Algorithmic and Theoretical Foundations of RL

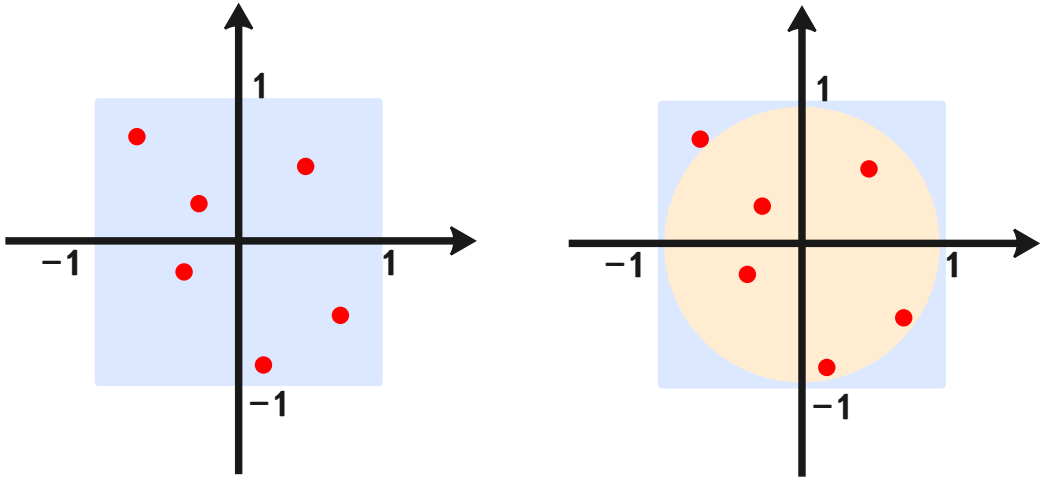
Monte Carlo Methods

A Typical Example

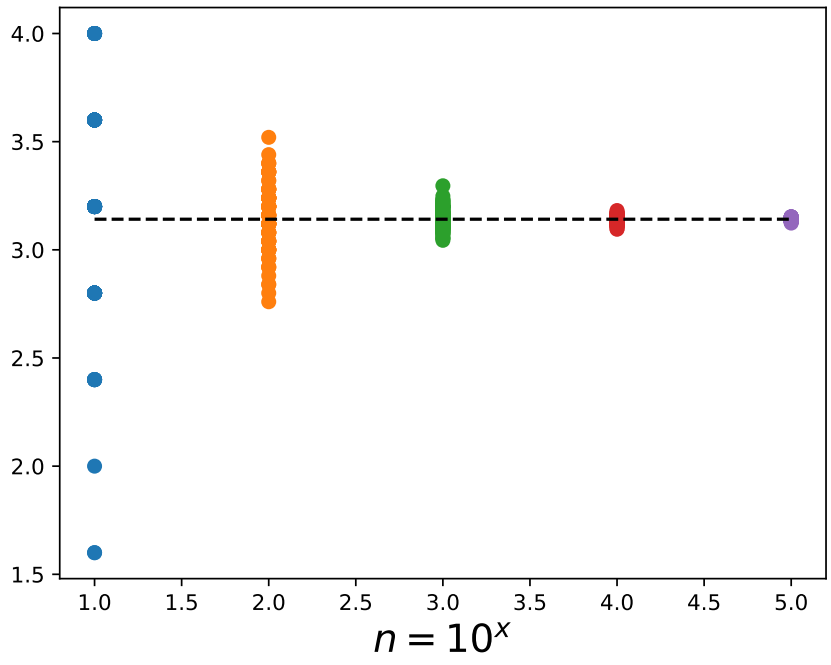
Monte Carlo (MC) methods refers to a collection of computational methods where simulation is used. A typical example is the computation of π.

Example 1 (Approximation of π)

- *Ratio of the area of circle to the area of square:* $\frac{A_C}{A_S} = \frac{\pi}{4}$
- *Simulation steps:*
  - *Randomly generate n points inside the square;*
  - *Count the number of points inside the circle (satisfying* $x^2 + y^2 < 1$*):* n_c*;*
  - $\pi \approx 4\frac{n_c}{n}$.



Simulation Result



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Compute Expectation or Integration

Computing the expectation or integration

$$\mu = \mathbb{E}_p\left[f(X)\right] = \int_\Omega f(x)p(x)dx$$

is a ubiquitous task in science and engineering.

