ETHz PAI Cheat Sheet

Probability & BLR

- Gaussian

$P(\mathcal{N}|\mathcal{N}) \sim \mathcal{N}(\mu_{A|B}, \Sigma_{A|B})$

$$\mu_{A|B} = \mu_A + \Sigma_{AB}\Sigma_{BB}^{-1}(x_B - \mu_B)$$
$$\Sigma_{A|B} = \Sigma_{AA} - \Sigma_{AB}\Sigma_{BB}^{-1}\Sigma_{BA}$$

$P(M\mathcal{N}) \sim \mathcal{N}(\mu_Y, \Sigma_Y)$

$$\mu_Y = M\mu_X$$
$$\Sigma_{YY} = M^\top \Sigma_{XX} M$$

$P(\mathcal{N}+\mathcal{N}) \sim P(\mu_Y, \Sigma_Y)$

$$\mu_Y = \mu_X + \mu_{X'}$$
$$\Sigma_{YY} = \Sigma_X + \Sigma_{X'}$$

$P(\mathcal{N}\mathcal{N}) \sim P(\mu_Y, \Sigma_Y)$

$$\Sigma_{YY} = (\Sigma_{XX}^{-1} + \Sigma_{X'X'}^{-1})^{-1}$$
$$\mu_Y = \Sigma_{YY}\Sigma_{XX}^{-1}\mu_X + \Sigma_{YY}\Sigma_{X'X'}^{-1}\mu_{X'}$$

entropy: $ln(\sigma\sqrt{2\pi e})$ (max in all distribution at μ, Σ)

- KL-Divergence:

$$D_{KL}(p\|q) = \int p(x) log\frac{p(x)}{q(x)}dx = H(p|q) - H(p)$$

- $D_{KL}(p||q)$(backward) : mode averageing
- $D_{KL}(q||p)$(forward) : mode seeking
  $p \sim \mathcal{N}(0, diag(\sigma_1^2, \sigma_2^2)) \Rightarrow \sigma_q^2 = \frac{2}{\sigma_1^{-2} + \sigma_2^{-2}}$
  $D_{KL}(q||p)$ is well defined if q is a subset of p
- $q \sim \mathcal{N}(\mathbb{E}(p), Var(p)) \Rightarrow H(p|q) = H(q)$

- Bayesian Linear Regression:

$$y = w^\top x + \epsilon \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2) \; w \sim \mathcal{N}(0, \sigma_p^2)$$
$$P(w|Y, X) \sim \mathcal{N}(\mu, \Sigma)$$
$$\mu = \frac{1}{\sigma_n^2}\Sigma X^\top Y \quad \Sigma = \left(\frac{1}{\sigma_n^2}X^\top X + \frac{1}{\sigma_p^2}I\right)^{-1}$$

uncertainty: aleartoric(rand) + epistemic(know)

Online

$$X_{new}^\top X_{new} = X^\top X + x_{t+1}x_{t+1}^\top$$
$$X_{new}^\top Y_{new} = X^\top Y + y_{t+1}x_{t+1}$$

Fast : $\mathcal{O}(d^3) \to \mathcal{O}(d^2)$

$$(A + xx^\top)^{-1} = A^{-1} - \frac{(A^{-1}x)(A^{-1}x)^\top}{1 + x^\top A^{-1} x}$$
$$(X_{new}^\top X_{new} + \sigma_n^2 I)^{-1} = (\underbrace{X^\top X + \sigma_n^2}_{A} + x_{t+1}x_{t+1}^\top)^{-1}$$

Bayesian Logistic Regression

- posterior is not gaussian
- posterior is not closed
- posterior log-density is convex
- $\sigma \uparrow \to$ standard logistic regression
- posterior cannot cover by $\mathcal{N}$ variational infer

GP & Kalman Filter

- Gaussian Process

$$y = f(x) + \epsilon \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$
$$P(f|X, Y) \sim GP(f; \mu', k')$$
$$\mu'_{x^*} = \mu_{x^*} + K_{x^*X}(K_{XX} + \sigma_n^2 I)^{-1}Y$$
$$k'_{x^*x^*} = K_{x^*x^*} - K_{x^*X}^\top(K_{XX} + \sigma_n^2 I)^{-1}K_{x^*X}$$

