

Probability review

Product rule:  $P(X_{1:n}) = P(X_1) \prod_{i=2}^n P(X_i | X_{1:i-1})$ .

Sum rule:  $P(X,Y) = \sum_y P(X,Y=y)$ .

Bayes rule:  $P(X|Y) = \frac{P(Y|X)P(X)}{P(Y)}$ .

Independence:  $P_{XY} = P_X P_Y$ .

Conditional independence:  $P_{XY|Z} = P_{X|Z} P_{Y|Z}$ .

Linearity of expectation:  $\mathbb{E}_{x,y}[aX + bY] = a\mathbb{E}_x[X] + b\mathbb{E}_y[Y]$ .

Expectation:  $\mathbb{E}_p[f(X)] = \sum_{i=0}^n p(x)f(x)$  (don't forget  $p(x)$ ).

Variance:  $\text{Var}[X] = \mathbb{E}[(X - \mathbb{E}[X])^2] = \mathbb{E}[X^2] - \mathbb{E}[X]^2$ .

Linearity of variance:

$\text{Var}[aX + bY + c] = a^2\text{Var}[X] + b^2\text{Var}[Y] + 2ab\text{Cov}(X,Y)$ .

Covariance:  $\text{Cov}(X,Y) = \mathbb{E}[(X - \mathbb{E}[X])(Y - \mathbb{E}[Y])]$ .

Cum. dist. function:  $\mathbb{P}(x \leq t) = F(t)$ , where  $F$  is CDF.

Matrix inversion:  $\begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1} = \frac{1}{ad-bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$ .

Multivariate Gaussian:

$$\mathcal{N}(x;\mu,\Sigma) = \frac{1}{\sqrt{(2\pi)^d |\Sigma|}} \exp\left(-\frac{1}{2}(x-\mu)^\top \Sigma^{-1}(x-\mu)\right).$$

A random vector is Gaussian if (1) the RVs are Gaussian, and (2) any linear combination of the RVs is Gaussian.

Properties:

$$\begin{aligned} X_A &\sim \mathcal{N}(\mu_A, \Sigma_{AA}) \\ X_A | X_B &\sim \mathcal{N}(\mu_{A|B}, \Sigma_{A|B}) \\ \mu_{A|B} &= \mu_A + \Sigma_{AB} \Sigma_{BB}^{-1} (x_B - \mu_B) \\ \Sigma_{A|B} &= \Sigma_{AA} - \Sigma_{AB} \Sigma_{BB}^{-1} \Sigma_{BA} \\ MX &\sim \mathcal{N}(M\mu, M\Sigma M^\top) \\ X + X' &\sim \mathcal{N}(\mu + \mu', \Sigma + \Sigma') \end{aligned}$$

If asked about conditional distribution of linear functions of Gaussians, notice that the functions can be jointly computed by a matrix operation, which results in a Gaussian, or use LoV.

Kalman filters: Motion model updates the state  $X_{t+1} = FX_t + \epsilon_t$ . Sensor model computes observation  $Y_t = HX_t + \eta_t$ .  $\epsilon_t \sim \mathcal{N}(0, \Sigma_\epsilon)$ ,  $\eta_t \sim \mathcal{N}(0, \Sigma_\eta)$ .  $\epsilon_t \uparrow \Rightarrow K_{t+1} \uparrow$ ,  $\eta_t \uparrow \Rightarrow K_{t+1} \downarrow$ ,  $\Sigma_t \uparrow \Rightarrow K_{t+1} \uparrow$ . Update:

$$\begin{aligned} X_{t+1} | y_{1:t+1} &\sim \mathcal{N}(\mu_{t+1}, \Sigma_{t+1}) \\ \mu_{t+1} &= F\mu_t + K_{t+1}(y_{t+1} - HF\mu_t) \\ \Sigma_{t+1} &= (I - K_{t+1}H)(F\Sigma_t F^\top + \Sigma_\epsilon) \\ K_{t+1} &= (F\Sigma_t F^\top + \Sigma_\epsilon)H^\top (H(F\Sigma_t F^\top + \Sigma_\epsilon)H^\top + \Sigma_y)^{-1} \end{aligned}$$

Entropy:  $H[p] = \mathbb{E}_p[-\log p(x)]$ .

d-Gaussian:  $H[\mathcal{N}(\mu, \Sigma)] = \frac{d}{2}(1 + \log(2\pi)) + \frac{1}{2}\log|\Sigma|$ .

