Probabilistic Artificial Intelligence summary

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Basics (iid ⇔ uncorrelated, $S=-\log u$)
$P(X_{1:n}) = P(X_1)P(X_2|X_1)\cdots P(X_n|X_{1:n-1})$
Bayes: $P(X|Y)=\frac{P(X,Y)}{P(Y)}=\frac{P(Y|X)P(X)}{P(Y)}$
$\mathrm{var}(X\pm Y)=\mathrm{var}(X)+\mathrm{var}(Y)\pm 2\mathrm{cov}(X,Y)$
$\mathbb{E}[(X-\mathbb{E}[X])(Y-\mathbb{E}[Y])]=\mathbb{E}[XY]-\mathbb{E}[X]\mathbb{E}[Y]$
Gauss: $\frac{1}{\sqrt{(2\pi)^d|\Sigma|}}\exp(-\frac12(x-\mu)^T\Sigma^{-1}(x-\mu))$
Cond: $P(X_A|X_B=x_B)=\mathcal{N}(\mu_{A|B},\Sigma_{A|B})$
$\mu_A+\Sigma_{AB}\Sigma_{BB}^{-1}(x_B-\mu_B)$, $\Sigma_{AA}-\Sigma_{AB}\Sigma_{BB}^{-1}\Sigma_{BA}$
$H(\prod p_i)=\sum_i H(p_i)$; $H(N(\mu,\Sigma))=\frac12 ln|2\pi e\Sigma|$
$H(p,q)=H(p)+H(q|p)$, $H[p||q]=H[p]+KL(p||q)$
Convex: g(x) $\smile\Leftrightarrow x_1,x_2\in\mathbb{R},\lambda\in[0,1]$: $g''(x)>0$; $g(\lambda x_1+(1-\lambda)x_2)\le\lambda g(x_1)+(1-\lambda)g(x_2)$ **Egg:** $g\smile$: $g(E[X])\le E[g(X)]$
Bayes: *Prior:* $p(\theta)$, *Like:* $p(y_{1:n}|x_{1:n},\theta)=\prod_{i=1}^n p(y_i|x_i,\theta)$, *Post:* $p(\theta|x_{1:n},y_{1:n})=\frac1Z p(\theta)\prod_{i=1}^n p(y_i|x_i,\theta)$, $Z=\int(*)d\theta$, *Pred:* $p(y^*|x^*,x_{1:n},y_{1:n})=\int p(y^*|x^*,\theta)p(\theta|x_{1:n},y_{1:n})d\theta$

BLR (Gauss prior/noise, ass. same as Ridge)
BayI $w_{ls}=w_{MLE}, w_{ridg}=w_{MAP}(\lambda=\sigma_n^2/\sigma_p^2)$
Test x^*, $f^*=w^Tx^*$, $y^*=f^*+\epsilon$, $\epsilon\sim\mathcal N(0,\sigma_n^2)$
$p(\mathbf w)=\mathcal N(0,\sigma_p^2\mathbf I)$, $p(\mathbf w|X,y)=\mathcal N(\mathbf w;\overline\mu,\overline\Sigma)$
$p(y_i|x_i,w,\sigma_n)=\mathcal N(y_i;w^Tx_i,\sigma_n^2)$, $\overline\mu=\sigma_n^{-2}\overline\Sigma X^Ty$
$\overline\Sigma=(\sigma_n^{-2}\mathbf X^TX+\sigma_p^{-2}I)^{-1}$, $p(f^*y^*|\mathbf X,\mathbf y,\mathbf x^*)=\mathcal N(\mathbf x^{*T}\overline\mu,\mathbf x^{*T}\overline\Sigma\mathbf x^*+\sigma_n^2)$, epistem/ aleator (irr)
$\mathrm{var}[y^*|x^*]=\mathbb E_\theta[\mathrm{var}_{y^*}[y^*|x^*,\theta]]+\mathrm{var}_\theta[\mathbb E_{y^*}[y^*|x^*,\theta]]$
RecUpt: giv. prior $p(\theta)$, obs $y_{1:n}$, $p^{(t)}(\theta)=p(\theta|y_{t+1})$ post. aftr t obs, $p^{(t+1)}(\theta)=p(\theta|y_{1:t+1})=p^{(t)}\cdot p(y_{t+1}|\theta)$, $X_{t+1}^TX_{t+1}=X_t^TX_t+x_{t+1}x_{t+1}^T$
$X_{t+1}^Ty_{t+1}=X^Ty_t+y_{t+1}x_{t+1}$ **Func View:** instead of $w\sim\mathcal N(0,\sigma_p^2I)$, f prior $f|X\sim\mathcal N(\Phi\mathbb E[w],\Phi\,\mathrm{var}[w]\Phi^\top)=\mathcal N(0,\sigma_p^2\Phi\Phi^\top)$,
$k(x,x')=\sigma_p^2\cdot\phi(x)^\top\phi(x')=\mathrm{cov}[f(x),f(x')]$
CV: $\lambda=\hat{\sigma_n^2}/\hat{\sigma_p^2}$, $\hat{\sigma_n^2}$ (MSE), find $\hat{\sigma_p^2}=\hat{\sigma_n^2}/\hat\lambda$
$X_{t+1}\perp X_{1:t-1},Y_{1:t-1}|X_t, Y_t\perp Y_{1:t-1}|X_{t-1}, Y_t\perp X_{1:t-1}|X_t$
State X_t obs Y_t Prior $P(X_1)\sim\mathcal N(\mu,\Sigma)$
Mot: $X_{t+1}=FX_t+\epsilon_t$, $\epsilon_t\sim\mathcal N(0,\Sigma_x)$ **Sens:** $Y_t=HX_t+\eta_t$, $\eta_t\sim\mathcal N(0,\Sigma_y)$ **Kupdt 4 pred:** $\mu_{t+1}=F\mu_t+K_{t+1}(y_{t+1}-HF\mu_t)$ $\Sigma_{t+1}=(I-K_{t+1}H)(F\Sigma_tF^T+\Sigma_x)$ **Kgain:** $K_{t+1}=(F\Sigma_tF^T+\Sigma_x)H^T(H(F\Sigma_tF^T+\Sigma_x)H^T+\Sigma_y)^{-1}$

