# Deep Jump Q-Evaluation for Personalized Decision Making with Continuous Treatments



 $^1 \rm Department$  of Statistics, North Carolina State University, North Carolina, USA  $^2 \rm Department$  of Statistics, London School of Economics and Political Science, London, UK

#### ENAR 2021 Spring Meeting

Cai, H., Shi, C., Lu, W., Song, R.

Deep Jump Q-Evaluation

Consider a decision making problem to assign individuals with appropriate treatment options in a continuous domain:



An illustration of a simple decision rule that always assigns individuals to a fixed best treatment option:



Due to individuals' heterogeneity in outcome to different treatment options, there may not exist a unified best treatment.



An individualized decision rule (IDR) is to assign individuals with a treatment option according to their baseline covariates.



Prior to adopting any decision rule in practice, it is crucial to know the impact of implementing such a rule.



It is risky to apply an IDR online to estimate its mean outcome. Policy evaluation proposes to use the offline data from a different historical rule.



- Baseline covariates  $X \in \mathcal{X}$  is  $p \times 1$  vector;
- <u>Treatment</u> A belongs to a continuous bounded space, say  $\mathcal{A} = [0, 1]$ ;
- <u>Outcome</u> of interest Y, the larger the better by convention;
- Observed Offline Dataset  $\{(X_i, A_i, Y_i)\}_{1 \le i \le n}$  where n is sample size;
- <u>A decision rule</u>  $\pi(\bullet)$  is a deterministic function that maps  $\mathcal{X}$  to  $\mathcal{A}$ .
- Propensity score / behavior policy  $b(\bullet|x)$  is the probability density function of A given X = x that generates the observed data.
- Q-function the expected outcome function conditional on the feature-treatment pair: Q(x, a) = E(Y|X = x, A = a).
- Under SUTVA, no unmeasured confounders, and the positivity assumptions, for a decision rule  $\pi$  of interest, its value is  $V(\pi) = E[Q\{X, \pi(X)\}].$
- Our goal is to estimate the value  $V(\pi)$  based on the observed data.

- Baseline covariates  $X \in \mathcal{X}$  is  $p \times 1$  vector;
- <u>Treatment</u> A belongs to a continuous bounded space, say  $\mathcal{A} = [0, 1]$ ;
- Outcome of interest Y, the larger the better by convention;
- Observed Offline Dataset  $\{(X_i, A_i, Y_i)\}_{1 \le i \le n}$  where n is sample size;
- <u>A decision rule</u>  $\pi(\bullet)$  is a deterministic function that maps  $\mathcal{X}$  to  $\mathcal{A}$ .
- Propensity score / behavior policy  $b(\bullet|x)$  is the probability density function of A given X = x that generates the observed data.
- Q-function the expected outcome function conditional on the feature-treatment pair: Q(x, a) = E(Y|X = x, A = a).
- Under SUTVA, no unmeasured confounders, and the positivity assumptions, for a decision rule  $\pi$  of interest, its value is  $V(\pi) = E[Q\{X, \pi(X)\}].$
- Our goal is to estimate the value  $V(\pi)$  based on the observed data.

- Baseline covariates  $X \in \mathcal{X}$  is  $p \times 1$  vector;
- <u>Treatment</u> A belongs to a continuous bounded space, say  $\mathcal{A} = [0, 1]$ ;
- Outcome of interest Y, the larger the better by convention;
- Observed Offline Dataset  $\{(X_i, A_i, Y_i)\}_{1 \le i \le n}$  where n is sample size;
- <u>A decision rule</u>  $\pi(\bullet)$  is a deterministic function that maps  $\mathcal{X}$  to  $\mathcal{A}$ .
- Propensity score / behavior policy  $b(\bullet|x)$  is the probability density function of A given X = x that generates the observed data.
- <u>Q-function</u> the expected outcome function conditional on the feature-treatment pair: Q(x, a) = E(Y|X = x, A = a).
- Under SUTVA, no unmeasured confounders, and the positivity assumptions, for a decision rule  $\pi$  of interest, its **value** is  $V(\pi) = E[Q\{X, \pi(X)\}].$

• Our goal is to estimate the value  $V(\pi)$  based on the observed data.