1-Gaussian:  $H[\mathcal{N}(\mu, \sigma^2)] = \frac{1}{2}\log(2\pi\sigma^2) + \frac{1}{2}$ .

$H[p,q] = H[p] + H[q|p]$ .  $H[X|Y] = \mathbb{E}_p\left[\log \frac{p(x,y)}{p(x)}\right]$ .

KL-divergence:  $KL(q||p) = \mathbb{E}_q\left[\log \frac{q(x)}{p(x)}\right] = \mathbb{E}_q\left[-\log \frac{p(x)}{q(x)}\right]$ . Non-negative (0 if  $p=q$ ,  $\infty$  if  $p(x)=0$  for  $x$  with  $q(x)>0$ ). Additional expected surprise when observing  $q$  samples while assuming  $p$ .

Mutual information:  $I(X;Y) = H[X] - H[X|Y]$ . Symmetric:  $I(X;Y) = I(Y;X)$ . Information never hurts:  $I(X;Y) \geq 0$ .

Jensen's inequality: If  $f$  convex:  $f(\mathbb{E}[X]) \leq \mathbb{E}[f(X)]$ .

MLE:  $\hat{\theta} = \text{amax}_\theta p(y|X, \theta) = \text{amax}_\theta \sum_{i=1}^n \log p(y_i | x_i, \theta)$ .

MAP:  $\hat{\theta} = \text{amax}_\theta p(\theta|X, y) = \text{amax}_\theta \log p(\theta) + \sum_{i=1}^n \log p(y_i | x_i, \theta)$ .

Bayesian learning: Prior:  $p(\theta)$ . Likelihood:  $p(y|X, \theta) = \prod_{i=1}^n p(y_i | x_i, \theta)$ . Posterior:  $p(\theta|X, y) = \frac{1}{Z} p(\theta) \prod_{i=1}^n p(y_i | x_i, \theta)$ .  $Z = \int p(\theta) \prod_{i=1}^n p(y_i | x_i, \theta) d\theta$ . Prediction:  $p(y^* | x^*, X, y) = \int p(y^* | x^*, \theta) p(\theta|X, y) d\theta$ . In general, intractable: GP, VI, and MCMC solve.

Aleatoric uncertainty: Uncertainty due to irreducible noise in data. Epistemic uncertainty: Uncertainty due to lack of data.

LoTV:  $\text{Var}[y^* | x^*] = \mathbb{E}_\theta[\text{Var}_{y^*}[y^* | x^*, \theta]] + \text{Var}_\theta[\mathbb{E}_{y^*}[y^* | x^*, \theta]]$ .

Bayesian Linear Regression  $f^* = w^\top x^*$ ,  $y^* = f^* + \epsilon$ ,  $\epsilon \sim \mathcal{N}(0, \sigma_n^2)$ . Prior:  $w \sim \mathcal{N}(0, \sigma_p^2 I)$ . Posterior:

$$\begin{aligned} w | X, y &\sim \mathcal{N}(\bar{\mu}, \bar{\Sigma}), \quad \bar{\mu} = (X^\top X + \sigma_n^2 \sigma_p^{-2} I)^{-1} X^\top y = \sigma_n^{-2} \Sigma X^\top y, \\ \bar{\Sigma} &= (\sigma_n^{-2} X^\top X + \sigma_p^{-2} I)^{-1}. \end{aligned}$$

Inference:  $y^* = x^{*\top} w + \epsilon \Rightarrow f^* | x^*, X, y \sim \mathcal{N}(x^{*\top} \bar{\mu}, x^{*\top} \bar{\Sigma} x^* + \sigma_n^2)$ .