- Numerical Integration: Trapezium rule, Simpson's rule, ...
- Monte Carlo Integration: Statistical methods based on **random** samples.

Simple Monte Carlo Integration

Let $X_1, \cdots, X_n \sim p(x)$ be i.i.d random samples. Then approximate μ by a (random) sample mean

$$\bar{\mu}_n = \frac{1}{n} \sum_{k=1}^{n} f(X_k).$$

- Un-bias and strong consistency

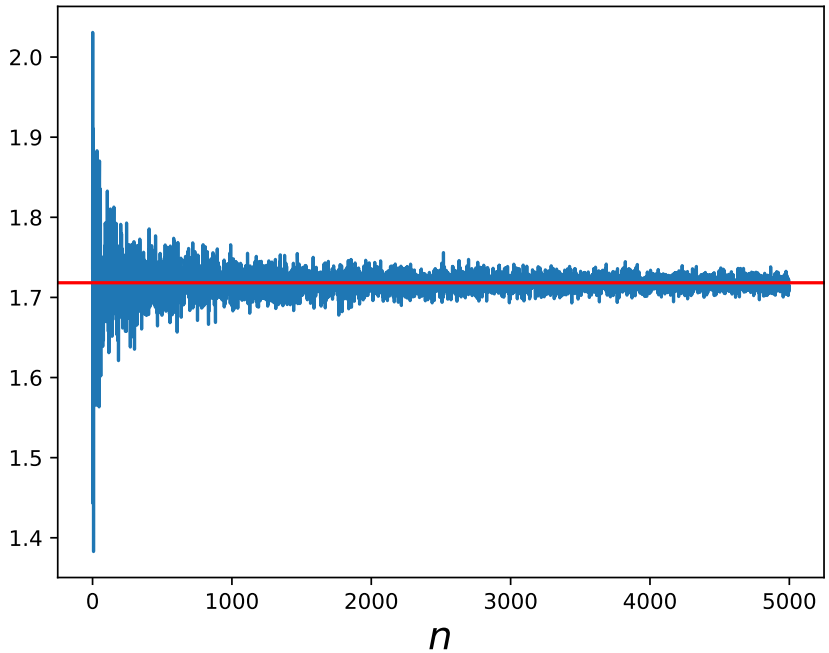
$$\mathbb{E}\left[\frac{1}{n} \sum_{k=1}^{n} f(X_k)\right] = \mu \quad \text{and} \quad \lim_{n \to \infty} \frac{1}{n} \sum_{k=1}^{n} f(X_k) \xrightarrow{a.s.} \mu.$$

- Finite sample variance

$$\mathrm{Var}_p\left[\frac{1}{n} \sum_{k=1}^{n} f(X_k)\right] = \frac{\mathrm{Var}_p\left[f(X)\right]}{n}.$$

Illustrative Example

Estimate the integral $\int_0^1 e^x dx$.



Variance Reduction

Variance reduction is an important component in statistical computing.

数学上等价，计算上未必等效. — 冯康

Consider equivalent problems with more information, structure or control.

- Control variates

$$\mathbb{E}_p\left[f(X)\right] = \mathbb{E}_p\left[h(X)\right], \quad \text{where } h(X) = f(X) + c \cdot \left(g(X) - \mathbb{E}\left[g(X)\right]\right).$$

  May choose c such that $\mathrm{Var}\left[h(X)\right] < \mathrm{Var}\left[f(X)\right]$ and evaluate $\mathbb{E}_X\left[h(X)\right]$.

- Importance sampling

$$\mathbb{E}_p\left[f(X)\right] = \int_\Omega f(x)p(x)dx = \int_\Omega \frac{f(y)p(y)}{q(y)}q(y)dy = \mathbb{E}_q\left[\frac{f(Y)p(Y)}{q(Y)}\right].$$

  May choose q such that $\mathrm{Var}_q\left[\frac{f(Y)p(Y)}{q(Y)}\right]$ is smaller and evaluate $\mathbb{E}_q\left[\frac{f(Y)p(Y)}{q(Y)}\right]$.