- Baseline covariates  $X \in \mathcal{X}$  is  $p \times 1$  vector;
- <u>Treatment</u> A belongs to a continuous bounded space, say  $\mathcal{A} = [0, 1]$ ;
- <u>Outcome</u> of interest Y, the larger the better by convention;
- Observed Offline Dataset  $\{(X_i, A_i, Y_i)\}_{1 \le i \le n}$  where n is sample size;
- <u>A decision rule</u>  $\pi(\bullet)$  is a deterministic function that maps  $\mathcal{X}$  to  $\mathcal{A}$ .
- Propensity score / behavior policy  $b(\bullet|x)$  is the probability density function of A given X = x that generates the observed data.
- <u>Q-function</u> the expected outcome function conditional on the feature-treatment pair: Q(x, a) = E(Y|X = x, A = a).
- Under SUTVA, no unmeasured confounders, and the positivity assumptions, for a decision rule  $\pi$  of interest, its **value** is  $V(\pi) = E[Q\{X, \pi(X)\}].$
- Our goal is to estimate the value  $V(\pi)$  based on the observed data.

- Most of current works on personalized decision making focus on policy optimization not policy evaluation;
- Less attention has been paid to the continuous treatment setting.
- Available methods rely on the use of a <u>kernel function</u>, and suffer from three limitations.
- Kallus & Zhou (2018), Colangelo & Lee (2020):

$$\frac{1}{n}\sum_{i=1}^{n} \left[ \widehat{Q}\{X_i, \pi(X_i)\} + \frac{K\{\frac{A_i - \pi(X_i)}{h}\}}{\widehat{b}(A_i|X_i)} \{Y_i - \widehat{Q}(X_i, A_i)\} \right].$$

Require the mean outcome to be smooth over the treatment space;

- Sensitive to the choice of the bandwidth parameter;
- Use a single bandwidth parameter, which may be sub-optimal.

- Most of current works on personalized decision making focus on policy optimization not policy evaluation;
- Less attention has been paid to the continuous treatment setting.
- Available methods rely on the use of a <u>kernel function</u>, and suffer from three limitations.
- Kallus & Zhou (2018), Colangelo & Lee (2020):

$$\frac{1}{n}\sum_{i=1}^{n} \left[ \widehat{Q}\{X_i, \pi(X_i)\} + \frac{K\{\frac{A_i - \pi(X_i)}{h}\}}{\widehat{b}(A_i|X_i)} \{Y_i - \widehat{Q}(X_i, A_i)\} \right].$$

- Require the mean outcome to be smooth over the treatment space;
- Sensitive to the choice of the bandwidth parameter;
- Use a single bandwidth parameter, which may be sub-optimal.

- Most of current works on personalized decision making focus on policy optimization not policy evaluation;
- Less attention has been paid to the continuous treatment setting.
- Available methods rely on the use of a <u>kernel function</u>, and suffer from three limitations.
- Kallus & Zhou (2018), Colangelo & Lee (2020):

$$\frac{1}{n}\sum_{i=1}^{n} \left[\widehat{Q}\{X_{i}, \pi(X_{i})\} + \frac{K\{\frac{A_{i}-\pi(X_{i})}{h}\}}{\widehat{b}(A_{i}|X_{i})}\{Y_{i} - \widehat{Q}(X_{i}, A_{i})\}\right].$$

- Require the mean outcome to be smooth over the treatment space;
- Sensitive to the choice of the bandwidth parameter;
- Use a single bandwidth parameter, which may be sub-optimal.

- Most of current works on personalized decision making focus on policy optimization not policy evaluation;
- Less attention has been paid to the continuous treatment setting.
- Available methods rely on the use of a <u>kernel function</u>, and suffer from three limitations.
- Kallus & Zhou (2018), Colangelo & Lee (2020):

$$\frac{1}{n}\sum_{i=1}^{n} \left[ \widehat{Q}\{X_i, \pi(X_i)\} + \frac{K\{\frac{A_i - \pi(X_i)}{h}\}}{\widehat{b}(A_i|X_i)} \{Y_i - \widehat{Q}(X_i, A_i)\} \right].$$

- Require the mean outcome to be smooth over the treatment space;
- Sensitive to the choice of the bandwidth parameter;
- Use a single bandwidth parameter, which may be sub-optimal.