GP $f\sim GP(\mu(x),K(x)$ (∞-dim Gaussian)
∞ set of RVs X s.t. $\forall A\subseteq X, A=\{x_1,..,x_m\}$ it holds $Y_A=[Y_{x_1},..,Y_{x_m}]\sim\mathcal N(\mu_A,K_{AA})$ w\ $K_{AA}^{(ij)}=k(x_i,x_j)$ and $\mu_A^{(i)}=\mu(x_i)$ (join Gaus)
Kern: *sqrd exp* anal, ∞ dif *exp* cont nodif, *Mat(ν)* ν mal dif, $\nu=1/2$ Lapl, $\nu=\infty$ Gaus
Cov k: symmetric, PSD, *statry:* $k(x,x')=k(x-x')$, *isotropic:* $k(x,x')=k(||x-x'||_2)$.
Pred $p(f)=GP(f;\mu(x),k(x,x'))$, observe $y_i=f(x_i)+\epsilon_i$, $\epsilon_i\sim\mathcal N(0,\sigma^2)$, $A=\{x_1,..,x_m\}$. Often $\mu(x)=0$, $p(f|x_{1:m},y_{1:m})=GP(f;\mu',k')$ with $k_{x,A}=[k(x,x_1)..k(x,x_m)]$, $\mu'(x)=\mu(x)+\mathbf k_{x,A}(\mathbf K_{AA}+\sigma^2\mathbf I)^{-1}(\mathbf y_A-\mu_A)$ $k'(x,x')=k(x,x')-\mathbf k_{x,A}(\mathbf K_{AA}+\sigma^2\mathbf I)^{-1}\mathbf k_{x',A}^T$, *Pred post:* at $x^\star$, $p(y^*|x_{1:m},y_{1:m},x^*)=\mathcal N(\mu_n^*,\sigma_n^{2*})$, $\mu_n^*=\mu'(x^*)$, $\sigma_n^{2*}=\sigma^2+k'(x^*,x^*)$, **Samp:** 1) discrete set to sample $\mathbf f=[f_1...f_n]$, $\mathbf f\sim\mathbf K^{1/2}\epsilon=\mathbf L\epsilon$ 2) $p(f_1..f_n)=\prod_{i=1}^n p(f_i|f_{1:i-1})$, sample $f_n\sim p(f_n|f_{1:n-1})$ **ModelSel:** 1) MLE $\hat\theta=\mathrm{amax}_\theta\, p(y|X,\theta)$, $\int p(y|X,f)p(f|\theta)df$, $\exp\{-\frac12\mathbf y^T\mathbf K_y^{-1}\mathbf y-\frac12\log|\mathbf K_y|\}$ 2) place hyper-prior $p(\theta)$, MAP $\hat\theta=\mathrm{amax}_\theta\, p(y|x,\theta)p(\theta)$, FullB $p(y^\star|x^\star,x_{1:n},y_{1:n})=\int p(y^\star|x^\star,f)p(f|x,y,\theta)p(\theta)d\theta$
Cost: n variables, req. lin system time $\mathcal O(n^3)$, space $\mathcal O(n^2)$, **BLR:** $\mathcal O(nd^2)$. **Fast GP:** 1) *GPU* 2) *Local:* distance decaying kernel (e.g. RBF), only condition on points x' where $|k(x,x')|>\tau$ 3)a) k approx: $k(x,x')\approx\phi(x)^T\phi(x')$, $\phi\in\mathbb R^m$, then BLR $\mathcal O(nm^2+m^3)$ 3)b) stat kern→ *Bochner*, **Random FF** $k_{x,x'}=\int_{\mathbb R^d}p(\omega)e^{j\omega^T(x-x')}d\omega=\mathbb E_{\omega,b}[z_{\omega,b}(x)z_{\omega,b}(x')]\approx\frac1m\sum_i z_{w^{(i)},b^{(i)}}(x)z_{w^{(i)},b^{(i)}}(x')$, $\omega\sim p(\omega)$, $b\sim\mathcal U[0,2\pi]$, $z_{\omega,b}(x)=(2/D)^{1/2}\cos(\omega^Tx+b)$ → draw samples ω_i,b_i, $k(x,x')\approx\phi(x)^T\phi(x')$ with $\phi_i(x)=\frac{1}{\sqrt m}z_{w^{(i)},b^{(i)}}(x)$
Rahimi: $M\subset\mathbb R^d$ compact, for RFFs $z(x)$, $\sigma_p^2=\mathbb E[\omega^T\omega]$, $\mathbb P[\sup_{x,x'\in M}|z(x)^\top z(x')-k(x,x')|\ge\epsilon]\le 2^8(\frac{\sigma_p\,\mathrm{diam}(M)}{\epsilon})^2\exp(-\frac{D\epsilon^2}{4(d+2)})$
4) *Inducing Points methods:* Summarz data via values of f at inducing points $\mathbf u=[u_1,..,u_m]$.
$p(\mathbf f^*,\mathbf f)=\int p(\mathbf f^*,\mathbf f,\mathbf u)d\mathbf u=\int p(\mathbf f^*,\mathbf f|\mathbf u)p(\mathbf u)d\mathbf u$
$p(\mathbf f^*,\mathbf f)\approx q(\mathbf f^*,\mathbf f)=\int q(\mathbf f^*|\mathbf u)q(\mathbf f|\mathbf u)p(\mathbf u)d\mathbf u$ with $u=f(z)$, z-inducing location, train conditional: $p(\boldsymbol f|\mathbf u)=\mathcal N(\boldsymbol K_{\mathbf f,\mathbf u}\boldsymbol K_{\mathbf u,\mathbf u}^{-1}\mathbf u,\boldsymbol K_{\mathbf f,\mathbf f}-\boldsymbol Q_{\mathbf f,\mathbf f})$, w\ $\mathbf Q_{\mathbf a,\mathbf b}=\mathbf K_{\mathbf a,\mathbf u}\mathbf K_{\mathbf u,\mathbf u}^{-1}\mathbf K_{\mathbf u,\mathbf b}$, test cond: $p(\boldsymbol f^*|\mathbf u)=\mathcal N(\boldsymbol K_{\mathbf f^*,\mathbf u}\boldsymbol K_{\mathbf u,\mathbf u}^{-1}\mathbf u,\boldsymbol K_{\mathbf f^*,\mathbf f^*}-\boldsymbol Q_{\mathbf f^*,\mathbf f^*})$
4)a) *Subset of Regressors:* assume $\mathbf K_{\mathbf f,\mathbf f}-\mathbf Q_{\mathbf f,\mathbf f}=0$, replace $p(\mathbf f|\mathbf u)$ by $q_{SoR}(\mathbf f|\mathbf u)=\mathcal N(\mathbf K_{\mathbf f,\mathbf u}\mathbf K_{\mathbf u,\mathbf u}^{-1}\mathbf u,0)$ resulting model is degenerate GP with covariance function $k_{SoR}(\mathbf x,\mathbf x')=k(x,\mathbf u)\mathbf K_{\mathbf u,\mathbf u}^{-1}k(\mathbf u,\mathbf x')$ *FITC:* Assume $\mathbf f_i\perp\mathbf f_j|\mathbf u,\forall i\ne j$ $q_{FITC}(\mathbf f|\mathbf u)=\mathcal N(\mathbf K_{\mathbf f,\mathbf u}\mathbf K_{\mathbf u,\mathbf u}^{-1}\mathbf u,\mathrm{diag}(\mathbf K_{\mathbf f,\mathbf f}-\mathbf Q_{\mathbf f,\mathbf f}))$, $q_{FITC}(\boldsymbol f^*|\mathbf u)=\mathrm p(\boldsymbol f^*|\mathbf u)$, cost cubic in # inducing pts, dominated inv $K_{\mathbf u,\mathbf u}$. *Pick inducing pts* by chose randly/greed criterion (var)/det grid, $\mathbf u$ as hyperpar, max marg like (ensure $\mathbf u$ repr data).