Logistic regression: Bernoulli likelihood  $(\pi^y (1 - \pi)^{1-y})$ .

Recursive update:  $p^{(t+1)}(\theta) = p(\theta | y_{1:t+1}) = \frac{1}{2} p^{(t)}(\theta) p(y_{t+1} | \theta)$ .

Online data recursion:  $X^\top X = \sum_{i=1}^n x_i x_i^\top$ ,  $X^\top y = \sum_{i=1}^n y_i x_i$ .

Gaussian Processes Problem: BLR can only make linear predictions. Solution: GP describes distributions over (non-linear) functions. In function space,  $f = Xw$ , which can be sampled by  $f \sim \mathcal{N}(0, X^\top X) \Rightarrow$  data points enter as inner products  $\Rightarrow$  use kernel function  $f \sim \mathcal{N}(0, k(X, X))$ .  $\mathcal{GP}(\mu, k)$  is formally defined as an infinite collection of RVs, of which any finite number are jointly Gaussian.

Kernel: Formally,  $k(x, x') = \phi(x)^\top \phi(x')$  for some feature function  $\phi \Rightarrow$  kernel function is more efficient. Intuitively,  $k(x, x')$  describes how  $f(x)$  and  $f(x')$  are related.  $k(X, X)$  is symmetric and positive semidefinite ( $z^\top M z \geq 0$  for all  $z \neq 0$ ). Must satisfy  $k(x, x') \leq \sqrt{k(x, x)k(x', x')}$ . Stationary:  $k(x, x') = k(x - x')$ . Isotropic:  $k(x, x') = k(\|x - x'\|_2)$  (same as stat. in 1D). Linear: Line. Gaussian (RBF): Smooth, larger  $\ell$ : smoother. Laplace (exponential): Non-smooth, larger  $\ell$ : smoother. Matérn:  $\nu = 1/2$ : Laplace,  $\nu \rightarrow \infty$ : Gaussian. Addition, multiplication, scaling, polynomial function of kernel functions are also kernel functions.

Inference:  $y^* | x^*, X, y \sim \mathcal{N}(\mu^*, k^* + \sigma_n^2)$  with data  $X_A$ :

$$\begin{aligned} \mu^* &= \mu(x^*) + k_{x^*, A}^\top (K_{AA} + \sigma_n^2 I)^{-1} (y - \mu_A) \\ k^* &= k(x^*, x^*) - k_{x^*, A}^\top (K_{AA} + \sigma_n^2 I)^{-1} k_{x^*, A}. \end{aligned}$$

GP posterior:  $\mathcal{GP}(\mu', k')$  such that:

$$\begin{aligned} \mu'(x) &= \mu(x) + k_{x, A}^\top (K_{AA} + \sigma_n^2 I)^{-1} (y - \mu_A) \\ k'(x, x') &= k(x, x') - k_{x, A}^\top (K_{AA} + \sigma_n^2 I)^{-1} k_{x', A}. \end{aligned}$$

Forward sampling: Iter sample 1-d Gaussian with prod. rule  $p(f_1, \dots, f_n)$ . Model selection: Hyperparameters matter a lot  $\Rightarrow$  Can be learned by maximizing marginal likelihood,

$$\hat{\theta} = \text{amin}_\theta y^\top K_{y, \theta}^{-1} y + \log \det(K_{y, \theta}),$$

which balances the goodness of the fit (term 1) and model complexity (term 2).

Problem: To learn a GP, need to invert matrices, which take  $\mathcal{O}(n^3)$  (BLR:  $\mathcal{O}(dn^2)$ ). Local methods: Stationary kernels depend on distance, so only condition if  $|k(x, x')| \geq \tau$ . Approximation: Approximate stationary kernel with Random Fourier Transform. Inducing point (FITC): Throw away data where there is a lot (cubic in inducing points, linear in data points).