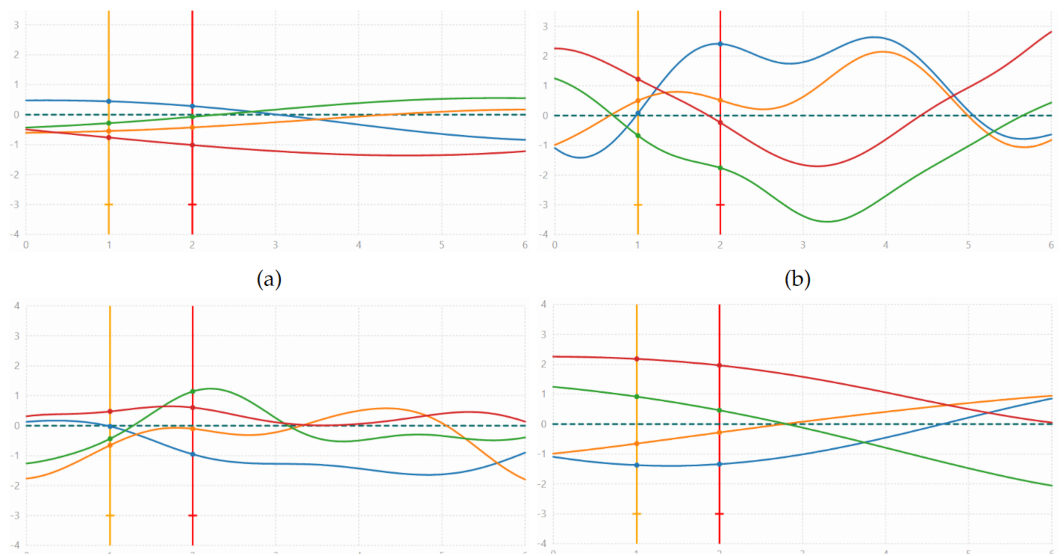
$\mathcal{O}(n^3)$ for the inverse operation
prediction in closed form

Kernel

RBF
$$k(u, v) = \sigma_F^2 exp\left(-\frac{(u-v)^2}{2l^2}\right)$$

l: length scale control the distance of data
σ_F : output scale control the magnitude

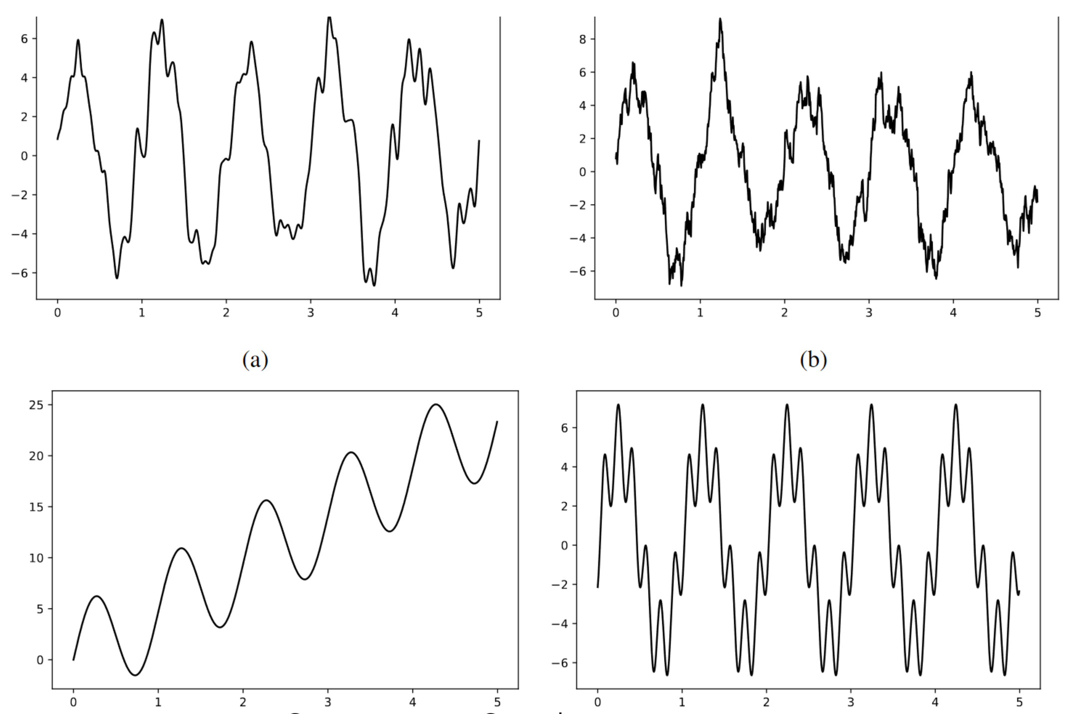
$$\lim_{l \to 0} k(u, v) = \sigma_F^2 \delta(u - v)$$
$$\lim_{l \to 0} k'(x, x) = k(x, x) - k_{xX}(K_{XX} + \sigma_n^2 I)^{-1}k_{xX}^\top$$
$$= \frac{\sigma_F^2\sigma_n^2}{\sigma_F^2 + \sigma_n^2}$$