Variatnl Inf (rev greed sel mode, fwd sel var)
$\mathrm{amin}_\lambda KL(p\|q_\lambda)=\mathrm{amax}_\lambda\lim_{n\to\infty}\sum_{i=1}^n\log q(x^{(i)}|\lambda)$
$q=\arg\min_{q\in\mathcal Q}KL(p||q)$ match 1, 2 mom of p
Laplace: $p(\theta|(x,y)_{1:n})\approx q_\lambda(\theta)=\mathcal N(\hat\theta,\Lambda^{-1})$
$\hat\theta=\arg\max_\theta p(\theta|y)$, $\Lambda=-\nabla^2\log p(\hat\theta|y),0=\nabla\log p(\hat\theta|y)$, *Pred* BL, greed fit mode (overcnf), match curv, pres MAP est, can diff from post
GVI: $0=\mathbb E_{q(\boldsymbol\theta)}[\nabla_{\boldsymbol\theta}\log p(\mathcal D,\boldsymbol\theta)]$, $\boldsymbol\Sigma^{-1}=-\mathbb E_{q(\boldsymbol\theta)}[\nabla^2_{\boldsymbol\theta}\log p(\mathcal D,\boldsymbol\theta)]$ **PVI:** $KL(\mathcal N\|Po)\propto -d/2\ln(2\pi e)$-$d\ln\sigma$-$1/m\sum_{j,i=1}^{m,n}[y_i\boldsymbol w^\top\boldsymbol x_i$-$e^{\boldsymbol w^\top\boldsymbol x_i}$-$\|\boldsymbol w\|_2^2/2\sigma_p^2]_{\boldsymbol w=\boldsymbol\mu+\sigma\epsilon^{(j)}}$ **BLR:** $P(y|x,w)=\mathrm{Ber}(y;\sigma(w^Tx))$, $\hat w=\mathrm{amin}_w\sum_{i=1}^n\log(1+\exp(-y_iw^Tx_i))+\lambda\|w\|_2^2$, $\mathcal N(\hat w,\Lambda^{-1})$, $\Lambda=\sum_{i=1}^n x_ix_i^T\sigma(\hat w^Tx_i)(1-\sigma(\hat w^Tx_i))$
Variational Inf: $p(\theta|y)=\frac1Z p(\theta,y)\approx q_\lambda(\theta)$
$q^*\in\arg\min_{q\in\mathcal Q}KL(q||p)$: $q\approx p$ where q large
$\mathrm{amin}_q KL(q||p)=\mathrm{amax}_q\mathbb E_{\theta\sim q}[\log p(\theta,y)]+H(q(\theta))$ $=\mathrm{amax}_q\mathbb E_{\theta\sim q_\lambda(\theta)}[\log p(y|\theta)]-KL(q(\theta)||p(\theta))$
$\max_\epsilon\mathbb E_\epsilon[\ln p(\mathcal D,\mu+\Sigma^{1/2}\epsilon)]+\frac12\ln|\Sigma|+\frac D2\log 2\pi e$
ELBO, $L(\lambda)\le\log p(y)$. $\nabla_\lambda L(\lambda)$ hard, *score* ∇: $\nabla_\lambda L=\mathbb E_{\theta\sim q_\lambda}[\nabla_\lambda\log q(\theta|\lambda)(\log p(y,\theta)$-$\log q(\theta|\lambda))]$ $\theta\sim q_\lambda(\cdot)$ dep on var param. **Reparam.:** let $\epsilon\sim\phi$, $\theta=g(\epsilon,\lambda)$, $q(\theta|\lambda)=\phi(\epsilon)|\nabla_\epsilon g(\epsilon;\lambda)|^{-1}$ and $\mathbb E_{\theta\sim q_\lambda}[f(\theta)]=\mathbb E_{\epsilon\sim\phi}[f(g(\epsilon;\lambda))]$, which yield $\nabla_\lambda\mathbb E_{\theta\sim q_\lambda}[f(\theta)]=\mathbb E_{\epsilon\sim\phi}[\nabla_\lambda f(g(\epsilon;\lambda))]$ *Blackbox VI:* max ELBO using stoch opt., for diagonal q, 2x expensive as MAP, only need to diff joint prob p and q, also use Natural Grad, Variance reduct tech. **GP Class:** $P(f)=GP(\mu,k)$, $P(y|f,\mathbf x)=\sigma(y\cdot f(\mathbf x))$ max (*) w\ $q(f_i):=\int p(f_i|\mathbf u)q(\mathbf u)d\mathbf u$, $\mathbf u$ *pseudo in.* $\sum_{i=1}^n\mathbb E_{q(f_i)}[\log p(y_i|f_i)]-KL(q(\mathbf u)\|p(\mathbf u))$

