### Robot grocery shopping (in partially observable settings)

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# How can we best learn parameters in a latent variable model?

In statistical estimation theory, the ideal estimator satisfies for	ır
requirements:	

- □ consistency
- statistical efficiency
- computational efficiency
- numerical stability

#### The EM algorithm satisfies:

- consistency X
- □ statistical efficiency 🗸 (assuming global)
- computational efficiency X
- 🗆 numerical stability 🗸

#### Motivation<sup>1</sup>

#### Variational inference satisfies:

- consistency X
- □ statistical efficiency ✓ (assuming global; SVI with averaging)
- □ computational efficiency 🗸 (SVI)
- □ numerical stability **✓** (implicit/proximal SVI)

#### Markov chain Monte carlo satisfies:

- □ consistency ✓
- statistical efficiency 🗸
- computational efficiency X
- □ numerical stability **X**(??)

#### What are spectral methods?

They are matrix (tensor) decompositions which generate sample moments, i.e., observable representations that are functions of the parameters.

- Can solve for them and asymptotically recover the ground truth in expectation, i.e., lead to consistent estimators
- Are consistent estimators for (certain) nonconvex problems!

#### Spectral methods satisfy:

- □ consistency ✓
- statistical efficiency 🗴
- computational efficiency
  - numerical stability 🗴

## Can we leverage the optimization viewpoint to

obtain statistical efficiency and numerical stability?

Given a cost function  $\ell(\theta; Y)$ , can:

- $\Box$  Add regularization / priors  $f(\theta)$
- Add weighted distance (generalized method of moments)
- Use efficient and numerically stable optimization routines (stochastic gradient methods)

#### Background: Generalized method of moments (GMMs)

Let  $Y_1, ..., Y_N$  be (d+1)-dimensional observations generated from some model with unknown parameters  $\theta \in \Theta$ .

The *k* moment conditions for a vector-valued function  $g(Y, \cdot) : \Theta \to \mathbb{R}^k$  is

$$m(\theta^*) \stackrel{\text{def}}{=} \mathbb{E}[g(Y, \theta^*)] = 0_{k \times 1}$$

The observable representations, or sample moments, are

$$\widehat{m}(\theta) \stackrel{\text{def}}{=} \frac{1}{N} \sum_{n=1}^{N} g(Y_n, \theta)$$

#### Background: Generalized method of moments (GMMs)

We aim to minimize the normed distance  $\|\widehat{m}(\theta)\|$  for some choice of  $\|\cdot\|$ . Define the *weighted Frobenius norm* as

$$\|\widehat{m}(\theta)\|_W^2 \stackrel{\text{def}}{=} \widehat{m}(\theta)^T W \widehat{m}(\theta),$$

where *W* is a positive definite matrix. The *generalized method of moments* (GMM) estimator is

$$\theta^{gmm} = \underset{\theta \in \Theta}{\arg \min} \|\widehat{m}(\theta)\|_{W}^{2}$$

#### Background: Generalized method of moments (GMMs)

Under standard assumptions\*, the GMM estimator  $\theta^{gmm}$  is consistent and asymptotically normal. Moreover, if

$$W \stackrel{\text{\tiny def}}{=} \mathbb{E}[g(Y_n, \theta^*)g(Y_n, \theta^*)^T]^{-1}$$

then  $\theta^{gmm}$  is statistically efficient in the class of asymptotically normal estimators (and conditioned only on the information in the moment!).

Time  $t \in \{1, 2, ...\}$ 

- □ Hidden states  $h_t \in \{1, ..., m\}$
- Observations  $x_t \in \{1, ..., n\}$   $(m \le n)$

Given full rank matrices  $T \in \mathbb{R}^{m \times m}$ ,  $O \in \mathbb{R}^{n \times m}$ , the dynamical system for HMMs is given by

$$T_{ij} \stackrel{\text{def}}{=} P[h_{t+1} = i \mid h_t = j] \iff P[h_{t+1}] = TP[h_t]$$

$$O_{ij} \stackrel{\text{def}}{=} P[x_t = i \mid h_t = j] \iff P[x_t] = OP[h_t]$$

and  $\pi \stackrel{\text{\tiny def}}{=} P[h_1] \in \mathbb{R}^m$  the initial state distribution.

Goal: Estimate the joint distribution  $P[x_{1:t}]$ , which also allows one to make predictions:  $P[x_{t+1} \mid x_{1:t}] = [x_{1:t+1}]/P[x_{1:t}]$ .