Control Variates

Notice that

$$\begin{aligned}&\operatorname{Var}\left[f(X)+c\cdot\left(g(X)-\mathbb{E}\left[g(X)\right]\right)\right]\\&=\operatorname{Var}\left[f(X)\right]+c^2\cdot\operatorname{Var}\left[g(X)\right]+2c\cdot\operatorname{Cov}\left(f(X),g(X)\right).\end{aligned}$$

The best c^* is given by

$$c^*=-\frac{\operatorname{Cov}\left(f(X),g(X)\right)}{\operatorname{Var}\left[g(X)\right]}.$$

Then variance is reduced by

$$\frac{\left[\operatorname{Cov}\left(f(X),g(X)\right)\right]^2}{\operatorname{Var}\left[g(X)\right]}.$$

The subscript p is dropped whenever the distribution is clear from context.

Illustrative Example

Estimate the integral $\int_0^1 e^x dx$. Let $n = 1000$. Take $g(x) = x$ and $c = -1.5$.

```
import numpy as np
```

```
n = 1000
x = np.random.rand(n)
y = np.exp(x)
mu = np.mean(y)
var = np.var(y)
print('Simple MC Integration: mu = %.5f,' % mu, 'var = %.5f' % var)
```

```
Simple MC Integration: mu = 1.70772, var = 0.24851
```

```
c = - 1.5
y = np.exp(x)+c*(x-1/2)
mu = np.mean(y)
var = np.var(y)
print('Control variate: mu = %.5f,' % mu, 'var = %.5f' % var)
```

```
Control variate: mu = 1.71893, var = 0.00715
```

Importance Sampling

Monte Carlo Integration via Importance Sampling

$$\underbrace{\mathbb{E}_p\left[f(X)\right]}_{\mu} = \mathbb{E}_q\left[\frac{f(Y)p(Y)}{q(Y)}\right] \approx \underbrace{\frac{1}{n}\sum_{k=1}^{n} f(Y_k)\frac{p(Y_k)}{q(Y_k)}}_{\bar{\mu}_{IS}},$$

where $Y_1, \cdots, Y_n \sim q(y)$.

- If a region is important for evaluation of $\mathbb{E}_p\left[f(X)\right]$, more data should be obtained from this region. This can be achieved by an importance sampling distribution, followed by correction of bias caused by distinction between target distribution and importance sampling distribution via $w(y) = p(y)/q(y)$.
- The expression for importance sampling indeed indicates that evaluation of $\mathbb{E}_p\left[f(X)\right]$ is not intrinsically associated with target distribution. This is particularly useful when only data from a different distribution are available, **which is often the case in RL**.

Selection of Importance Sampling Distribution

In order to reduce variance, $q(y)$ should be selected such that $f(y)p(y)/q(y)$ varies not much over the integration region.

Theorem 1

The minimum variance of $\bar{\mu}_{IS}$ under q is achieved at

$$q^*(y) = \frac{|f(y)|p(y)}{\mathbb{E}_p\left[|f(Y)|\right]},$$

with the minimum variance given by

$$\mathrm{Var}_{q^*}\left[\bar{\mu}^*_{IS}\right] = \frac{1}{n}\left(\left[\mathbb{E}_p\left[|f(Y)|\right]\right]^2 - \mu^2\right).$$

- Though $q^*(y)$ is not available since $\mathbb{E}_p\left[|f(y)|\right]$, the theorem does provide a principle for selecting $q(y)$: $q(y)$ should be "similar" to $|f(y)|p(y)$ in shape.

Proof of Theorem 1

First note that for any $q(y)$, the variance $\mathrm{Var}_q\left[\bar{\mu}_{IS}\right]$ is given by

$$\begin{aligned} n \cdot \mathrm{Var}_q\left[\bar{\mu}_{IS}\right] &= \int \frac{f(y)^2 p(y)^2}{q(y)} dy - \mu^2 \\ &= \int \frac{(f(y)p(y) - \mu q(y))^2}{q(y)} dy, \end{aligned}$$

which suggest that $q(y) \propto f(y)p(y)$ if $f(y) \geq 0$. Moreover, from it we can see that

$$\begin{aligned} n \cdot \mathrm{Var}_{q^*}\left[\bar{\mu}^*_{IS}\right] + \mu^2 &= \left(\int |f(y)| p(y) dy \right)^2 \\ &= \left(\int \frac{|f(y)| p(y)}{q(y)} q(y) dy \right)^2 \\ &\leq \int \frac{f(y)^2 p(y)^2}{q(y)} dy \\ &= n \cdot \mathrm{Var}_q\left[\bar{\mu}_{IS}\right] + \mu^2, \quad \forall\, q(y). \end{aligned}$$