Variational Inference In some cases, not realistic to assume Gaussian  $\Rightarrow$  Approximate  $p(\theta|y) = \frac{1}{Z} p(\theta, y) \approx q_\lambda(\theta) \Rightarrow$  Minimize  $KL(q_\lambda || p) \Rightarrow q^* = \text{amax}_\lambda \mathbb{E}_{\theta \sim q_\lambda} [\log p(y|\theta)] - KL(q_\lambda || p_{\text{prior}})$ . I.e., minimizing  $KL(q_\lambda || p) \equiv$  maximizing expected likelihood, while remaining close to prior. ELBO: Lower bounds  $\log p(y)$ , so it is a good method of model selection.

Forward KL  $KL(p || q_\lambda)$ : covers full prob. density, but intractable. Backward KL  $KL(q_\lambda || p)$ : greedily covers mode.

Laplace approximation:  $q_\lambda(\theta) = \mathcal{N}(\hat{\theta}, \Lambda)$ , where  $\hat{\theta} = \text{amax}_\theta p(\theta|y)$  and  $\Lambda = -H_\theta \log p(\theta|y)$ . Matches shape of the true posterior around its mode  $\Rightarrow$  Extremely overconfident predictions, because it is greedy.

Problem: Want to compute gradient w.r.t.  $\lambda$  of an expectation w.r.t.  $\lambda$ . Reparameterization trick: Suppose  $\epsilon \sim \phi$ ,  $\theta = g(\epsilon, \lambda)$  (diff. and inv.), then  $\mathbb{E}_{\theta \sim q_\lambda} [f(\theta)] = \mathbb{E}_{\epsilon \sim \phi} [f(g(\epsilon, \lambda))]$ . (Can be used for MC obj, unbiased.) Gaussian:  $\theta = g(\epsilon, \lambda) = \Sigma^{1/2} \epsilon + \mu \sim \mathcal{N}(\mu, \Sigma)$ . Inference:  $p(y^* | x^*, y) \approx \int p(y^* | f^*) q_\lambda(f^* | x^*) df^*$  (intractable, but single dimension).

Markov Chain Monte Carlo Markov chain: Seq. of RVs s.t.  $X_{t+1} \perp X_{1:t-1} | X_t$ . Stationary dist.:  $\pi(x) = \sum_{x'} p(x | x') \pi(x')$ . (Solve by  $\pi = P^\top \pi$ ,  $\mathbf{1}^\top \pi = 1$ .) Ergodicity:  $\exists t [\forall x, x' [p^{(t)}(x' | x) > 0]]$ , where  $p^{(t)}$  is prob. to reach  $x'$  from  $x$  in exactly  $t$  steps. (Terminal states  $\Rightarrow$  not ergodic.) (Ensure ergodicity by self-loops.) Fundamental theorem of ergodic MCs: Ergodic MC always converges to a unique pos. stat. dist. Detailed balance equation: For an unnormalized dist.  $q$  an MC satisfies DBE iff  $q(x)p(x' | x) = q(x')p(x | x') \Rightarrow$  stat. dist.  $= \frac{1}{Z} q$ . Sampling: Sample MC's stat. dist. by first doing a burn-in  $t_0$  to reach stat. dist. Idea: Approximate intractable  $p$  by drawing  $m$  samples from MC with stat. dist.  $p(\theta|y) \Rightarrow p(y^* | x^*, y) = \mathbb{E}_{p(\cdot|y)} [p(y^* | x^*, \theta)] = \frac{1}{m} \sum_{i=1}^m p(y^* | x^*, \theta_i)$ .