Notation: 
$$P[x, y, \dots]_{ij} \stackrel{\text{def}}{=} P(x = i, y = j, \dots)$$

Theorem

The joint probability matrix  $P[x_{t+1}, x_t]$  satisfies the following for all columns  $j \in \{1, ..., n\}$ :

$$P[x_{t+1}, x_t]_{.j} = \Phi_j P[x_t] \qquad \Phi_j \stackrel{\text{def}}{=} OT \operatorname{diag}(O_{j.})O^{\dagger}$$

Furthermore,

$$P[x_{t+1}, x_t, x_{1:t-1}]_{,j\vec{k}} = \Phi_j P[x_t, x_{1:t-1}]_{,\vec{k}}$$

where  $\vec{k}$  represents a sequence of states for  $x_{1:t-1}$ , i.e.,  $x_1 = k_1, \dots, x_{t-1} = k_{t-1}$ .

We aim to solve

$$\min_{\Phi_{j}} \|\widehat{P}[x_{t+1}, x_{t}, x_{1:t-1}]_{.j\vec{k}} - \Phi_{j}\widehat{P}[x_{t}, x_{1:t-1}]_{.\vec{k}}\|_{F}$$

such that  $\operatorname{rank}(\Phi_j) \leq m$  for all  $j \in \{1, ..., n\}$ . By the Eckart-Young-Mirsky theorem, this is equivalent to solving

$$\min_{\Phi_j} \| U_j^T \widehat{P}[x_{t+1}, x_t, x_{1:t-1}]_{.j\vec{k}} - \Phi_j U_j^T \widehat{P}[x_t, x_{1:t-1}]_{.\vec{k}} \|_F$$

where  $U_i$  is the matrix of m left-singular vectors of

$$\mathbb{E}[\widehat{P}[\boldsymbol{x}_{t+1}, \boldsymbol{x}_t, \boldsymbol{x}_{1:t-1}]_{.j\vec{k}} \widehat{P}[\boldsymbol{x}_t, \boldsymbol{x}_{1:t-1}]_{.\vec{k}}^T]$$

- ☐ It's convex! (optimization leads to consistent estimator)
- This recovers the same (???) parameters as the method of moments estimation derived in Hsu et al. (2009).

Use weighted Frobenius norm instead for GMM estimation:

$$\min_{\Phi_j} \|\widehat{P}[x_{t+1}, x_t, x_{1:t-1}]_{.j\vec{k}} - \Phi_j \widehat{P}[x_t, x_{1:t-1}]_{.\vec{k}}\|_W^2$$

such that rank( $\Phi_j$ )  $\leq m$ .

And add your favorite regularizers/priors!

$$\min_{\Phi_j} \|\widehat{P}[x_{t+1}, x_t, x_{1:t-1}]_{.j\vec{k}} - \Phi_j \widehat{P}[x_t, x_{1:t-1}]_{.\vec{k}} \|_W^2 + \alpha \|\Phi_j\|_1 + (1 - \alpha) \|\Phi_j\|_F^2$$

such that rank( $\Phi_j$ )  $\leq m$ .

$$\min_{\Phi_{j}} \|\widehat{P}[x_{t+1}, x_{t}, x_{1:t-1}]_{j\vec{k}} - \Phi_{j}\widehat{P}[x_{t}, x_{1:t-1}]_{\vec{k}}\|_{W}^{2} \qquad \operatorname{rank}(\Phi_{j}) \leq m$$

- 1. This extends naturally to predictive state representations (Boots and Gordon, 2010) (??? work in progress).
- 2. Remark on local optima in the optimization
- ☐ In the unweighted case (MoM), any local optima are necessarily global
- In the weighted case (GMM), this no longer holds (Nati and Jaakola, 2003)

$$\min_{\Phi_{j}} \|\widehat{P}[x_{t+1}, x_{t}, x_{1:t-1}]_{.j\vec{k}} - \Phi_{j}\widehat{P}[x_{t}, x_{1:t-1}]_{.\vec{k}}\|_{W}^{2} \qquad \text{rank}(\Phi_{j}) \leq m$$

If the weighting introduces local optima, then what's the point?

#### Conclusion

Reframing moment estimation from spectral methods as optimization leads to an alternative viewpoint on improving estimation:

- □ consistency ✓ (???)
- □ statistical efficiency 🗸 (GMM estimator, using SGD with averaging)
- □ computational efficiency ✓ (SGD)
- □ numerical stability ✔ (implicit/proximal SGD)