# Toy Example: Adaptive Discretization



Oracle Q-function

Figure 1: Left panel: the oracle Q-function on the feature-treatment space for the toy example. Right panel: the green curve presents the oracle Q-function  $Q\{x, \pi(x)\}$  under decision rule  $\pi(x) = x$  in the toy example; and the red curve is the fitted mean value by the deep jump Q-evaluation and the pink dash line corresponds to the 95% confidence bound.



Figure 2: Left: example of piece-wise constant function. Middle: illustration of a deep neural network. Right: demonstration of policy evaluation.

Model 1: Piecewise function:  $Q(x, a) = \sum_{\mathcal{I} \in \mathcal{D}_0} \{q_{\mathcal{I},0}(x) \mathbb{I}(a \in \mathcal{I})\}$ , for some partition  $\mathcal{D}_0$  of [0, 1] and a collection of functions  $\{q_{\mathcal{I},0}\}_{\mathcal{I} \in \mathcal{D}_0}$ . Model 2: Continuous function: Q is a continuous function of a and x.

- Divide the treatment space  $\mathcal{A}$  into m disjoint initial intervals  $[0,1/m), [1/m,2/m), \ldots, [(m-1)/m,1].$
- Define  $\mathcal{B}(m)$  as the set of <u>candidate discretizations</u>  $\mathcal{D}$  so each interval  $\mathcal{I} \in \mathcal{D}$  corresponds to a union of some of the m initial intervals.
- Each discretization  $\mathcal{D} \in \mathcal{B}(m)$  is associated with a set of functions  $\{q_{\mathcal{I}}\}_{\mathcal{I} \in \mathcal{D}}$ , which **depend on** <u>features</u>, but not on the <u>treatment</u>.
- Model these q<sub>I</sub> in some function class of <u>deep neural networks</u> Q<sub>I</sub>, to capture the complex dependence between the outcome and features.
- Estimate Discretization by:

$$\left( \widehat{\mathcal{D}}, \{ \widehat{q}_{\mathcal{I}} : \mathcal{I} \in \widehat{\mathcal{D}} \} \right) = \operatorname*{arg\,min}_{(\mathcal{D} \in \mathcal{B}(m), \{ q_{\mathcal{I}} \in \mathcal{Q}_{\mathcal{I}} : \mathcal{I} \in \mathcal{D} \})} \\ \left( \sum_{\mathcal{I} \in \mathcal{D}} \left[ \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}(A_i \in \mathcal{I}) \{ Y_i - q_{\mathcal{I}}(X_i) \}^2 \right] + \gamma_n |\mathcal{D}| \right),$$

for some regularization parameter  $\gamma_n$ .

- Divide the treatment space  $\mathcal{A}$  into m disjoint initial intervals  $[0,1/m), [1/m,2/m), \ldots, [(m-1)/m,1].$
- Define  $\mathcal{B}(m)$  as the set of <u>candidate discretizations</u>  $\mathcal{D}$  so each interval  $\mathcal{I} \in \mathcal{D}$  corresponds to a union of some of the m initial intervals.
- Each discretization  $\mathcal{D} \in \mathcal{B}(m)$  is associated with a set of functions  $\{q_{\mathcal{I}}\}_{\mathcal{I} \in \mathcal{D}}$ , which **depend on** <u>features</u>, but not on the <u>treatment</u>.
- Model these q<sub>I</sub> in some function class of deep neural networks Q<sub>I</sub>, to capture the complex dependence between the outcome and features.
- Estimate Discretization by:

$$\left( \widehat{\mathcal{D}}, \{ \widehat{q}_{\mathcal{I}} : \mathcal{I} \in \widehat{\mathcal{D}} \} \right) = \operatorname*{arg\,min}_{(\mathcal{D} \in \mathcal{B}(m), \{ q_{\mathcal{I}} \in \mathcal{Q}_{\mathcal{I}} : \mathcal{I} \in \mathcal{D} \})} \\ \left( \sum_{\mathcal{I} \in \mathcal{D}} \left[ \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}(A_i \in \mathcal{I}) \{ Y_i - q_{\mathcal{I}}(X_i) \}^2 \right] + \gamma_n |\mathcal{D}| \right),$$

for some regularization parameter  $\gamma_n$ .