**Hoeffding's inequality:** Compute bound on error.  
 $p(|\mathbb{E}_{p(\cdot|y)}[p(y^* | x^*, \theta)] - \frac{1}{m} \sum_{i=1}^m p(y^* | x^*, \theta_i)| > \epsilon) \leq 2 \exp(-2m\epsilon^2/C^2)$ , where  $C$  is the upper bound of values (1 for prob. dist.). To get a prob.  $\leq \delta$  of error  $> \epsilon$ , we need  $m \geq \log 2 - \log \delta / 2\epsilon^2$  samples.

**Metropolis-Hastings:** Arbitrary proposal dist.  $r(x' | x)$ . Follow proposal with prob.  $\alpha(x' | x) = \min\left\{1, \frac{q(x')r(x|x')}{q(x)r(x'|x)}\right\} \Rightarrow$  satisfies DBE to get stat. dist.  $\frac{1}{Z}q(x)$ . Arbitrary proposal influences how fast we converge to stat. dist. **Gaussian:** Prob. dist. has form  $p(x) = \frac{1}{Z} \exp(-f(x)) \Rightarrow \alpha(x' | x) = \min\left\{q, \frac{r(x|x')}{r(x'|x)} \exp(f(x) - f(x'))\right\}$ . If  $r(x' | x) = \mathcal{N}(x'; x, \tau I) \Rightarrow \frac{r(x|x')}{r(x'|x)} = 1$  (symmetry). If  $r$  proposes low energy (high prob) region, acceptance is 1. **Problem:** Uninformed  $\Rightarrow$  Use gradient information (MALA requires full access to  $f$ ).

**Bayesian Deep Learning** **Non-linear dependencies.**

**Prior:**  $\theta \sim \mathcal{N}(0, \sigma_p^2 I)$ . **Likelihood:**  $y | x, \theta \sim \mathcal{N}(\mu_\theta(x), \sigma_\theta^2(x))$ .

**Homoscedastic:** Same noise for all data points,  $\sigma_\theta^2(x) = c$ .

**Heteroscedastic:** Varying noise.

**MAP:**  $\text{amin}_\theta \frac{1}{2\sigma_p^2} \|\theta\|^2 - \sum_{i=1}^n \log \sigma_\theta^2(x_i) + \frac{(y_i - \mu_\theta(x_i))^2}{2\sigma_\theta^2(x_i)}$ . Attenuate loss for certain data points by attributing error to large variance. Fails to model epistemic uncertainty  $\Rightarrow$  VI (Gaussian in expectation) and Monte Carlo or MCMC:

$\mathbb{E}[y^* | x^*, y] \approx \frac{1}{m} \sum_{j=1}^m \mu_{\theta_j}(x^*)$ .

$\text{Var}[y^* | x^*, y] \approx \frac{1}{m} \sum_{j=1}^m \sigma_{\theta_j}^2(x^*) + \frac{1}{m-1} \sum_{j=1}^m (\mu_{\theta_j}(x^*) - \bar{\mu}(x^*))^2$

**MCMC:** Produce seq.  $\theta_1, \dots, \theta_T$ , then  $p(y^* | x^*, y) \approx \frac{1}{T} \sum_{j=1}^T p(y^* | x^*, \theta_j)$ . **Problem:** Cannot store  $T$  times params of network. **Solution:** Approx. with Gaussian and running mean/var.

**MC dropout:** Dropout during inference  $\Leftrightarrow$  VI with Bernoulli.

**Prob. ensembles:** Train networks on rand. subsets, average.

**Calibration:** Well-calibrated  $\Leftrightarrow$  confidence (assigned prob.)  $\approx$  frequency. **Reliability diagram:** Bin according to class pred. probs. (assume class 1). Above line: underconfident, below line: overconfident. (No samples  $\Rightarrow$  empty bin in diagram).  $\text{freq}(B_m) = \frac{1}{|B_m|} \sum_{i \in B_m} \mathbb{1}\{Y_i = 1\}$ ,  $\text{conf}(B_m) = \frac{1}{|B_m|} \sum_{i \in B_m} p(Y_i = 1 | x_i)$ . **ECE:** avg. deviation from perfect calibration:  $\ell_{\text{ECE}} = \sum_{m=1}^M \frac{|B_m|}{n} |\text{freq}(B_m) - \text{conf}(B_m)|$ .