MCMC (MC: seq of RV $X_{1:n}$ with (*))
TV Dist: $\|\mu-v\|_{\mathrm{TV}}=2\sup_{A\subseteq\mathcal A}|\mu(A)-v(A)|$
Mix.Time: $\tau_{\mathrm{TV}}(\epsilon)=\min\{t|\forall q_0:\|q_t-\pi\|_{\mathrm{TV}}\le\epsilon\}$
Rapidly mix: $\tau_{\mathrm{TV}}(\epsilon)\in\mathcal O(\mathrm{poly}(n,\log(1/\epsilon)))$
(*) Stat MC w\ prior $P(X_1)$, trans $P(X_{t+1}|X_t)$ indep of t. *ergodic* $\exists\, t<\infty$ s.t. all states reachable from every state in *exactly* t steps. **Mark Ass:** $X_{t+1}\perp\!\!\!\perp X_{1:t-1}|X_t\forall t$ **Stat Distrib:** $\pi(P-I)=0$. Stat Ergodic MC is unique stat distr $\pi(X)>0$ s.t. $\forall x$: $\lim_{N\to\infty}P(X_N=x)=\pi(x)$, $\pi(X)$ indep of prior $P(X_1)$. **Sim MC** fwd sampl $x_N\sim P(X_N|X_{N-1}=x_{N-1})$ **MCMC:** Approx pred. distr. $p(y^*|x^*,x_{1:n},y_{1:n})=\int p(y^*|x^*,\theta)p(\theta|(x,y)_{1:n})d\theta=\mathbb E_{\theta\sim p(\cdot|(x,y)_{1:n})}[p(y^*|x^*,\theta)]\approx\frac1m\sum_{i=1}^m p(y^*|x^*,\theta^{(i)})$, sample $\theta^{(i)}\sim p(\theta|(x,y)_{1:n})$ from MC with stat distr (*).
Hoeffding: Let f be bounded in $[0,C]$:
$\mathbb P(|\mathbb E[f(X)]$- $\frac1N\sum_1^N f(x_i)|>\epsilon)\le 2\exp(\text{-}2N\epsilon^2/C^2)$
Given unnormalized distr. $Q(x)>0$, design MC s.t. $\pi(x)=\frac1ZQ(x)$. **DB (reversible):** $Q(x)P(x'|x)=Q(x')P(x|x')\to\pi(x)=\frac1ZQ(x)$.

Gibbs Sampling: Asympt. correct but slow
1. Init $\mathbf x^{(0)}$, fix observed RVs X_B to $\mathbf x_B$
2. Repeat: set $\mathbf x^{(t)}=\mathbf x^{(t-1)}$; sel $j\in[1:m]\setminus B$ $x_j^{(t)}\sim P(X_j|\mathbf x^{(t)}_{[1:m]\setminus\{j\}})$ Rand: ful. DB, find cor distr. Determin: not ful. DB, corr distr.

$P(X_i=x_i|\boldsymbol x_{-i})=\frac1ZQ(X_i=x_i,\boldsymbol x_{-i})=\frac1ZQ(\boldsymbol x_{1:n})$ re-sampl X_i only requires eval unnorm joint distrib and renorm. **Expectations via MCMC**: Joint sample at t dep only on t-1 → LLN, HB not apply. *Thm:* $X_{1:n}$ EMC on finite D, $f\in D$, $\lim_{N\to\infty}\frac1N\sum_{i=1}^N f(x_i)=\sum_{x\in D}\pi(x)f(x)$
Use MCMC to get samples $\mathbf X^{(1:T)}$. After burn-in time t_0: $\mathbb E[f(\mathbf X)]\approx\frac{1}{T-t_0}\sum_{\tau=t_0+1}^T f(\mathbf X^{(\tau)})$
MetroH: Gen MC → DB 1) Proposal $R(X'|X)$, given $X_t=x$, sample $x'\sim R(X'|X=x)$; 2) For $X_t=x$, w.p. $\alpha=\min\{1,\frac{Q(x')R(x|x')}{Q(x)R(x'|x)}\}$: $X_{t+1}=x'$; else $X_{t+1}=x$ **Cont RVs:** log-concave $p(x)=\frac1Z\exp(-f(x))$, f convex. M/H: $\alpha=\min\{1,\frac{R(x|x')}{R(x'|x)}\exp(f(x)-f(x'))\}$, Simple uninf dir. **Improved prop:** *MALA/LMC:* $R(x'|x)=\mathcal N(x';x-\eta_t\nabla f(x);2\tau I)$ MALA converg to stat distr for log concave (locall also non convex) func (for general distrib convergence slow), mixing time $\mathcal O(d)$. *Improve efficiency:* both proposal step and accept step requires full acces to energy function f → SGD, decaying step size, skip accept/reject → *SGLD*
$\theta\sim\frac1Z\exp(\log p(\theta)+\sum_{i=1}^n\log p(y_i|x_i,\theta))$ 1) θ_0 2) For t do $i_1..i_m\sim U(1,n)$, $\epsilon_t\sim\mathcal N(0,2\eta_tI)$, $\theta_{t+1}=\theta_t$-$\eta_t(\nabla\ln p_{\theta_t}+\frac nm\sum_1^m\nabla\ln p(y_{i_j}|\theta_t,x_{i_j}))+\epsilon_t$ SGLD = SGD + Gauss noise, convergence if $\eta_t\in\mathcal O(t^{-1/3})$, const step boost mixing, improve perf. via Adagrad, *HMC* (mom)