Illustrative Example

Estimate the integral $\int_0^1 1_{[3/4,1]}(x)dx$. Let $n = 1000$. Take

$$p(x) = 1 \text{ for } 0 \leq x \leq 1 \quad \text{and } q(x) = \begin{cases} 0 & \text{if } 0 \leq x < 0.5 \\ 2 & \text{if } 0.5 \leq x < 1. \end{cases}$$

```
import numpy as np
```

```
n = 1000
x = np.random.rand(1,n)
fx = (x>=0.75)
mu = np.mean(fx)
var = np.var(fx)
print('Simple MC Integration: mu = %.5f,' % mu, 'var = %.5f' % var)
```

```
Simple MC Integration: mu = 0.23900, var = 0.18188
```

```
y = 0.5*np.random.rand(1,n)+0.5
fy = (y>=0.75)/2
mu = np.mean(fy)
var = np.var(fy)
print('Importance Sampling: mu = %.5f,' % mu, 'var = %.5f' % var)
```

```
Importance Sampling: mu = 0.25450, var = 0.06248
```

A Word about Bias-Variance Tradeoff

Let $\bar{\mu} \in \mathbb{R}^d$ be a statistical estimator of a parameter $\mu \in \mathbb{R}^d$ (not necessarily $\mathbb{E}[\bar{\mu}] = \mu$). Then the MSE is given by

$$\begin{aligned}\mathbb{E}\left[\|\bar{\mu} - \mu\|_2^2\right] &= \mathbb{E}\left[\|\bar{\mu} - \mathbb{E}[\bar{\mu}] + \mathbb{E}[\bar{\mu}] - \mu\|_2^2\right] \\ &= \underbrace{\|\mathbb{E}[\bar{\mu}] - \mu\|_2^2}_{\text{bias}^2} + \underbrace{\mathbb{E}\left[\|\bar{\mu} - \mathbb{E}[\bar{\mu}]\|_2^2\right]}_{\text{variance}}.\end{aligned}$$

- Unbiased estimator is not always the one the achieves a smaller MSE.

A Word about Bias-Variance Tradeoff

Example

Consider the problem of estimating a vector $x \in \mathbb{R}^d$ from the noisy observation

$$y = x + e,$$

where $e \sim \mathcal{N}(0, \sigma^2 I_d)$. Suppose x is k-sparse, i.e., it only has k-nonzero entries.

- Least squares (LS) estimator: $\bar{x}_1 = y$. Unbiased; MSE is variance, given by

$$\mathbb{E}\left[\|\bar{x}_1 - x\|_2^2\right] = d \cdot \sigma^2.$$

- Zero estimator $\bar{x}_2 = 0$. Clearly, $\mathbb{E}\left[(\bar{x}_2)_j\right] \neq x_j$ if $x_j \neq 0$ and $\mathrm{Var}\left[\bar{x}_2\right] = 0$. Moreover,

$$\mathbb{E}\left[\|\bar{x}_2 - x\|_2^2\right] = \|x\|_2^2 \leq k\|x\|_\infty^2.$$

  Assume $\|x\|_\infty < \sigma$. Then it can be seen that the MSE of $\bar{x}_2$ can be much smaller than that of $\bar{x}_1$.

Without the assumption $\|x\|_\infty < \sigma$, one can use the soft-thresholding denoiser $\bar{x} = \mathrm{sgn}(y)(|y| - \lambda)_+$ for suitable λ. See "Ideal spatial adaptation by wavelet shrinkage" by Donoho and Johnstone, 1994.

Incremental Update for Sample Mean

Calculate sample mean $\bar{\mu}_n = \frac{1}{n}\sum_{k=1}^{n} X_k$ in an incremental manner rather than wait until all the samples are collected:

$$\bar{\mu}_{k+1} = \bar{\mu}_k + \frac{1}{k+1}\left(X_{k+1} - \bar{\mu}_k\right).$$

A more general form

$$\bar{\mu}_{k+1} = \bar{\mu}_k + \alpha_k\left(X_{k+1} - \bar{\mu}_k\right), \quad \alpha_k > 0.$$

- The incremental update can be viewed as a special case of the Robbins-Monro Algorithm that will be discussed next.