**Active Learning** **Decide which data to collect:**  $\mathcal{NP}$ -hard.

**Uncertainty sampling:** Greedily pick points with maximal mutual information  $\Rightarrow x_{t+1} = \text{amax}_x I(f_x; y_x | \mathcal{Y}_{S_t})$ . If Gaussian:  $x_{t+1} = \text{amax}_x \sigma_{x|S_t}^2 / \sigma_n^2(x)$ .  $\gamma_T = \max_{x_{1:T}} I(f(x_{1:T}); y_{1:T})$ . Monotone submodular. Constant factor approx:  $I(f(x_{1:T}); y_{1:T}) \geq (1 - 1/e) \gamma_T$  (near-optimal,  $1 - 1/e \approx 0.63$ ).

**BALD:**  $x_{t+1} = \text{amax}_x I(y_x; \theta | x_{1:t}, y_{1:t}) = \text{amax}_x H[y_x | x_{1:t}, y_{1:t}] - \mathbb{E}_{\theta | x_{1:t}, y_{1:t}}[H[y_x | \theta]]$ . Want points where the post. is uncertain because all  $\theta$  are certain about their differing pred. Approximate term 2 using VI and MC.

**Bayesian Optimization** **Not only reduce uncertainty, but also maximize objective.**  $x_{t+1} = \text{amax}_x a(x)$ .

**Regret:**  $R_T = \sum_{t=1}^T (\max_x f(x) - f(x_t))$ . Want algorithm with sublinear regret:  $\lim_{T \rightarrow \infty} R_T/T = 0$ .  $f^* = \max_x f(x)$ .

**GP-UCB:** Optimism in the face of uncertainty: pick point where we can hope for best outcome:  $a_{\text{UCB}} = \mu_t(x) + \beta_t \sigma_t(x)$ .  $\mu, \sigma$  from GP.  $R_T \in \mathcal{O}(\sqrt{\gamma_T/T})$ . **GP bounds:** Linear:  $\gamma_T \in \mathcal{O}(d \log T)$ , Gaussian:  $\mathcal{O}((\log T)^{d+1})$ , Matérn:  $\mathcal{O}(T^{d/2v+d} (\log T)^{2v/2v+d})$ .

**PI:**  $a_{\text{PI}}(x) = \Phi((\mu_t(x) - f^*)/\sigma_t(x))$  is prob. to improve  $f^*$ . Greedy.

**EI:**  $a_{\text{EI}}(x) = (\mu_t(x) - f^*) \Phi((\mu_t(x) - f^*)/\sigma_t(x)) + \sigma_t(x) \phi((\mu_t(x) - f^*)/\sigma_t(x))$  is expectation of improvement.

**Thompson sampling:** Draw sample from GP and select max.

**Markov Decision Processes** **Env. that makes Markov ass.** (states  $\mathcal{X}$ , actions  $\mathcal{A}$ , transitions  $p(x' | x, a)$ , rewards  $r(x, a)$ ). **Policy:**  $\pi$  maps states to actions (induces MC with  $p(x' | x) = \sum_a \pi(a | x) p(x' | x, a)$ ), want to find  $\pi$  that max. long-term rewards. Horizon  $T$  reward:  $\mathbb{E}_\pi[\sum_{t=0}^T r(x_t, a_t)]$ . Horizon  $\infty$  reward:  $\mathbb{E}_\pi[\sum_{t=0}^\infty \gamma^t r(x_t, a_t)]$ . **Geo series:**  $\sum_{t=0}^\infty \gamma^t = 1/(1-\gamma)$ .

$V^\pi(x) = \mathbb{E}_x[\sum_{t=0}^\infty \gamma^t r(X_t, \pi(X_t)) | X_0 = x]$   
 $= r(x, \pi(x)) + \gamma \sum_{x'} p(x' | x, \pi(x)) V^\pi(x')$  (Bellman eq).

