}{N(a|x)}$ ,  $\hat{r}(x, a) = \text{avg rewards}$  Converges but needs many samples

**Q-Learning (Off-policy):**  $Q(s, a) \leftarrow Q(s, a) + \alpha(r + \gamma \max_{a'} Q(s', a') - Q(s, a))$  Uses max (ideal best  $a'$ ); off-policy

**SARSA (On-policy):**  $Q(s, a) \leftarrow Q(s, a) + \alpha(r + \gamma Q(s', a') - Q(s, a))$  Uses actual  $a'$  from policy; on-policy

**TD Learning:**  $V(s) \leftarrow V(s) + \alpha(r + \gamma V(s') - V(s))$  As **SGD:**  $\ell = \frac{1}{2}(V(s) - (r + \gamma V(s')))^2$  Converges if Robbins-Monro:  $\sum \alpha_t = \infty$ ,  $\sum \alpha_t^2 < \infty$

**Exploration:  $\varepsilon$ -greedy:** prob  $\varepsilon$  random, else best

**Optimistic Init:**  $Q = \frac{R_{\max}}{1-\gamma}$  **Rmax:** unknown( $s, a$ )  $\rightarrow R_{\max}$ , PAC guarantee

## Deep RL

**DQN:**  $\mathcal{L} = (r + \gamma \max_{a'} Q_{\theta-(s', a')} - Q_{\theta(s, a)})^2$  **Target Net  $\theta^-$ :** stabilize; **Experience Replay:** break correlation

**Double DQN:** selection  $\theta$ , eval  $\theta^-$ ; reduces overestimation

## Policy

$\nabla_\theta J = \mathbb{E}_{\tau \sim \pi_\theta} \left[ \sum_t \nabla \log \pi_{\theta(a_t|s_t)} G_t \right]$   $\nabla \log P(\tau) = \sum_t \nabla \log \pi(a_t|s_t)$  (dynamics cancel!) **REINFORCE:** MC estimate, high variance

**Baseline:**  $G_t = b(s_t)$ ,  $b = V(s)$  optimal; unbiased

**Actor-Critic:** **Actor:**  $\pi_{\theta(a|s)}$ ; **Critic:**  $V_{\varphi(s)}$  or  $Q_{\varphi(s,a)}$   $\nabla J \approx \mathbb{E}[\nabla \log \pi(a|s)(Q(s, a) - V(s))]$  Critic bootstrap  $\downarrow$  variance  $\rightarrow$  bias

**Advanced:** **TRPO:**  $\max \mathbb{E} \left[ \left( \frac{\pi_\theta}{\pi_{\text{old}}} \right) A^{\pi_{\text{old}}} \right]$  s.t. KL  $\leq \delta$

**DDPG:** continuous actions, deterministic  $\mu_{\theta(s)}$  **Adv Fnc:**  $A^{\pi(s,a)} = Q^{\pi(s,a)} - V^{\pi(s)}$

## Bayesian Networks

**Def:** DAG  $G$  + CPDs  $P(X_v | \text{Pa}_{X_v})$  **Joint:**  $P(X_{1:n}) = \prod_i P(X_i | \text{Pa}_i)$  Variable order 重要 for compact representation

**D-Separation:**  $X \perp Y | Z$  iff all paths blocked by  $Z$   
**Active trails** (path 通): Chain  $X \rightarrow Y \rightarrow Z$ :  $Y$  not observed Fork  $X \leftarrow Y \rightarrow Z$ :  $Y$  not observed Collider  $X \rightarrow Y \leftarrow Z$ :  $Y$  or descendant is observed

**Inference:** VE: Sum out non-query vars; complexity = treewidth  
**BP (Sum-Product):**  $\mu_{v \rightarrow u} \propto \prod_{u' \sim v} \mu_{u' \rightarrow v}$  Exact on trees; loopy 可能不 converge  
**Max-Product:** replace  $\sum$  with max for MPE/ MAP

**Approx Inference:** Rejection Sampling: discard samples 不符 evidence, inefficient if rare **Likelihood Weighting**: weight by evidence prob **Gibbs**: sample each var from conditional given rest

**Learning:** Params:  $\hat{\theta}_{X_i | \text{Pa}_i} = \frac{\text{count}(X_i, \text{Pa}_i)}{\text{count}(\text{Pa}_i)}$  (MLE)  
**Structure:** Score-based, MLE score 偏好 fully connected BIC:  $S_{\text{BIC}} = \sum \hat{I}(X_i; \text{Pa}_i) - \frac{\log N}{2N} |G|$  **Chow-Liu:** max spanning tree on MI weights → optimal tree BN

## Diffusion Models

**Setup:** Forward: data → noise (fixed, no learning)  
**Backward:** noise → data (learned generation) Latent var model:  $x_{1:T}$  are latents,  $x_0$  is data

**Forward Process:**  $q(x_t | x_{t-1}) = \mathcal{N}(x_t; \sqrt{1-\beta_t}x_{t-1}, \beta_t I)$   $x_t = \sqrt{1-\beta_t}x_{t-1} + \sqrt{\beta_t}\varepsilon_t$  Schedule:  $\beta_t \in (0, 1)$  单调增,  $\beta_1 \approx 10^{-4}$ ,  $\beta_T \approx 0.02$