BDL (Prior: $p(\theta)=\mathcal N(\theta;0,\sigma_p^2I)$, Gauss = *)
* weig decay, *Like:* $p(y|x,\theta)=\mathcal N(y;f(x,\theta),\sigma^2)$ MAP: $\hat\theta=\mathrm{amin}_\theta-\log p(\theta)-\sum_i\log p(y_i|x_i,\theta)$ hetero ϵ well, fails pred epistemic, use *VI (BbB)*. **Etero:** $y|\boldsymbol x,\boldsymbol\theta\sim\mathcal N(\mu(\boldsymbol x;\boldsymbol\theta),\sigma^2(\boldsymbol x;\boldsymbol\theta))$, $f_1(\boldsymbol x;\boldsymbol\theta)$, $\exp(f_2(\boldsymbol x;\boldsymbol\theta))$ **VI:** SGD-opt ELBO via $\nabla_\lambda L(\lambda)$. Find VI approx q_λ. Draw m weights $\theta^{(j)}\sim q_\lambda(\cdot)$. *Pred* $p(y^*|\mathbf x^*,\mathbf x_{1:n},y_{1:n})\approx\mathbb E_{\theta\sim q_\lambda}[p(y^*|\mathbf x^*,\theta)]\approx\frac1m\sum_j p(y^*|\mathbf x^*,\theta^{(j)})$, $\mathrm{Var}[y^*|\cdot]\approx\frac1m\sum_1^m\sigma^2(x^*,\theta^{(j)})+\frac1m\sum_1^m(\mu(x^*,\theta^{(j)})-\overline\mu(x^*))^2$
MC wghts $\theta^{(1:T)}$ SGLD, LD, SGHMC; pred by avg $\theta^{(1:T)}$. *Summ:* subsmpl/GVI $q(\theta|\mu_{1:d},\sigma^2_{1:d})$ $\mu_i=\frac1T\sum_{j=1}^T\theta_i^{(j)}$; $\sigma_i^2=\frac1T\sum_{j=1}^T(\theta_i^{(j)}-\mu_i)^2$
DropVI: $q_j(\theta_j|\lambda_j)=p\delta_0(\theta_j)+(1\text{-}p)\delta_{\lambda_j}(\theta_j)$, $\theta^{(j)}$ NN w\ wght giv by λ, $\theta^{(j)}=0$ wp p.
Prob. Ensbles: train multiple models bootstrap, **Cal:** confidence=accuracy on heldout
Reliability Diag: plot expected sample acc

as func of confidence 1) group pred in M bin, 2) freq$(B_m) = 1/|B_m| \sum_{i\in B_m} [\hat y_i = 1]$ 3) conf$(B_m) = 1/|B_m|\sum_{i\in B_m}\hat p_i$ 4) $MECE = \max \sum_{m=1}^M \frac{|B_m|}{n}|\text{freq}(B_m) - \text{conf}(B_m)|$ *Improve* via histo bin, isotonic regr., platt (temp) scaling

Active Learn (min $\#x$ reducing uncertainty)

MutInf: $I(X;Y) = I(Y;X) = H(X)$-$H(X|Y)$ $X\sim N(\mu,\Sigma), Y = X + N(0,\sigma^2)$, $I = \frac12 \ln|I + \frac{1}{\sigma^2}\Sigma|$

InfGain: $f(S)$, $S\subseteq D$, $F(S) = H(f) - H(f|y_S) = I(f;y_S) = \frac12\log|I+\sigma^{-2}K_S|$, obs at S
Thm: $F(S_T) \ge (1-1/e)\max_{S\subseteq D,|S|\le T} F(S)$

Greed MIopt: $F(S)$ NP hard, $S_t = \{x_1,..,x_t\}$ $x_{t+1} = \arg\max_{x\in D} F(S_t\cup\{x\})$ =arg max$_{x\in D}\sigma^2_{x|S_t}$

UncSmpl: $x_t = \arg\max_{x\in D}\sigma^2_{t-1}(x)$, (homo, $\mathcal N$) Fail distepist/aleat, *Etero:* amax$_x$ $\sigma_f^2(x)/\sigma_n^2(x)$
Or: trAce/Eigval/log-Determinant designs

BALD: (class) $x_{t+1} = \text{amax}_x I(\theta; y_x|x_{1:t}, y_{1:t}) = \text{amax}_x H(y|x,(x,y)_{1:t}) - \mathbb E_{\theta\sim p(\cdot|(x,y)_{1:t})}[H(y|x,\theta)]$

Bayesian Opt (seq. pick $x_1,..,x_T\in D$ (*))

(*), $y_t = f(x_t)+\epsilon_t$, find $\max_x f(x)$ st T smal

CumReg: $R_T = \sum_{t=1}^T \max_{x\in D} f(x) - f(x_t)$ sublin if $R_T/T\to 0$ (obj) $\Leftrightarrow f(x_t)\to\max f(x)$ (UCB $\ge$ best lower bound if well cal) **GP-UCB:** $x_t = \arg\max_{x\in D}\mu_{t-1}(x) + \beta_t\sigma_{t-1}(x)$ $\mu(x),\sigma(x)$ from GP marginal, β_t EE-tradeoff. non-convex usually, low D use Lipschitz, high D. grad ascent (w\ rand init) *Thm:* $f\sim GP$,if correct β_t: $\frac1T R_T = \mathcal O(\sqrt{\gamma_T/T})$, with $\gamma_T = \max_{|S|\le T} I(f;y_S)$ (max. info gain)

Thomp sampl: at t, draw from GP post. $\tilde f\sim P(f|x_{1:t},y_{1:t})$, select $x_{t+1}\in\arg\max_{x\in D}\tilde f(x)$ datasets in BO/AL small, data pts selected dependend on prior obs, *sol:* hyperprior on hyperparam, select pts at random occasionally.