$Q(x, a) = r(x, a) + \gamma \sum_{x'} p(x' | x, a) V^\pi(x')$ .  $V(x) = \max_a Q(x, a)$ .

**Bellman theorem:**  $\pi$  is optimal  $\Leftrightarrow$  greedy w.r.t.  $V^\pi$ .

**Policy iteration:**  $\pi \Rightarrow V^\pi, V \Rightarrow \pi_V$  (alternate).  $\pi_V(x) = \text{amax}_a r(x, a) + \gamma \sum_{x'} p(x' | x, a) V(x')$  (greedy). Converges monotonically, **guaranteed to converge** in  $\mathcal{O}(|\mathcal{X}|^2 |\mathcal{A}| / (1-\gamma))$  iterations, expensive (computed efficiently by solving single LSoE).

**Value iteration:** Dynamic programming:  
 $V_t(x) = \max_a r(x, a) + \gamma \sum_{x'} p(x' | x, a) V_{t-1}(x')$ . Iterates until  $\|v_t - v_{t-1}\|_\infty \leq \epsilon$ :  **$\epsilon$ -optimal convergence**, in polynomial in iterations, per iteration:  $\mathcal{O}(|\mathcal{X}|^2 |\mathcal{A}|)$ , inexpensive. Then, pick greedy policy.

**Reinforcement Learning** **Learn within unknown MDP. On-policy:** Learn from own data, **Off-policy:** Learn from other policy data, **Model-based:** Learn MDP and solve, **Model-free:** Learn value function directly. Data points:  $\langle x, a, r, x' \rangle$ .

**Robbins-Monro:**  $\sum_{t=0}^\infty x_t = \infty, \sum_{t=0}^\infty x_t^2 < \infty$ . E.g.  $1/t$ .

**$\epsilon$ -greedy (based):** Pick random action with prob.  $\epsilon_t$ , or best action according to MDP with prob.  $1 - \epsilon_t$ . **Guaranteed to converge to optimal policy if  $\epsilon_t$  satisfies RM.** Problem: does not quickly eliminate suboptimal actions.

$R_{\max}$  (based): Solves problem. Add fairy tale  $p(x^* | x^*, a) = 1, r(x^*, a) = R_{\max}$ , assume unexplored go there.

**TD-learning (on, free):**  $V^\pi(x) \leftarrow (1 - \alpha_t) V^\pi(x) + \alpha_t (r + \gamma V^\pi(x'))$ . **Guaranteed to converge if  $\alpha_t$  satisfies RM and all states are visited infinitely often.** Space:  $\mathcal{O}(|\mathcal{X}|)$ .

**Q-learning (off, free):**  $Q(x, a) \leftarrow (1 - \alpha_t) Q(x, a) + \alpha_t (r + \gamma \max_{a'} Q(x', a'))$ . **Guaranteed to converge if  $\alpha_t$  satisfies RM and all state-action pairs are visited infinitely often.** Space:  $\mathcal{O}(|\mathcal{X}| |\mathcal{A}|)$ .

**DQN (off, free, cont. states):** GD on  $\frac{1}{2} (Q(x, a; \theta) - (r + \gamma \max_{a'} Q(x', a'; \theta^{\text{old}})))^2$  (Bellman error). **Slow to converge:** maintain constant target network. **DDQN:** Maximization bias makes DQN overestimate. Solution: 2 Q networks where we take minimum to be value.