- Divide the treatment space  $\mathcal{A}$  into m disjoint initial intervals  $[0,1/m), [1/m,2/m), \ldots, [(m-1)/m,1].$
- Define  $\mathcal{B}(m)$  as the set of <u>candidate discretizations</u>  $\mathcal{D}$  so each interval  $\mathcal{I} \in \mathcal{D}$  corresponds to a union of some of the m initial intervals.
- Each discretization  $\mathcal{D} \in \mathcal{B}(m)$  is associated with a set of functions  $\{q_{\mathcal{I}}\}_{\mathcal{I} \in \mathcal{D}}$ , which **depend on** <u>features</u>, but not on the <u>treatment</u>.
- Model these  $q_{\mathcal{I}}$  in some function class of deep neural networks  $Q_{\mathcal{I}}$ , to capture the complex dependence between the outcome and features.
- Estimate Discretization by:

$$\left(\widehat{\mathcal{D}}, \{\widehat{q}_{\mathcal{I}} : \mathcal{I} \in \widehat{\mathcal{D}}\}\right) = \operatorname*{arg\,min}_{(\mathcal{D} \in \mathcal{B}(m), \{q_{\mathcal{I}} \in \mathcal{Q}_{\mathcal{I}} : \mathcal{I} \in \mathcal{D}\})} \left( \sum_{\mathcal{I} \in \mathcal{D}} \left[ \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}(A_{i} \in \mathcal{I}) \{Y_{i} - q_{\mathcal{I}}(X_{i})\}^{2} \right] + \gamma_{n} |\mathcal{D}| \right),$$

for some regularization parameter  $\gamma_n$ .

Deep Jump Q-Evaluation

- Divide the treatment space  $\mathcal{A}$  into m disjoint initial intervals  $[0,1/m), [1/m,2/m), \ldots, [(m-1)/m,1].$
- Define  $\mathcal{B}(m)$  as the set of <u>candidate discretizations</u>  $\mathcal{D}$  so each interval  $\mathcal{I} \in \mathcal{D}$  corresponds to a union of some of the m initial intervals.
- Each discretization  $\mathcal{D} \in \mathcal{B}(m)$  is associated with a set of functions  $\{q_{\mathcal{I}}\}_{\mathcal{I} \in \mathcal{D}}$ , which **depend on** <u>features</u>, but not on the <u>treatment</u>.
- Model these  $q_{\mathcal{I}}$  in some function class of deep neural networks  $Q_{\mathcal{I}}$ , to capture the complex dependence between the outcome and features.
- Estimate Discretization by:

$$\begin{pmatrix} \widehat{\mathcal{D}}, \{\widehat{q}_{\mathcal{I}} : \mathcal{I} \in \widehat{\mathcal{D}}\} \end{pmatrix} = \underset{(\mathcal{D} \in \mathcal{B}(m), \{q_{\mathcal{I}} \in \mathcal{Q}_{\mathcal{I}} : \mathcal{I} \in \mathcal{D}\})}{\operatorname{arg min}} \\ \left( \sum_{\mathcal{I} \in \mathcal{D}} \left[ \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}(A_{i} \in \mathcal{I}) \{Y_{i} - q_{\mathcal{I}}(X_{i})\}^{2} \right] + \gamma_{n} |\mathcal{D}| \right),$$

for some regularization parameter  $\gamma_n$ .