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Robbins-Monro (RM) Algorithm

Consider the fixed point problem

$$x = h(x),$$

where $h : \mathbb{R}^d \to \mathbb{R}^d$ is a function. The fixed point iteration after introducing stepsize is given by

$$x_{k+1} = x_k + \alpha_k(h(x_k) - x_k).$$

RM considers the case where only a perturbation or noisy oracle of $h(x)$, denoted $\tilde{h}(x) = h(x) + e$, can be returned for every input x.

$$x_{k+1} = x_k + \alpha_k \left(\tilde{h}(x_k) - x_k\right) = x_k + \alpha_k \left(h(x_k) - x_k + e_k\right).$$

When $h(x_k)$ cannot be accurately known, using $\alpha_k = 1$ may be too aggressive. Then adjusting the stepsize becomes necessary, which is also one reason that it is introduced.

Special Cases

- Incremental update for sample mean: $h(\bar{\mu}) = \mu$. For each $\bar{\mu}$ only the X ($\mathbb{E}[X] = \mu$) can be obtained. Thus RM reduces to

$$\bar{\mu}_{k+1} = \bar{\mu}_k + \alpha_k \cdot (X_{k+1} - \mu_k).$$

- Stochastic gradient: $\min_x \mathbb{E}_\xi [f(x;\xi)]$ is equivalent to $x - \mathbb{E}_\xi [\nabla f(x;\xi)] = x$. For each x only $\nabla f(x;\xi)$ can be returned. Then RM reduces to

$$x_{k+1} = x_k - \alpha_k \nabla f(x_k;\xi_k).$$

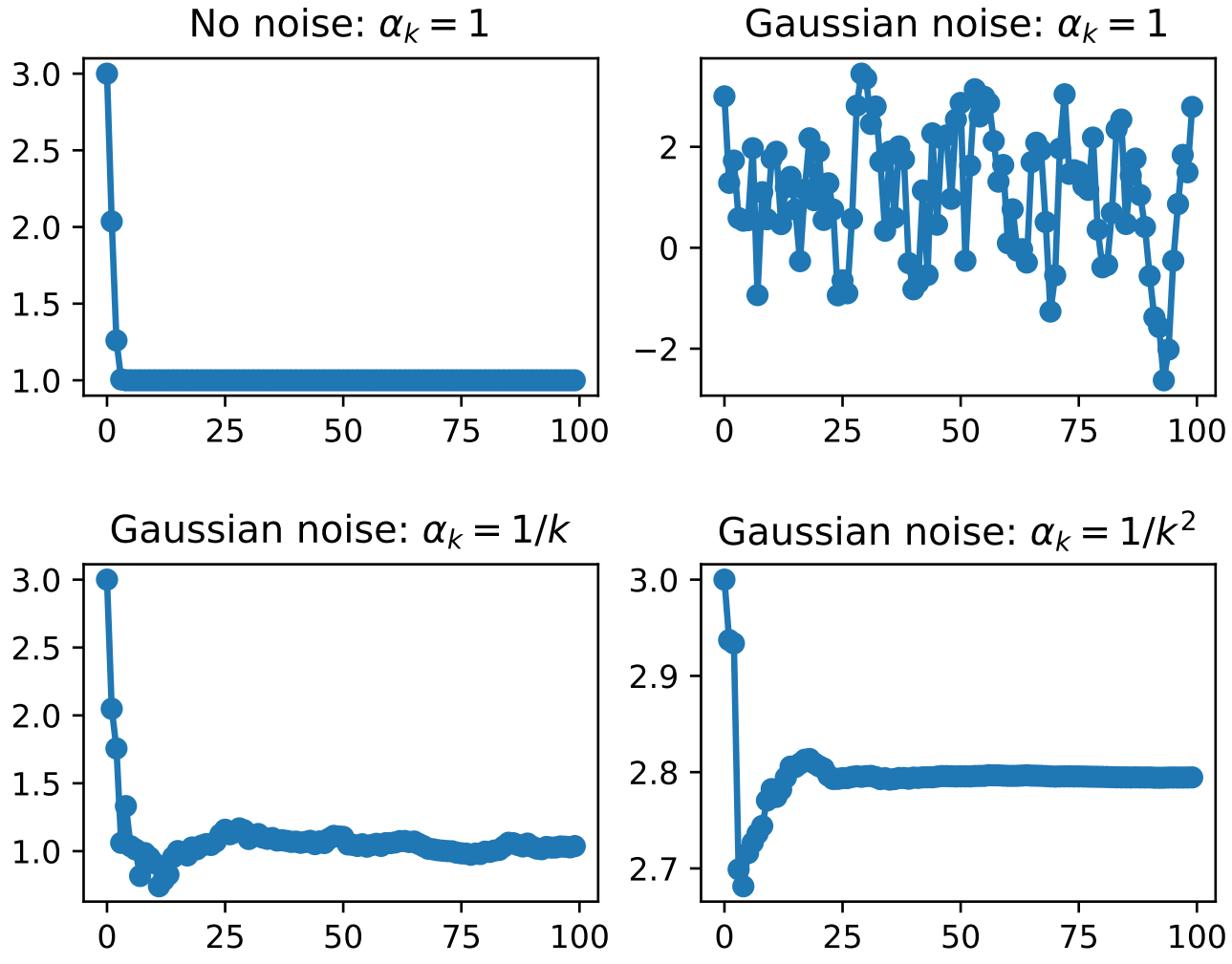
- Finding the root of $f(x) = 0$ is equivalent to fixed point problem $x - f(x) = x$. Suppose only denoted $f(x) + e$ can be obtained for each x. Then, RM reduces to