$\sigma_F^2 = 0.5 \quad l = 4$	$\sigma_F^2 = 2 \quad l = 1$
$\sigma_F^2 = 0.5 \quad l = 1$	$\sigma_F^2 = 2 \quad l = 4$

Linear
$$k(u, v) = \lambda uv$$

equals to BLR with $\lambda = \sigma_p^2$



$exp(-\lambda^2(x-y)^2)$	$exp(-\lambda\|x-y\|)$
λxy	$cos(2\lambda\|x-y\|)$

GP & Kalman Filter

Fast

- $k(x, x') = \phi(x)\phi(x)^\top \; \mathcal{O}(n^3) \to \mathcal{O}(nm^2 + m^3)$
- fourier features: $k(x, x') \approx k(x - x')$
  $= \int_{\mathbb{R}^d} p(\omega)e^{j\omega^t op(x-x')}dw$ (stationary)
  Bochner Theorem:$p(\omega) \geq 0 \Rightarrow k \geq 0$
- inducing points: $\mathcal{O}(n^3)$
  cubic inducing points, linear point
  SoR: subset of regressor (zero)
  FITC: (diag)

- Kalman Filter

$$x_{t+1} = F_t x_t + \Sigma_{x,t} \quad y_t = H_t x_t + \Sigma_y$$

$P(x_{t+1}|x_t) \sim \mathcal{N}(F x_t, \Sigma_{x,t}) \; P(y_t|x_t) \sim \mathcal{N}(H_t x_t, \Sigma_y)$

predict
$$\hat{x}_{t+1} = F_t x_t \quad \hat{\Sigma}_{x,t+1} = H_t\Sigma_{x,t}H_t^\top + \Sigma_{d_t}$$
$$P(x_t|y_{1:t}) \sim \mathcal{N}(\mu_t, \Sigma_{d_t}^2)$$

correct
$$K_{t+1} = \hat{\Sigma}_{x,t}H_t^\top(H_t\hat{\Sigma}_{x,t}H_t^\top + \Sigma_y)^{-1}$$
$$x_{t+1} = \hat{x}_{t+1} + K_{t+1}(y_{t+1} - H_t\hat{x}_{t+1})$$
$$\Sigma_{x,t+1} = (I - K_{t+1}H_t)\hat{\Sigma}_{x,t}$$