**Closed-Form Marginal** ★: Define:  $\alpha_t = 1 - \beta_t$ ,  $|(\alpha)_t = \prod_{s=1}^t \alpha_s$   $q(x_t | x_0) = \mathcal{N}(\sqrt{|(\alpha)_t}x_0, (1 - |(\alpha)_t)I)$  **Reparam:**  $x_t = \sqrt{|(\alpha)_t}x_0 + \sqrt{1 - |(\alpha)_t}\varepsilon$ ,  $\varepsilon \sim \mathcal{N}(0, I)$  As  $t \rightarrow T$ :  $|(\alpha)_T \rightarrow 0$ ,  $x_T \sim \mathcal{N}(0, I)$  indep of  $x_0$

**Reverse Process:**  $p_{\lambda(x_{t-1}|x_t)} = \mathcal{N}(\mu_{\lambda(x_t,t)}, \sigma_t^2 I)$   
Prior:  $p(x_T) = \mathcal{N}(0, I)$  Generate: sample  $x_T$ , iteratively denoise to  $x_0$

**Forward Posterior:**  $q(x_{t-1} | x_t, x_0) = \mathcal{N}(\tilde{\mu}_t, \tilde{\beta}_t I)$   
 $\tilde{\mu}_t = \frac{\sqrt{|(\alpha)_{t-1}}\beta_t}{1 - |(\alpha)_t}x_0 + \frac{\sqrt{\alpha_t}(1 - |(\alpha)_{t-1})}{1 - |(\alpha)_t}x_t$   $\tilde{\beta}_t = \frac{(1 - |(\alpha)_{t-1})\beta_t}{1 - |(\alpha)_t}$   
Key: given  $x_0, x_t$ , forward posterior is Gaussian (tractable)

**ELBO & Loss:**  $\mathcal{L} = \text{const} - \sum_{t=2}^T \underbrace{\text{KL}(q(x_{t-1} | x_t, x_0) \| p_{\lambda(x_{t-1}|x_t)})}_{L_t}$  Two Gaussians same var:  $\text{KL} \propto \|\mu_1 - \mu_2\|^2$

★**Noise Prediction** : Predict  $\varepsilon$  instead of  $\mu$  (more stable): From  $x_t = \sqrt{|(\alpha)_t}x_0 + \sqrt{1 - |(\alpha)_t}\varepsilon$ :  
 $\tilde{\mu}_t = \frac{1}{\sqrt{\alpha_t}}(x_t - \frac{\beta_t}{\sqrt{1 - |(\alpha)_t}}\varepsilon)$  **Simple Loss:**  $L_{\text{simple}} = \mathbb{E}_{t,x_0,\varepsilon} [\|\varepsilon - \varepsilon_{\lambda(x_t,t)}\|^2]$

**Training Algo:** Repeat: sample  $x_0 \sim p_{\text{data}}$ ,  $t \sim \text{Unif}\{1, \dots, T\}$ ,  $\varepsilon \sim \mathcal{N}(0, I)$   $x_t = \sqrt{|(\alpha)_t}x_0 + \sqrt{1 - |(\alpha)_t}\varepsilon$   $\nabla_{\lambda} \|\varepsilon - \varepsilon_{\lambda(x_t,t)}\|^2$

**Sampling Algo:**  $x_T \sim \mathcal{N}(0, I)$  For  $t = T, \dots, 1$ :  $z \sim \mathcal{N}(0, I)$  if  $t > 1$  else  $z = 0$   $x_{t-1} = \frac{1}{\sqrt{\alpha_t}}(x_t - \frac{\beta_t}{\sqrt{1 - |(\alpha)_t}}\varepsilon_{\lambda(x_t,t)}) + \sigma_t z$

**Connection:**  $\varepsilon_{\lambda(x_t,t)} \approx -\sqrt{1 - |(\alpha)_t} \nabla_{x_t} \log q(x_t)$   
**Denoising = Score matching**

**Variants:** LDM: diffusion in VAE latent space, more efficient DDIM: deterministic sampling, fewer steps  
**Cond Gen:**  $\varepsilon_{\lambda(x_t,t,c)}$ , Classifier-Free Guidance:  $\tilde{\varepsilon} = (1 + w)\varepsilon_{\lambda(x_t,t,c)} - w\varepsilon_{\lambda(x_t,t)}$

## QuickCheck:

- VI: Approx posterior via ELBO. Laplace MAP, Reparam for grad.
- MCMC: Sample posterior. MH accept/reject, Gibbs coordinate, Langevin uses  $\nabla$ .
- GP: Prior over fncts, closed-form posterior. RBF smooth, Matérn tunable.
- BNN: Prior on weights, MC predictive. Aleatoric=data noise, Epistemic=model.
- Active: Max MI, BALD for disagreement, submodular→greedy( $1 - \frac{1}{e}$ ).
- BO: UCB balance explore/exploit, EI expected gain, Thompson sample.
- BN: DAG factorization, d-sep for indep, BP exact on trees.
- KF: Linear Gaussian, Kalman gain trades predict vs observe.
- Diffusion: Forward=noise, Backward=denoise, train predict  $\varepsilon$ .
- On/Off: On=SARSA,REINFORCE,PPO; Off=Q-learn,DQN,SAC
- Bellman:  $V = R + \gamma PV$ ;