Perturbation Methods

① Correlated Sampling

- motivation is doing parametric studies
- goal is to estimate how a response/QoI changes when model parameters change using a single calculation

② Differential Operator Sampling

- motivation are sensitivity studies
- formulate estimators to compute derivatives of responses/QoIs w.r.t. model parameters

Correlated Sampling

$\Rightarrow$ apply to a discrete-time Markov Chain, but more general random processes can be used as well

Define: R = response/QoI

α = input model parameter

ω = index for a random walk/realization

$R = \sum_{\omega} r(\omega) f(\omega)$, $r(\omega)$ = scoring/response fcn for r.w. ω

$f(\omega)$ = prob. of r.w. ω occurring

R' = perturbed response b/c of some change α, call it $\Delta\alpha$

$\Rightarrow$ $\Delta\alpha$ leads to the following changes to the simulation process

① **Direct Effect**: changes $r(\omega)$ by Δr independent of changes to the random walks

② **Indirect Effect**: changes $f(\omega)$ by Δf, change in the r.w. probability

Perturbed Response: $R' = \sum_{\omega'} r'(\omega') f'(\omega')$ ⇒ perturbations are NOT derivatives

r.w.'s for perturbed case

⇒ expand $f(\omega)$ as the product of probabilities of taking individual steps

$$f(\omega) = \prod_{k=1}^{n(\omega)} p_k(\omega),$$

$n(\omega)$ = # steps in r.w. ω

$p_k(\omega)$ = prob. of the kth step in r.w. ω

⇒ Insert into expression for R'

$$R' = \sum_{\omega'} r'(\omega') \prod_{k=1}^{n'(\omega')} p_k'(\omega')$$

⇒ Our desire is to use the r.w.'s ω in the base/unperturbed case vs. the perturbed r.w.'s ω'

$$R' \approx \sum_{\omega} r'(\omega) \prod_{k=1}^{n(\omega)} p_k'(\omega)$$

approximate b/c changing a model parameter could "open up" new parts of the sample space not in the base case

$$R' \approx \sum_{\omega} r'(\omega) \prod_{k=1}^{n(\omega)} \underbrace{\left(\frac{p_k'(\omega)}{p_k(\omega)}\right)}_{a_k(\omega) = \text{adjustment factor for kth step}} p_k(\omega)$$

$$= \sum_{\omega} r'(\omega) \prod_{k=1}^{n(\omega)} a_k(\omega) p_k(\omega)$$

$$= \sum_{\omega} r'(\omega) \underbrace{\left(\prod_{k=1}^{n(\omega)} a_k(\omega)\right)}_{a(\omega)} \underbrace{\left(\prod_{k=1}^{n(\omega)} p_k(\omega)\right)}_{f(\omega)}$$

$$\boxed{R' \approx \sum_{\omega} \underbrace{r'(\omega) a(\omega)}_{\text{scoring/response fxn for the perturbed response}} \underbrace{f(\omega)}_{\text{handled by the frequency of r.w. } \omega \text{ occurring}}}$$

$\Rightarrow$ assume an additive scoring fxn:

$$r(w) = \sum_k r_k(w)\,, \quad r_k(w) = \text{response/scoring contribution for } k\text{th step}$$

$$r'(w) = \sum_k r_k'(w) = \sum_k \Big(r_k(w) + \underbrace{\Delta r_k(w)}_{\text{change b/c of DDx}}\Big)$$

$\Rightarrow$ change in response

$$\Delta R = R' - R$$

$$\approx \sum_w r'(w)\,a(w)\,f(w) - \sum_w r(w)\,f(w)$$

$$= \sum_w \left(\frac{r'(w)}{r(w)}\,a(w)\,r(w) - r(w) \right) f(w)$$

$$= \sum_w \left(\frac{r'(w)}{r(w)}\,a(w) - 1 \right) r(w)\,f(w)$$

put in terms of Δr

$$\boxed{\Delta R \approx \sum_w \underbrace{\left[\underbrace{\left(1 + \frac{\Delta r(w)}{r(w)}\right)}_{\text{direct effect}} \underbrace{a(w)}_{\text{indirect effect}} - 1 \right] r(w)}_{\text{scoring fxn for } \Delta R} f(w)}$$

Modification of DTMC Algorithm

⇒ at the start of each random walk/sample we set $a_m = 1$, $\Delta r_m = 0$ for each perturbation $m = 1, \ldots, M$

a_m = multiplicative accumulator for the adjustment factor for pert. m

Δr_m = additive accumulator for the change in scoring fxn for pert. m

⇒ sample each step in random walk as before

- now for each step $k = 1, \ldots, n$

$$a_m \mathrel{*}= \frac{p'_{m,k}}{\underbrace{p_k}_{\text{element of transition matrix for kth step}}} = \frac{\text{perturbed transition prob}}{\text{unperturbed / base " " (the one we are simulating)}}$$

$$\Delta r_m \mathrel{+}= \Delta r_{m,k} = \text{change in response/score contribution for kth step}$$

⇒ at the end of the random walk

make the score for pert m:

$$\Delta R_m \mathrel{+}= \left[\left(1 + \frac{\Delta r_m}{r}\right) a_m - 1 \right] r$$

NOT each STEP!

⇒ repeat for numerous random walks/samples and divide ΔR_m by the # samples to get the estimate

Ex: geometric distribution

$$f(n) = \lambda^{n-1}(1-\lambda), \quad n=1,2,3,\dots$$

$$P = \begin{bmatrix} \lambda & 0 \\ 1-\lambda & 1 \end{bmatrix}$$

⇒ let R = expected # steps to reach state 2

$$R = \sum_{n=1}^{\infty} r(n) f(n) = \sum_{n=1}^{\infty} n \lambda^{n-1} \cancel{f}(1-\lambda) = \frac{1}{1-\lambda}$$

⇒ for perturbed r.w. w/ $\lambda \rightarrow \lambda'$

$$R' = \frac{1}{1-\lambda'}$$

⇒ will correlated sampling produce this value of R'?

$$R' \stackrel{?}{=} \sum_{n=1}^{\infty} \overbrace{r(n)}^{=r'(n)=n} a(n) f(n)$$

$$= (1)\left[\frac{1-\lambda'}{\cancel{1-\lambda}}\right]\cancel{(1-\lambda)}$$

$$+ (2)\left[\left(\frac{\lambda'}{\cancel{\lambda}}\right)\left(\frac{1-\lambda'}{\cancel{1-\lambda}}\right)\right]\cancel{\lambda(1-\lambda)}$$

$$+ (3)\left[\left(\frac{\lambda'}{\cancel{\lambda}}\right)^2\left(\frac{1-\lambda'}{\cancel{1-\lambda}}\right)\right]\cancel{\lambda^2(1-\lambda)}$$

$$= \sum_{n=1}^{\infty} n(\lambda')^{n-1}(1-\lambda') = \frac{1}{1-\lambda'} \checkmark$$

$\Rightarrow$ In simulation, if we step $1 \to 1$ we multiply an by $\frac{\lambda'}{\lambda}$,

if we step $1 \to 2$, we multiply an by $\frac{1-\lambda'}{1-\lambda}$

Remarks

⇒ works well when the cost of accruing the perturbed estimators is fast compared to the computational cost of the simulation (ex. particle transport) compared to seperate realizations

⇒ the estimator for adjustment factor is multiplicative and can be very large for some random walks → high variance, when $\Delta\alpha$ is large (keep the changes to model parameters modest)