kalman gain:K_{t+1}, can be computed offline

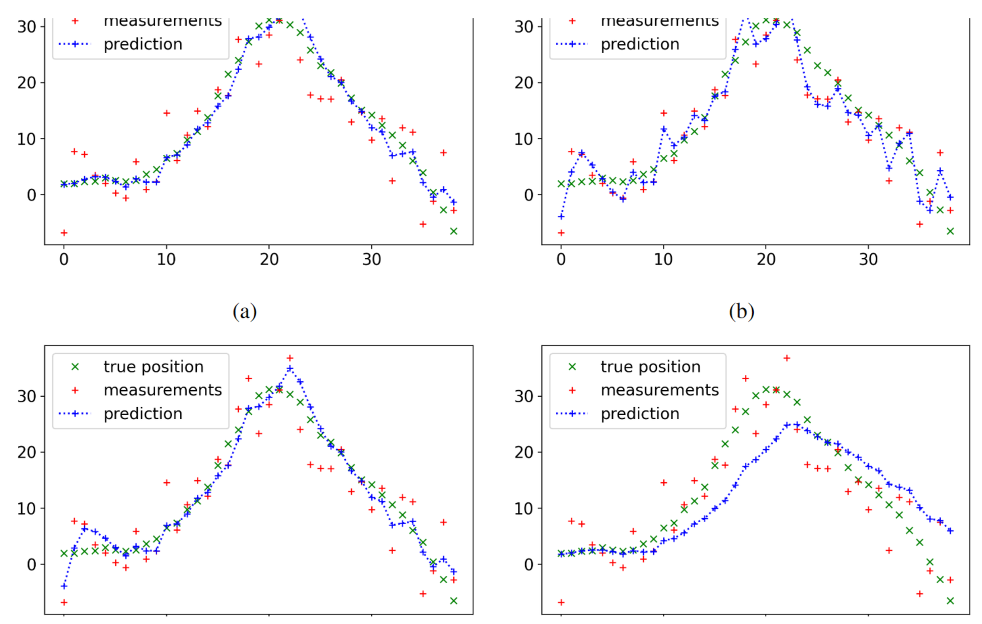
Linear Dynamic System

$$x_{k+1} \sim (ax_k, \sigma^2), x_0 = 0 \to MLE(a) = \frac{\sum_{i=0}^{n-1} x_i x^{i+1}}{\sum_{i=0}^{n-1} x_i^2}$$

if $a \sim \mathcal{N}(0, \frac{\sigma^2}{\lambda})$, $Var(a|x_0, \cdots, x_n) = \frac{\sigma^2}{\lambda + \sum_{i=0}^{n-1} x_i^2}$

Wiener process/Brownian motion

assume $P(x_{t+1}|x_t) \sim \mathcal{N}(x_t, \sigma_x^2) \quad x_0 \sim \mathcal{N}(0, \sigma_0^2)$,
the Kalman Filter can be seen as a GP
$f \sim \mathcal{GP}(0, k_{KF}) \quad k_{KF}(x, x') = \sigma_0^2 + \sigma_x^2 min\{x, x'\}$



$$x_0 \sim \mathcal{N}([^{2,0}]^\top, \sigma^2 I)$$
$$x_{t+1} = \begin{bmatrix} 1 & 1 \\ 0 & a \end{bmatrix} x_t \quad y_t \sim \mathcal{N}(\begin{bmatrix} 1 \\ 0 \end{bmatrix} x_t, \sigma_y^2)$$

$a = 1, \sigma = 1, \sigma_y = 1$	$a = 1, \sigma = 1, \sigma_y = 1$
$a = 1, \sigma = 10, \sigma_y = 10$	$a = 0.5, \sigma = 1, \sigma_y = 10$

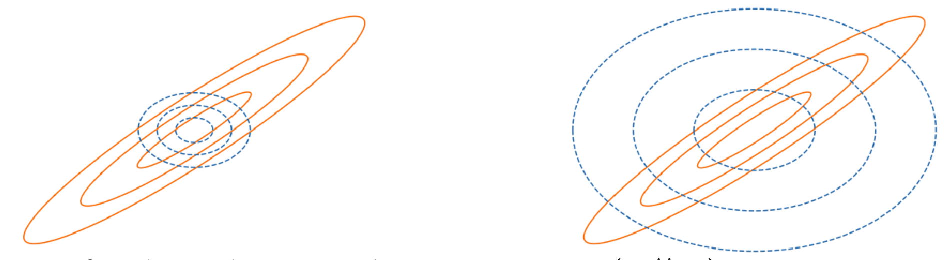
Approximation & MCMC

- Approximation

Laplacian approximation

$q(\theta) \sim (\hat{\theta}, \Lambda^{-1}) \; \hat{\theta} = \underset{\theta}{argmax}\, p(\theta|y) \; \Lambda = -\nabla\nabla p(\hat{\theta}|y)$