Markov Decision Processes (r, P known)

MDP: Finite MDP (control MC), state $X = \{1,..,n\}$, action $A = \{1,..,m\}$, trans $P(x'|x,a)$, init $P(x_0)$, reward $r(x,a,x')$, discount $\gamma\in[0,1]$

Planning in MDPs: Policy $\pi: X\to AP(A)$ (det./rand), induce MC w\ trans $P(X_{t+1} = x'|X_t = x) = P(x'|x,\pi(x)) \sum_a \pi(a|x)P(x'|x,a)$

Value fun: fixed π $V^\pi(x) = J(\pi|X_0=x) = \mathbb E[\sum_{t=0}^\infty \gamma^t r(X_t,\pi(X_t))|X_0=x] = r(x,\pi(x)) + \gamma\sum_{x'}P(x'|x,\pi(x))V^\pi(x')$, $V^\pi = (I-\gamma T^\pi)^{-1} r^\pi$ $V_i^\pi = V^\pi(i)$, $r_i^\pi = r^\pi(i,\pi(i))$, $T^\pi_{i,j} = P(j|i,\pi(i))$
$V^\pi(x) = \sum_{x'}P(x'|x,\pi(x))[r(x,\pi(x),x') + \gamma V^\pi(x')]$ $= Q^\pi(x,\pi(x)) = \mathbb E_{a'\sim\pi(x)}Q^\pi(x,a')$ det/rand

Fixed Point Iteration: 1) initialize V_0^π 2) for $t = 1:T$ do: $V_t^\pi = r^\pi + \gamma T^\pi V^\pi_{t-1}$ (converges)

Greedy policy w.r.t. V: V induces policy $\pi_V(x) = \text{amax}_a r(x,a) + \gamma\sum_{x'}P(x'|x,a)V(x')$

Greedy π w.r.t. Q: $\pi_Q(x) = \arg\max_a Q(x,a)$

BellThm: Opt $\pi^*\leftrightarrow$greedy wrt induced V^* $V^*(x) = \max_{a\in\mathcal A}[r(x,a) + \gamma\sum_{x'\in X}P(x'|x,a)V^*(x')]$ $= \text{mx}_{a\in\mathcal A}\mathbb E_{x'}[r(x,a)+\gamma V^*(x')] = \text{mx}_{a\in\mathcal A}Q^*(x,a)$

Policy Iter: 1) Init arbitry π 2) Until conv: calc $V^{\pi_t}(x)$, calc greedy pol π_t^G w.r.t. V^{π_t}, set $\pi_{t+1}\leftarrow\pi_t^G$ Stop if $V^{\pi_t}(x) = V^{\pi_{t+1}}(x)$. Monoton improves all val $V^{\pi_{t+1}}(x)\ge V^{\pi_t}(x)\forall x$. Converge exact optimal in $\mathcal O(n^2 m/(1-\gamma))$. **SAF:** $Q_t(x,a) = r(x,a) + \gamma\sum_{x'}P(x'|x,a)V_{t-1}(x')$

Value Iteration: 1) Init $V_0(x) = \max_a r(x,a)$ 2) for $t = 1:\infty$: $V_t(x) = \max_a Q_t(x,a)$. Stop if $||V_t - V_{t-1}||_\infty\le\epsilon$, pick grdy π_G w.r.t. V_t. Conv ϵ-opt sol in poly time. *Tradeoffs:* Pol/val $\mathcal O(n^3/nmk)$ per iter, k sprs **POMDP:**(X,A,P,R,γ,Y,Q), $O_{x,y,a} = P[Y_{t+1}=y|X_{t+1}=x, A_t = a]$

Belief state: $b_t(x) = P[X_t = x|y_{1:t}, A_{t-1} = a]$ $b_t(x)\in\Delta^{|X|} = \{b\ge0\in\mathbb R^{|X|}, \sum_{i=1}^{|X|}b_i = 1\}$ $b_{t+1}(x) = \frac1Z O(y_{t+1}, x)\Sigma_{x'}b_t(x')P(x|x',a), Z = \sum_x$

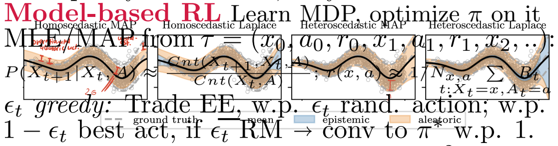
BMDP: $(\Delta^{|X|}, A, \tau(b'|b,a), \rho = \sum_x b(x)r(x,a))$

Solve POMDPs finite T: exp. #belif states. BUT: most belif states never reach → discretize space by sampling, PBVI, PBPI, dim reduction

RL (agent act. chang state, unknown MDP)

- **On**-policy: full control on actions/EE-trade
- **Off**-policy: no control, only observation data

Model-based RL Learn MDP, optimize π on it MLE/MAP from $\tau = (x_0, a_0, r_0, x_1, a_1, r_1, x_2, ..)$: $P(X_{t+1}|X_t,A) \approx \frac{Cnt(X_{t+1},X_t,A)}{Cnt(X_t,A)}$; $r(x,a) \approx 1/N_{x,a}\sum_{t:X_t=x,A_t=a} R_t$



ϵ_t *greedy:* Trade EE, w.p. ϵ_t rand. action; w.p. $1-\epsilon_t$ best act, if ϵ_t RM → conv to π^* w.p. 1.

RobMonro (RM): $\sum_t\epsilon_t = \infty$, $\sum_t\epsilon_t^2<\infty$

$R_{\max}$ Alg: Set unknown $r(x,a)$ to R_{max}, $r(x,a)\le R_{max},\forall x,a$, add fairy tale state x^*, set $P(x^*|x,a) = 1$, compute π. Repeat: run π while updtng $r(x,a)$, $P(x'|x,a)$, recompute π. $P(x^*|x^*,a) = 1, r(x^*,a) = R_{\max}$ *Lem:* evry T stps, whp $R_{\max}$ eithr obt near opt reward, or visit at least 1 unknwn state-action pair. *Thm:* wp 1-δ, $R_{\max}$ reach ϵ-opt policy in #steps poly in $|X|,|A|,T,1/\epsilon,\log(1/\delta),R_{\max}$. **Problms of MBRL:** *Mem require:* $P(x'|x,a)\approx\mathcal O(|X|^2|A|)$, $r(x,a)\approx\mathcal O(|X||A|)$ *Computate:* reptdly solve MDP (Val/Pol Iter)

Model-free RL Directly estim value function

TD-Learning: Follow policy π, get (x,a,r,x') Update: $\hat V^\pi(x)\leftarrow(1-\alpha_t)\hat V^\pi(x) + \alpha_t(r+\gamma\hat V^\pi(x'))$ *Thm:* If α_t is RM and all (x,a) pairs chosen ∞ often, then $\hat V^\pi$ converges to V^π w.p. 1.