$$x_{k+1} = x_k - \alpha_k (f(x_k) + e_k).$$

- **Bellman optimality equation is in the form of $x = h(x)$ and TD algorithms in RL are in the form of RM.**

Illustrative Example

Find the root of $f(x) = \tanh(x - 1)$ with starting point $x_1 = 3$.



Convergence of RM

Theorem 2 (Convergence of RM)

Assume the following conditions hold:

- $|h'(x)| \leq \gamma < 1$ *for all* x*;*
- $\sum_{k=1}^{\infty} \alpha_k = \infty$ *and* $\sum_{k=1}^{\infty} \alpha_k^2 < \infty$*;*
- $\mathbb{E}\left[e_k | \mathcal{F}_k\right] = 0$ *and* $\mathbb{E}\left[e_k^2 | \mathcal{F}_k\right] < \infty$ *with probability 1, where* $\mathcal{F}_k = \{x_k, x_{k-1}, \cdots\}$.

Then x_k *converges to the fixed point solution* x^* *with probability* 1.

The proof of this theorem relies on a powerful tool: Dvoretzky's Theorem.

For simplicity, we only consider the single variable case, i.e., $d = 1$.

Dvoretzky's Theorem

Theorem 3 (Dvoretzky's Theorem)
Consider the stochastic process

$$w_{k+1} = (1 - \alpha_k)w_k + \beta_k e_k,$$

where $\{\alpha_k\}$, $\{\beta_k\}$, $\{\eta_k\}$ *are stochastic sequences and* $\alpha_k \geq 0$, $\beta_k \geq 0$. *Suppose the following conditions hold:*

- $\sum_{k=1}^{\infty} \alpha_k = \infty$, $\sum_{k=1}^{\infty} \alpha_k^2 < \infty$, $\sum_{k=1}^{\infty} \beta_k^2 < \infty$ *uniformly with probability* 1;
- $\mathbb{E}\left[e_k | \mathcal{F}_k\right] = 0$ *and* $\mathbb{E}\left[e_k^2 | \mathcal{F}_k\right] < \infty$, *where*

$$\mathcal{F}_k = \{w_k, w_{k-1}, \cdots, e_{k-1}, \cdots, \alpha_{k-1}, \cdots, \beta_{k-1}, \cdots\}.$$

Then w_k *converges to* 0 *with probability* 1.

The proof of Dvoretzky's Theorem requires the knowledge of martingales, which will not be discussed; see "On the Convergence of Stochastic Iterative Dynamic Programming Algorithms" by Jaakkola et al., 1994.

Proof of Theorem 2

Since $|h'(x)| \leq \gamma < 1$, it is easy to see $h(x)$ is a contraction. Thus the fixed point solution x^* exists. Thus,

$$\begin{aligned} x_{k+1} - x^* &= x_k - x^* + \alpha_k(h(x_k) - h(x^*) + x^* - x_k) + \alpha_k e_k \\ &= x_k - x^* + \alpha_k(h(x_k')(x_k - x^*) + x^* - x_k) + \alpha_k e_k \\ &= x_k - x^* - \alpha_k(1 - h(x_k'))(x_k - x^*) + \alpha_k e_k. \end{aligned}$$

It is easy to verify that the conditions of Dvoretzky's Theorem holds for $w_k = x_k - x^*$. Thus $x_k \to x^*$ almost surely.