- not skewed
- only one modal
- no previous knowledge



- Left: backward KL $D_{KL}(q\|p)$
- Right: forward KL $D_{KL}(p\|q)$

Evidence Lower Bound(ELBO)

$$Q^* = \underset{Q \in \mathcal{Q}}{argmin}\, D_{KL}(Q(Z)\|P(Z|X))$$
$$= \underset{Q \in \mathcal{Q}}{argmax}\, \mathbb{E}_{Z \sim Q(Z)}[log(P(X|Z))]$$
$$- D_{KL}(Q(Z)||P(Z)) = \mathbb{E}_q p - D_{KL}(p\|p)$$

MLE $\quad \hat{\theta} = \underset{\theta}{argmax}\, P(X_{1:n}|\theta)$

sometimes add l_2 norm which is $\|\cdot - \mu\|_2^2$ for vector and $\|\cdot - \mu\|_F^2$ for matrix and $(\cdot - \mu)^2$ for scalar

MAP $\quad \hat{\theta} = \underset{\theta}{argmax}(X_{1:n}|\theta, X')$

reparameterization tricks

- random variable continous
- reduce variance by introducing bias
- automatic differentiation

- Markov Chain Monte Carlo

$$\pi = \pi P$$

π is the stationary state, P is the transition matrix

ergodic:$\exists t \in \mathbb{N} \to (P)^t > 0$

- MCMC used for any distribution
- $P(x|x') = P(x'|x) \to$ uniform distribution

Metropolis-Hastings (MH) Algorithm:

given proposal transition $R(x'|x)$ and unnormalized stationary distribution $Q(x)$

accept rate $\alpha = min\{1, \frac{Q(x')R(x|x')}{Q(x)R(x'|x)}\}$ from x to x'

Gibbs Sampling : random choose dimension

MALA: $\quad R(x'|x) = \mathcal{N}(x'|x - \tau\nabla f(x); 2\tau I)$

Stochastic Gradient Langevin Dynamics(SGLD)

$$\Delta\theta = -\eta(\nabla log\, p(\theta_t) + \frac{N}{n}\sum_{j=1}^{n}\nabla log p(y_{i_j}|\theta_t, x_{i_j})) + \epsilon_t$$
$$= -\eta(\theta_t + \nabla_\theta log\, L(\theta_t)) + \epsilon_t$$

$\epsilon_t \sim \mathcal{N}(0, 2\eta I)$

$L(\theta_t)$ is the likelihood

can guarantee convergence, need burn in step

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Bayesian DL & Optimization

- Bayesian DeepLearning

$$P(y|x,\theta) \sim \mathcal{N}(y|f_\mu(x;\theta_\mu), exp(f_\sigma(x;\theta_\sigma)))$$

train

$$\hat{\theta} = \underset{\theta}{argmin} - lnP(\theta) - \sum_{i=1}^{n} lnP(y_i|x_i,\theta)$$

$$= \underset{\theta}{argmin}\ \lambda||\theta||_2^2 + \frac{1}{2}\sum_{i=1}^{n}\Big[\frac{||y_i-\mu(x_i;\theta_\mu)||^2}{\sigma(x_i;\theta_\sigma)^2} + ln\ \sigma(x_i;\theta_\sigma)^2\Big]$$

predict $P(y'|x',X,Y) = \mathbb{E}_{\theta\sim q}[P(y'|x',\theta)]$

$$Var[y'|x',X,Y] = \mathbb{E}_{\theta\sim q}[Var[y'|x',\theta]] + Var[\mathbb{E}_{\theta\sim q}[y'|x',\theta]]$$

- Aleatoric uncertainty(random)
- Epistemic uncertainty(knowledge)

- MAP for BNN is not closed, unless likelihood and prior are $\mathcal{N}$
- MLE for BNN is closed
- $Var(C\theta|\theta) = 0 \quad \theta \sim p$

approximate inference for BNN: 1.SGLD, 2.Dropout, 3.Ensemble, 4.black-box stochastic variational inference