Optimistic Q-L Estimate $Q^*(x,a)$ 1) Init rand /zero $\hat Q^*(x,a) = \frac{R_{max}}{1-\gamma}\prod_{t=1}^{T_{init}}(1-\alpha_t)^{-1}$ 2) at t $a_t\in\text{amax}_a\hat Q^*(x_t,a)$, get (x_t,a_t,r,x'), $\hat Q^*(x_t,a_t)$ ← (1-α_t)$\hat Q^*(x_t,a_t) + \alpha_t(r+\gamma\max_{a'}\hat Q^*(x',a'))$
Thms for $R_{\max}$, TD-L → Time: $\mathcal O(|A|)$, Mem: $\mathcal O(|X||A|)$, $|X|,|A|$, exp #agents, state vars

RL via FuncAprox (parametric approx. of (*))

(*) val funct $V(x;\theta)$ or act val funct $Q(x,a;\theta)$

TD-Learning as SGD: Tabular TD update rule can be viewed as SGD on squared loss $l_2(\theta;x,x',r) = \frac12(V(x;\theta) - r - \gamma V(x';\theta_{old}))^2$, then $V\leftarrow V - \alpha_t\nabla_{V(x;\theta)}l_2$ is equiv to TD update.

Function Approx Q-learning: very slow Loss $l_2(\theta;x,a,r,x') = \frac12\delta^2$ with $\delta = Q(x,a;\theta) - r - \gamma\max_{a'}Q(x',a';\theta_{old})$. *Alg:* Until conv: In state x, pick action a, obsrv r,x'. Update: $\theta\leftarrow\theta - \alpha_t\nabla_\theta l_2 = \theta - \alpha_t\delta\nabla_\theta Q(x,a;\theta)$ **DQN:** Q-learn w\ NN as func aprox, *experience replay*, maintn data D, clone NN to stablze target opt $L(\theta) = \sum_{(x,a,r,x')\in D}(r+\gamma\max_{a'}Q(x',a';\theta^{old}) - Q(x,a;\theta))^2$

Double DQN: Use current NN to eval action arg max to prevents maximiz. bias of DQN. $L^{DDQN}(\theta) = \sum_{(x,a,r,x')\in D}[r+\gamma Q(x',a^*(\theta);\theta^{old}) - Q(x,a;\theta)]^2$ $a^*(\theta) = \arg\max_{a'}Q(x',a';\theta)$

Q-learn π $a_t = \text{amax}_a Q(x,a;\theta)$ bad if $|A|\uparrow$

Policy Search Methods: Param. policy π_θ Max $J(\theta) = \mathbb E_{\tau\sim\pi_\theta}[r(\tau)]$ $(\tau = x_{0:T}, a_{0:T}\sim\pi_\theta)$, $r(\tau) = \sum_{t=0}^T\gamma^t r(x_t,a_t)$); via ∇_θ. *Score Grad:* $\nabla_\theta J_\theta = \nabla_\theta\mathbb E_{\tau\sim\pi_\theta}r(\tau) = \mathbb E_{\tau\sim\pi_\theta}[r(\tau)\nabla_\theta\ln\pi_\theta(\tau)]$ *MDP:* $\pi_\theta(\tau) = p(x_0)\prod_0^T\pi(a_t|x_t;\theta)p(x_{t+1}|x_t,a_t)$ then: $\nabla_\theta J(\theta) = \mathbb E_{\tau\sim\pi_\theta}[r(\tau)\sum_{t=0}^T\nabla_\theta\log\pi(a_t|x_t;\theta)]$ *Reduce variance:* baselines (but ∇ unbiased) $\mathbb E_{\tau\sim\pi_\theta}[r(\tau)\nabla\log\pi_\theta(\tau)] = \mathbb E...[(r(\tau)-b)\nabla\log\pi_\theta(\tau)]$

R2Go: $G_t = \sum_{t'=t}^T\gamma^{t'-t}r_{t'}$; $b_t(x_t) = 1/T\sum_{t=0}^T G_t$ $\nabla J_T(\theta) = \mathbb E_{\tau\sim\pi_\theta}[\sum_{t=0}^T\gamma^t G_t\nabla_\theta\log\pi(a_t|x_t;\theta)]$ *Mean over returns:* replace G_t with $(G_t - b_t(x_t))$

REINFORCE: Input $\pi(a|x;\theta)$, init θ, repeat: gener episode $(x_i,a_i,r_i), i = 0:T$; for $t = 0:T$ set G_t to retrn from step t, update θ: $\theta = \theta + \eta\gamma^t G_t\nabla_\theta\log\pi(A_t|X_t;\theta)$ optimizes score-∇ using MC returns; high variance

Deep RL with policy grad and actor-critic

Advantge Func: $A^\pi(x,a) = Q^\pi(x,a) - V^\pi(x)$ π^*iff $\forall x,a: A^{\pi^*}(x,a)\le0; \forall\pi,x:\max_a A^\pi(x,a)\ge0$

Actor-Critic: Approx π_θ and V^π, e.g. 2 NNs Reinterpreting score-∇ = *Policy grad Thm* $\nabla J(\theta_\pi) = \mathbb E_{\tau\sim\pi_\theta}[\sum_{t=0}^\infty\gamma^t Q(x_t,a_t;\theta_Q)\nabla\log\pi(a_t|x_t;\theta_\pi)]$ $= \mathbb E_{(x,a)\sim\pi_\theta}[Q(x,a;\theta_Q)\nabla_{\theta_\pi}\log\pi(a|x;\theta_\pi)]$;