Finite Iteration Mean Square Error

Theorem 4

Assume the following conditions hold:

- $\|h(x) - h(y)\|_2 \leq \gamma \|x - y\|_2$ *for* $0 < \gamma < 1$;
- $\mathbb{E}\left[e_k | \mathcal{F}_k\right] = 0$ *and* $\mathbb{E}\left[e_k^2 | \mathcal{F}_k\right] < \infty$ *with probability 1, where* $\mathcal{F}_k = \{x_k, x_{k-1}, \cdots\}$.

Set $\alpha_k = \frac{1}{k}$. *Then,*

$$\mathbb{E}\left[\|x_k - x^*\|_2^2\right] \lesssim \begin{cases} \frac{1}{k} & \text{if } 0 \leq \gamma < 1/2 \\ \frac{\log k}{k} & \text{if } \gamma = 1/2 \\ \frac{1}{k^{2(1-\gamma)}} & \text{if } 1/2 < \gamma < 1. \end{cases}$$

- As a special case of RM, it is trivial that the iterate for mean estimation $\bar{\mu}_{k+1} = \bar{\mu}_k + \alpha_k \cdot (X_k - \mu_k)$ satisfies

$$\mathbb{E}\left[|\bar{\mu}_k - \mu|_2^2\right] \lesssim \frac{1}{k}.$$

The final convergence rate has been calculated with the help of Yuwen Wang.

Proof of Theorem 4

Without loss of generality, assume that e_k are chosen independently in each iteration. First we have

$$
\begin{aligned}
\|x_{k+1} - x^*\|_2^2 &= \|x_k - x^* + x_{k+1} - x_k\|_2^2 \\
&= \|x_k - x^*\|_2^2 + 2\langle x_k - x^*, x_{k+1} - x_k\rangle + \|x_{k+1} - x_k\|_2^2 \\
&= \|x_k - x^*\|_2^2 + 2\alpha_k\langle x_k - x^*, h(x_k) - x_k + e_k\rangle + \alpha_k^2\|h(x_k) - x_k + e_k\|_2^2 \\
&= \|x_k - x^*\|_2^2 + 2\alpha_k\langle x_k - x^*, h(x_k) - h(x^*)\rangle - 2\alpha_k\langle x_k - x^*, x_k - x^*\rangle \\
&\quad + 2\alpha_k\langle x_k - x^*, e_k\rangle + \alpha_k^2\|h(x_k) - x_k + e_k\|_2^2 \\
&\le \|x_k - x^*\|_2^2 - 2\alpha_k(1-\gamma)\|x_k - x^*\|_2^2 + 2\alpha_k\langle x_k - x^*, e_k\rangle \\
&\quad + \alpha_k^2\|h(x_k) - x_k + e_k\|_2^2 \\
&= \|x_k - x^*\|_2^2 - 2\alpha_k(1-\gamma)\|x_k - x^*\|_2^2 + 2\alpha_k\langle x_k - x^*, e_k\rangle \\
&\quad + \alpha_k^2\|h(x_k) - h(x^*) + x^* - x_k + e_k\|_2^2 \\
&\le \|x_k - x^*\|_2^2 - 2\alpha_k(1-\gamma)\|x_k - x^*\|_2^2 + 2\alpha_k\langle x_k - x^*, e_k\rangle \\
&\quad + \alpha_k^2\left(2\|x_k - x^*\|_2 + \|e_k\|_2\right)^2 \\
&\le \|x_k - x^*\|_2^2 - 2\alpha_k(1-\gamma)\|x_k - x^*\|_2^2 + 2\alpha_k\langle x_k - x^*, e_k\rangle \\
&\quad + 8\alpha_k^2\|x_k - x^*\|_2^2 + 2\alpha_k^2\|e_k\|_2^2.
\end{aligned}
$$

Proof of Theorem 4 (Cont'd)

Note that $\mathbb{E}\left[\langle x_k - x^*, e_k\rangle\right] = 0$. Taking an expectation on both sides yields that

$$\mathbb{E}\left[\|x_{k+1} - x^*\|_2^2\right] \leq (1 - 2\alpha_k(1-\gamma) + 8\alpha_k^2)\mathbb{E}\left[\|x_k - x^*\|_2^2\right] + 2\alpha_k^2 B.$$

Note that when k is sufficiently large $1 - 2\alpha_k(1-\gamma) + 8\alpha_k^2 < 1$. Then the rate can be established by some algebraic recursive inequalities.

Questions?