Stochastic Weight Averaging-Gaussian(SWAG)

$$\mu_{SWA} = \frac{1}{T}\sum_{1}^{T}\theta_i$$

$$\Sigma_{SWA} = \frac{1}{T-1}\sum_{1}^{T}(\theta_i - \mu_{SWA})(\theta_i - \mu_{SWA})^\top$$

Dropout

$$p(y^*|x^*,X,Y) \approx \mathbb{E}_{\theta\sim q(\cdot|\lambda)}[p(y^*|x^*,\theta)]$$

- dropout is also applied in prediction
- dropout can be seen as varational inference

- Bayesian Optimization

Mutual Information

$$F(s) = H(f) - H(f|y_s) = \frac{1}{2}log|I + \sigma^{-2}K_s|$$

$$F(S_T) \geq (1-\frac{1}{e})\max_{S\subseteq D,|S|\leq T} F(S)$$

regret

$$R_T = \sum_{t=1}^{T}(max_{x\in D}f(x) - f(x_t))$$

- sublinear(optimal) if $\frac{R_T}{T} \to 0$ $\lim_{t\to\infty} f(x_t) \to f(x^*)$
- $R_T^A \leq R_T^B$ cannot tell anything
- $\forall t\ R_t^A \leq R_t^B$ menas A is better
- $R \uparrow\to$ more exploration

Bayesian Optimization

- Bayesian Optimization

Uncertainty Sampling

$$x_t = \underset{x\in D}{argmax}\frac{\sigma_e^2(x)}{\sigma_a(x)}$$

- ✓ max info gain in homoscedastic noise case
- ✗ max info gain in heterodastic noise
- ✓ $\lim_{t\to\infty} \hat{x}_t = \underset{x\in D}{argmax}\ \mu_t(x)$, $f(\hat{x}) \to f(x^*)$
- ✗ $\lim_{t\to\infty} f(x_t) \to f(x^*)$

Upper Confidence Sampling(UCB)

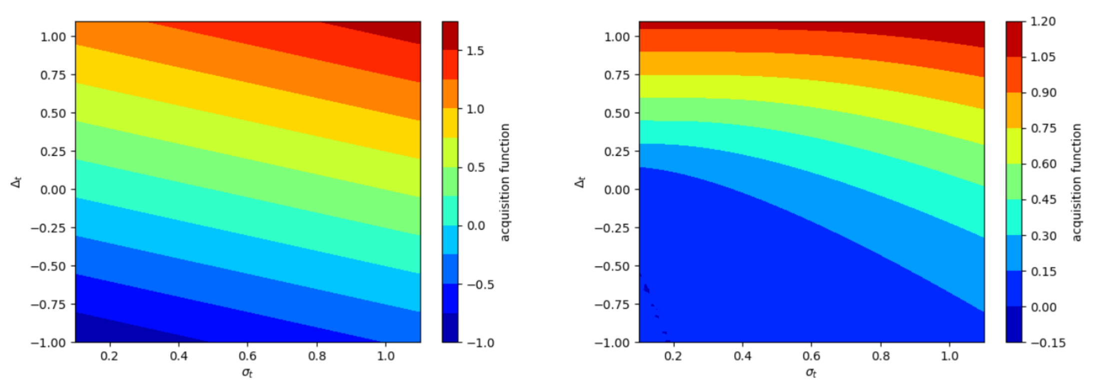
$$a = \mu_t(x) + \beta\sigma_t(x)$$

Probability of Improvement(PI)

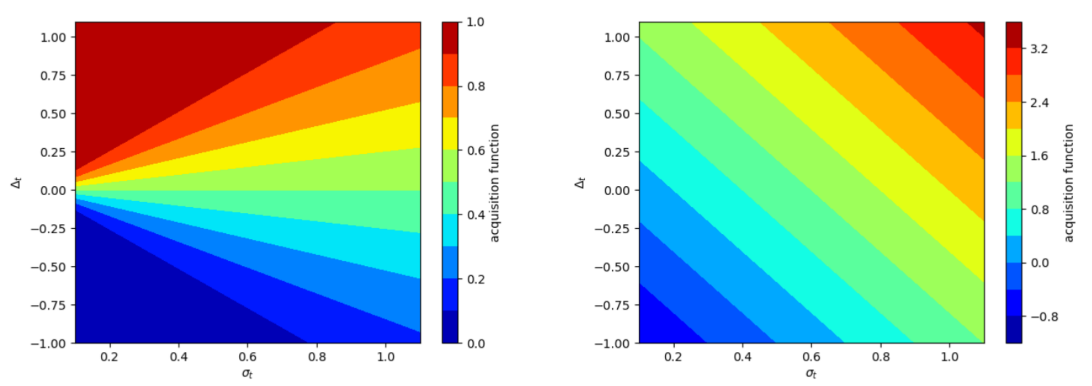
$$a = \Phi\left(\frac{\mu_t(x) - f^*}{\sigma_t(x)}\right)$$