Doubly Robust Estimator under Deep Jump Q-Evaluation Given  $\widehat{D}$  and  $\{\widehat{q}_{\mathcal{I}} : \mathcal{I} \in \widehat{D}\}$ , the value for any decision rule of interest  $\pi$  is

$$\widehat{V}(\pi) = \frac{1}{n} \sum_{\mathcal{I} \in \widehat{\mathcal{D}}} \sum_{i=1}^{n} \left( \mathbb{I}\{\pi(X_i) \in \mathcal{I}\} \left[ \frac{\mathbb{I}(A_i \in \mathcal{I})}{\widehat{b}_{\mathcal{I}}(X_i)} \{Y_i - \widehat{q}_{\mathcal{I}}(X_i)\} + \widehat{q}_{\mathcal{I}}(X_i) \right] \right)$$

where  $\hat{b}_{\mathcal{I}}(x)$  is some estimator of the generalized propensity score function  $\Pr(A \in \mathcal{I} | X = x)$ .

The complete algorithm consists of:

- Data Splitting: use different subsets of data samples to estimate the discretization and to construct the value estimator.
- Deep Discretization: apply pruned exact linear time method (Killick et al., 2012) in multi-scale change point detection.
- Cross-fitting: to remove the bias induced by overfitting.

Cai, H., Shi, C., Lu, W., Song, R.

Deep Jump Q-Evaluation

Doubly Robust Estimator under Deep Jump Q-Evaluation Given  $\widehat{D}$  and  $\{\widehat{q}_{\mathcal{I}} : \mathcal{I} \in \widehat{D}\}$ , the value for any decision rule of interest  $\pi$  is

$$\widehat{V}(\pi) = \frac{1}{n} \sum_{\mathcal{I} \in \widehat{\mathcal{D}}} \sum_{i=1}^{n} \left( \mathbb{I}\{\pi(X_i) \in \mathcal{I}\} \left[ \frac{\mathbb{I}(A_i \in \mathcal{I})}{\widehat{b}_{\mathcal{I}}(X_i)} \{Y_i - \widehat{q}_{\mathcal{I}}(X_i)\} + \widehat{q}_{\mathcal{I}}(X_i) \right] \right)$$

where  $\hat{b}_{\mathcal{I}}(x)$  is some estimator of the generalized propensity score function  $\Pr(A \in \mathcal{I} | X = x)$ .

The complete algorithm consists of:

- Data Splitting: use different subsets of data samples to estimate the discretization and to construct the value estimator.
- Deep Discretization: apply pruned exact linear time method (Killick et al., 2012) in multi-scale change point detection.
- Cross-fitting: to remove the bias induced by overfitting.

Deep Jump Q-Evaluation

Doubly Robust Estimator under Deep Jump Q-Evaluation Given  $\widehat{D}$  and  $\{\widehat{q}_{\mathcal{I}} : \mathcal{I} \in \widehat{D}\}$ , the value for any decision rule of interest  $\pi$  is

$$\widehat{V}(\pi) = \frac{1}{n} \sum_{\mathcal{I} \in \widehat{\mathcal{D}}} \sum_{i=1}^{n} \left( \mathbb{I}\{\pi(X_i) \in \mathcal{I}\} \left[ \frac{\mathbb{I}(A_i \in \mathcal{I})}{\widehat{b}_{\mathcal{I}}(X_i)} \{Y_i - \widehat{q}_{\mathcal{I}}(X_i)\} + \widehat{q}_{\mathcal{I}}(X_i) \right] \right)$$

where  $\hat{b}_{\mathcal{I}}(x)$  is some estimator of the generalized propensity score function  $\Pr(A \in \mathcal{I} | X = x)$ .

The complete algorithm consists of:

- Data Splitting: use different subsets of data samples to estimate the discretization and to construct the value estimator.
- Deep Discretization: apply pruned exact linear time method (Killick et al., 2012) in multi-scale change point detection.
- Cross-fitting: to remove the bias induced by overfitting.