Online A.C.: val fun apprx + pol grad thm $\delta = Q(x,a;\theta_Q) - r - \gamma Q(x',\pi(x',\theta_\pi);\theta_Q)$ $\theta_\pi\leftarrow\theta_\pi + \eta_t Q(x,a;\theta_Q)\nabla\log\pi(a|x;\theta_\pi)$ $\theta_Q\leftarrow\theta_Q - \eta_t\delta\nabla Q(x,a;\theta_Q)$ (**FA Q-learning**) *Var red:* baselines $Q(x,a;\theta_Q) - V(x;\theta_V)$: adv func estim → **A2/3C, GAE/GAAC**; **TRPO** opt surrogate obj in trust region, guarantees monoton improve $J(\theta)$, **PPO** heuristic variant

Off-policy AC: allow reuse of past data Replace in L_{DQN} a' by $\pi(x';\theta_\pi)$, π follows greedy pol., to model $\max_{a'}Q$. Equivalent to: $\theta_\pi^*\in\arg\max_\theta\mathbb E_{x\sim\mu}[Q(x,\pi(x;\theta);\theta_Q)]$, with $\mu(x)>0$ *explores all states.* If $Q(\cdot;\theta_Q),\pi(\cdot;\theta_\pi)$ diff, use backprop to get stoch-∇ (unbiased) $\nabla_\theta J(\theta) = \mathbb E_{x\sim\mu}[\nabla_\theta Q(x,\pi(x;\theta);\theta_Q)]$ $\nabla_\theta Q(x,\pi(x;\theta)) = \nabla_a Q(x,a)|_{a=\pi(x;\theta)}\nabla_\theta\pi(x;\theta)$ Needs *deterministic* π → inject additional action noise (ϵ_t greedy) to ensure explore →

DDPG: 1) init θ_Q,θ_π, set $\theta_Q^{old} = \theta_Q, \theta_\pi^{old} = \theta_\pi$ 2) repeat: observe x, execute $a = \pi(x;\theta_\pi)+\epsilon$ to observe r,x', store in D. If time to update: for iter: sample batch B from D, cmpt target $y = r+\gamma Q(x',\pi(x',\theta_\pi^{old}),\theta_Q^{old})$, updates: *Critic:* $\theta_Q\leftarrow\theta_Q - \eta\nabla1/|B|\sum_B(Q(x,a;\theta_Q)-y)^2$, *Actor:* $\theta_\pi\leftarrow\theta_\pi + \eta\nabla1/|B|\sum_B Q(x,\pi(x;\theta_\pi);\theta_Q)$, *Params:* $\theta_j^{old}\leftarrow(1-\rho)\theta_j^{old} + \rho\theta_j$ for $j\in\{\pi,Q\}$

TD3: DDPG with 2 Critics avoid maxim bias

Rand π DDPG: (DQN with reparam π grad) For *critic* $a'\sim\pi(x';\theta_\pi^{old})$, get unbias ∇, *actor* $\nabla_{\theta_\pi}\mathbb E_{a\sim\pi(x;\theta_\pi)}Q(x,a;\theta_Q)$reparam $a = \psi(x;\theta_\pi,\epsilon)$ $\nabla_{\theta_\pi}\mathbb E_{a\sim\pi_{\theta_\pi}}Q(x,a;\theta_Q) = \mathbb E_\epsilon\nabla_* Q(x,\psi(x;\theta_\pi,\epsilon);\theta_Q)$

EntrpyReg: $J_\lambda(\theta) = J(\theta) + \lambda H(\pi_\theta)\uparrow$ explor

SAC: variant of DDPG/TD3 for H reg MDPs

MB DipRL (approx dynamcs model $f\approx p$, r)

Init π, data (or {}), for epis: 1) use π, get data 2) lern f, r from data, 3) plan new π on estim

Plang: cont full obs X, nonlin trans, constr

DetDyn: $x_{t+1} = f(x_t,a_t)$, finit H, at t mxze: $J_H(a_{t:t+H-1}) = \sum_{\tau=t:t+H-1}\gamma^{\tau-t}r_\tau(x_\tau(a_{t:\tau-1}),a_\tau)$ $x_\tau(a_{t:\tau-1}) = f(f(...(f(x_t,a_t),a_{t+1})..))$ do a_t, replan. Opt via ∇ meth for diff r,f, cont A (local min, vanish/explod ∇) → use rand shoot. *Rand shot:* Gen rand $a_{(i),t:t+H-1}$, pick $i^* = \text{amax}_i J_H(a_{(i),t:t+H-1})$. If fin H, sparse r: *MPC ValEstim:* $J_H(a_{t:t+H-1}) = \sum_{\tau=t:t+H-1}\gamma^{\tau-t}r_\tau(x_\tau(a_{t:\tau-1}),a_\tau) + \gamma^H V(x_{t+H})$, **StocDyn:** $\max_{a_{t:t+H-1}}\mathbb E_{x_{t+1:t+H}}[\sum_{\tau=t:t+H-1}\gamma^{\tau-t}r_\tau + \gamma^H V(x_{t+H})|*]$

$\mathbb E$ via *MC traj smplng*, unbias estm of J_H, aprox via smpl avg. **Param π:** ($H=0\to$ DDPG) $J_H(\theta) = \mathbb E_{x_0\sim\mu}[\sum_{\tau=0:H-1}\gamma^\tau r_\tau + \gamma^H Q(x_H,\pi(x_H,\theta))|\theta]$

UnknownDyn: follow π, learn f,r,Q off-π from replay buf, replan π based on f,r,Q. Point est poor perf, err compound → use *BayL:* Model distrib over f (BNN, GP), use aprox inference (exact, VI, MC..) **Greedy exploi:** 1) $D = \{\}$, prior $P(f|\{\})$ 2) repeat: plan new π to $\max_\pi\mathbb E_{f\sim P(\cdot|D)}J(\pi,f)$, use π, add new data to D, update post $P(f|D)$ **PETS algo:** ensmbl of NNs to pred cond Gaus trans distr, MPC for plang. **Explor:** add noise/*/* **Thom Smplng:** Like Greedy but in 2) smpl model $f\sim P(\cdot|D)$ then $max_\pi J(\pi,f)$ Use epist noise, ↑ explor. **Opt explor:** Like Greedy but in 2) $\max_\pi\max_{f\in M(D)}J(\pi,f)$; w\ $M(D)$ set of plausible models given D.