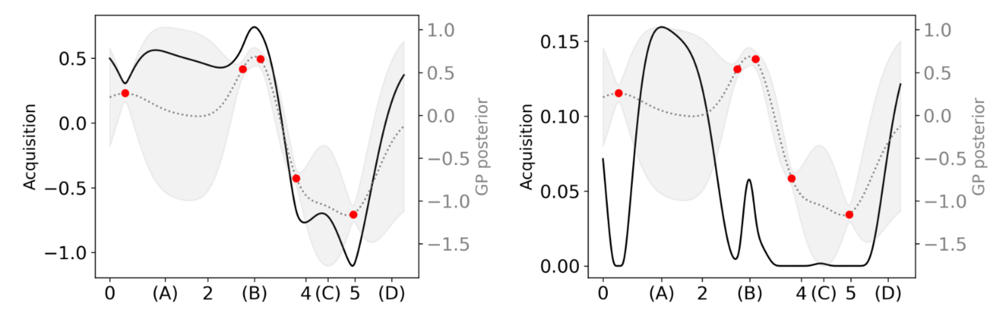
Expected Improvement(EI)

$$a = (\mu_t(x) - f^*)\Phi\left(\frac{\mu_t(x) - f^*}{\sigma_t(x)}\right) + \sigma_t(x)\phi\left(\frac{\mu_t(x) - f^*}{\sigma_t(x)}\right)$$

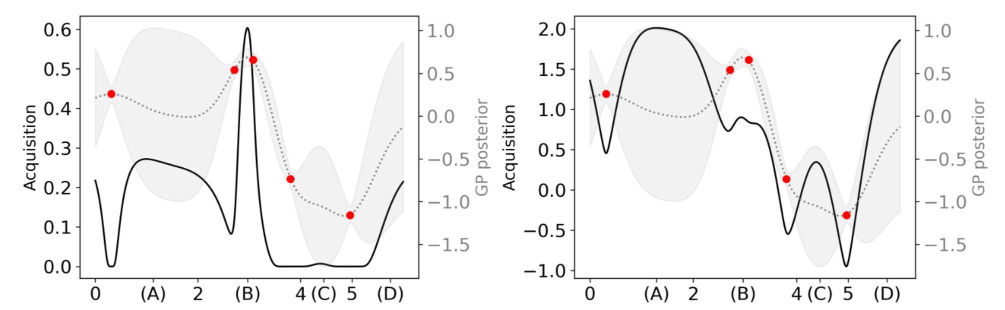


(a) (b)





(a) (b)



(c) (d)

UCB($\beta=0.5$)	EI
PI	UCB($\beta=2$)

$$acquisition \uparrow \Longleftrightarrow exploitation$$

$$acquisition \downarrow \Longleftrightarrow exploration$$

Reinforcement Learning

Bellman Theorem

$$V^*(x) = max_a(r(x,a) + \gamma\sum_{x'}P(x'|x,a)V^*(x'))$$

Hoeffding Bound

$$P(|\mu - \frac{1}{n}\sum_{i=1}^{n}Z_i| > \varepsilon) \leq 2exp(-\frac{2n\varepsilon^2}{C^2})$$

- cR do not change policy

- Model Based

Value Iteration

- guarantee converge to an ε optimal policy not the exact optimal policy
- polynomial time
- performance depend on the input