**Policy search (on, free, cont. actions):** Parametrize  $\pi(x; \theta)$ . Maximize expected trajectory reward.  $\nabla_\theta \mathbb{E}_{\tau \sim \pi_\theta} [r(\tau)] = \mathbb{E}_{t \sim \pi_\theta} [r(\tau) \nabla_\theta \log \pi_\theta(\tau)] = \mathbb{E}_{t \sim \pi_\theta} [r(\tau) \sum_{i=0}^T \nabla_\theta \log \pi_\theta(a_t | x_t)] \Rightarrow$  Do not need to know MDP to compute gradient. **Baselines:** Large variance  $\Rightarrow$  introduce baseline:  $\mathbb{E}_{\tau \sim \pi_\theta} [r(\tau) \nabla_\theta \log \pi_\theta] = \mathbb{E}_{\tau \sim \pi_\theta} [(r(\tau) - b(\tau)) \nabla_\theta \log \pi_\theta(\tau)]$ .

**REINFORCE (on, free):**  $\theta \leftarrow \theta + \eta \gamma^t G_t \nabla_\theta \log \pi_\theta(a_t | x_t)$ , where  $G_t = r(\tau) - b_t = \sum_{t'=t}^T \gamma^{t'-t} r_{t'}$ .

**Actor-critic (on, free):** REINFORCE gradient =  $\mathbb{E}_{(x,a) \sim \pi_\theta} [Q(x, a) \nabla_\theta \log \pi_\theta(a | x)]$ . So: parametrize actor  $\pi_\theta$  and critic  $Q_\theta$ . Use in each others' update equations:  
 $\theta_\pi \leftarrow \theta_\pi + \eta_t Q(x, a | \theta_Q) \nabla_\theta \log \pi_\theta(a | x)$ .  
 $\theta_Q \leftarrow \theta_Q - \eta_t (Q(x, a; \theta_Q) - r - \gamma Q(x', \pi(x'; \theta_\pi); \theta_Q)) \nabla_\theta Q(x, a; \theta)$ .

**A2C (on, free):** Add value network  $V_\theta$  for the baseline:  $A(x, a) = Q(x, a) - V(x, a)$  (advantage function). This centers the Q-values.

**DDPG (off, free):** Replace  $\max_{a'} Q(x', a'; \theta^{\text{old}})$  in DQN by  $\pi(x'; \theta_\pi)$ , where  $\pi$  should follow the greedy policy w.r.t.  $Q$ . **Key idea:** If we use a rich enough parameterization of policies, selecting the greedy policy w.r.t.  $Q$  is equivalent to  $\theta_\pi^* = \text{amax}_{\theta_\pi} \mathbb{E}_{x \sim \mu} [Q(x, \pi(x; \theta_\pi); \theta_Q)]$ .  $\mu(x) > 0$  is an exploration distribution with full support. This needs det.  $\pi$ , thus we inject noise for exploration (akin  $\epsilon$ -greedy).

**TD3 (off, free):** Add second critic network to address max. bias.

**SAC (off, free):** Add entropy regularization to loss  $\lambda H(\pi_\theta)$ .

**Planning:** Det. transition function  $x_{t+1} = f(x_t, a_t)$  and reward function  $r(x_t, a_t)$ . Cannot plan over infinite horizon  $\Rightarrow$  **Key idea:** plan over finite horizon  $H$ , carry out first action, repeat. Optimize  $J_H(a_{t:t+H-1}) = \sum_{t'=t}^{t+H-1} \gamma^{t'-t} r(x_{t'}, a_{t'})$ . Local minima, vanishing/exploding gradient  $\Rightarrow$  heuristics  $\Rightarrow$  Random shooting ( $m$  samples, pick best). Will not work if sparse rewards  $\Rightarrow$  Get access to value function to look further:  $J_H(a_{t:t+H-1}) = \sum_{t'=t}^{t+H-1} \gamma^{t'-t} r_{t'} + \gamma^H V(x_{t+H})$ .

**Model-based ML:** Estimate  $f$  and  $r$  off-policy with supervised learning ( $(x_t, a_t) \mapsto (r_t, x_{t+1})$ , regression). **Benefit:** Dramatically decreases sample complexity (need less data). Use MAP estimate  $\Rightarrow$  exploited by planning algos  $\Rightarrow$  Uncertainty (GP/BNN).