Policy Iteration

- monotonically improve the policy
- polynomial time, gaurantee converge

ϵ greedy

when random number $< \epsilon$ do the random action

Rmax method

set reward R and transition probability $P(x^*|x,a) = 1$ at first

- with probability $1-\sigma$,reach ε - optimal
- polynomial time in $|X|, |A|, T, \frac{1}{\varepsilon}, log(\frac{1}{\delta})$

- Model Free

Temporal Difference(TD) - Learning

$$\hat{V}^\pi(x) \leftarrow (1-\alpha_t)\hat{V}^\pi(x) + \alpha_t(r + \gamma\hat{V}^\pi(x'))$$

on-policy

Theorem: $\sum_t \alpha_t = \infty, \sum_t \alpha_t^2 < \infty \Rightarrow P(\hat{V}^\pi \to V^\pi) = 1$

Q-Learning

off-policy

$$\hat{Q}^* \leftarrow (1-\alpha_t)\hat{Q}^*(x,a) + \alpha_t(r + \gamma\max_{a'}\hat{Q}^*(x',a'))$$

init : $\hat{Q}^*(x,a) = \frac{R_{max}}{1-\gamma}\Pi_{t=1}^{T_{init}}(1-\alpha_t)^{-1}$

Theorem: $\sum_t \alpha_t = \infty, \sum_t \alpha_t^2 < \infty \Rightarrow P(\hat{Q}^* \to Q^*) = 1$

- with probability $1-\sigma$, R max will reach an ε - optimal
- polynomial time in $|X|, |A|, T, \frac{1}{\varepsilon}, log(\frac{1}{\delta})$
- decay learning rate guarantee convergence

Deep RL

- Model Free

Policy Search

REINFORCE

$$\nabla_\theta J(\theta) = \mathbb{E}_{\tau\sim p_\theta(\tau)}[\sum_{t=0}^{T}\gamma^t(\sum_{t'=t}^{T}\gamma^{t'-t}r_{t'})\nabla_\theta ln\pi_\theta(a_t|x_t)]$$

$$\theta \leftarrow \theta + \eta_t\nabla_\theta J(\theta)$$

Actor-Critic

$$\nabla_{\theta_\pi}J(\theta_\pi) = \mathbb{E}_{(x,a)\sim\pi_{\theta_\pi}}[Q_{\theta_Q}(x,a)\nabla_{\theta_\pi}ln\pi_{\theta_\pi}(a|x)]$$

$$\theta_\pi \leftarrow \theta_\pi + \eta_t\nabla_{\theta_\pi}J(\theta_\pi)$$

$$\theta_Q \leftarrow \theta_Q - \eta_t(Q_{\theta_Q}(x,a) - r - \gamma Q_{\theta_Q}(x', \pi_{\theta_\pi}(x')))\nabla_{\theta_Q}Q_{\theta_Q}(x,a)$$

- use a baseline to reduce variance in the gradient estimates

Proximal Policy Optimization(PPO)

$$L_{\theta_k}(\theta_k) = \mathbb{E}_{\tau\sim\pi_k}\sum_{t=0}^{\infty}\Big[\frac{\pi_\theta(a|x)}{\pi_{\theta_k}(a|x)}(r + \gamma Q^{\pi_{\theta_k}}(x',a) - Q^{\pi_{\theta_k}}(x,a))\Big]$$

$$\theta_k \leftarrow \theta_k - \eta_t\nabla_{\theta_k}L_{\theta_k}(\theta_k)$$

Deep Deterministic Policy Gradients(DDPG)

- randomly add noise ensure sufficient exploration

on-policy	REINFORCE, Actor-Critic, PPO
off-policy	DDPG, TD3, SAC

- Model Based

reduce sample complexity

Random Shooting Method

Monte Carlo Tree Search

PETS

- Other

Bernoulli distribution

$$Bernoulli(x;p) = p^x(1-p)^{1-x}$$

$$\mathbb{E}[Bernoulli(x;p)] = p$$

$$\mathbb{V}ar[Bernoulli(x;p)] = p(1-p)$$

Poisson distribution

$$Pr(x;\lambda) = \frac{\lambda^k e^{-\lambda}}{k!}$$

$$\mathbb{E}[Pr(x;\lambda)] = \lambda$$

$$\mathbb{V}ar[Pr(x;\lambda)] = \lambda$$