# **Convergence** Rates

Theorem 1 (under Model 1 (Piecewise Function))

Suppose *m* is proportional to *n* and  $\{\gamma_n\}_{n\in\mathbb{N}}$  satisfies  $\gamma_n \to 0$  and  $\gamma_n \gg n^{-\epsilon}$  for some  $\epsilon > -2\beta/(2\beta + p)$  for  $\beta$ -smoothness. Then, there exist some classes of deep neural networks such that for any decision rule  $\pi$ ,

$$\widehat{V}(\pi) = V(\pi) + O_p\{n^{-2\beta/(2\beta+p)}\log^8 n\} + O_p(n^{-1/2}).$$

Theorem 2 (under Model 2 (Continuous Function)) Suppose *m* is proportional to *n* and  $\gamma_n$  is proportional to  $\max\{n^{-3/5}, n^{-2\beta/(2\beta+p)}\log^9 n\}$ . Then for any decision rule  $\pi$ ,  $\widehat{V}(\pi) - V(\pi) = O_p(n^{-1/5}) + O_p\{n^{-2\beta/(6\beta+3p)}\log^3 n\}.$ 

Cai, H., Shi, C., Lu, W., Song, R.

#### • p = 81 baseline covariates X.

- <u>Continuous Treatment A</u>: the dose of Warfarin, converted into [0, 1].
- <u>Outcome of interest Y:</u> is defined as the absolute distance between the international normalized ratio (INR, a measurement of the time it takes for the blood to clot) after the treatment and the ideal value 2.5, i.e, Y = -|INR 2.5|.
- The goal is to evaluate the value function under a decision rule of interest offline, based on the Warfarin dataset.

- p = 81 baseline covariates X.
- <u>Continuous Treatment A</u>: the dose of Warfarin, converted into [0, 1].
- <u>Outcome of interest Y:</u> is defined as the absolute distance between the international normalized ratio (INR, a measurement of the time it takes for the blood to clot) after the treatment and the ideal value 2.5, i.e, Y = -|INR 2.5|.
- The goal is to evaluate the value function under a decision rule of interest offline, based on the Warfarin dataset.

- p = 81 baseline covariates X.
- <u>Continuous Treatment A</u>: the dose of Warfarin, converted into [0,1].
- <u>Outcome of interest Y:</u> is defined as the absolute distance between the international normalized ratio (INR, a measurement of the time it takes for the blood to clot) after the treatment and the ideal value 2.5, i.e, Y = -|INR 2.5|.
- The goal is to evaluate the value function under a decision rule of interest offline, based on the Warfarin dataset.

- p = 81 baseline covariates X.
- <u>Continuous Treatment A</u>: the dose of Warfarin, converted into [0,1].
- <u>Outcome of interest Y:</u> is defined as the absolute distance between the international normalized ratio (INR, a measurement of the time it takes for the blood to clot) after the treatment and the ideal value 2.5, i.e, Y = -|INR 2.5|.
- The goal is to evaluate the value function under a decision rule of interest offline, based on the Warfarin dataset.

#### Implementation and Results

- Decision rule of interest: the optimal decision rule  $\pi^*(X)$ ;
- Benchmarks (kernel-based methods): Kallus & Zhou (2018), Colangelo & Lee (2020).

Table 1: The bias, the standard deviation, and the mean squared error of the estimated values under the optimal decision rule via the proposed deep jump Q-evaluation and two kernel-based methods for the Warfarin data.

Methods	Bias	Standard deviation	Mean squared error
Deep Jump Q-Evaluation	0.259	0.416	0.240
Kallus & Zhou (2018)	0.662	0.742	0.989
Colangelo & Lee (2020)	0.442	1.164	1.550

Our deep jump Q-evaluation method for continuous treatments:

- integrates multi-scale change point detection, deep learning, and the doubly-robust value estimators in discrete domains;
- does not require kernel bandwidth selection, by adaptively discretizing the treatment space using deep discretization;
- has a better convergence rate for any decision rule of interest, allowing the conditional mean outcome to be either a <u>continuous</u> or piecewise function of the treatment.

Our deep jump Q-evaluation method for continuous treatments:

- integrates multi-scale change point detection, deep learning, and the doubly-robust value estimators in discrete domains;
- does not require kernel bandwidth selection, by adaptively discretizing the treatment space using deep discretization;
- has a better convergence rate for any decision rule of interest, allowing the conditional mean outcome to be either a <u>continuous</u> or piecewise function of the treatment.

Our deep jump Q-evaluation method for continuous treatments:

- integrates multi-scale change point detection, deep learning, and the doubly-robust value estimators in discrete domains;
- does not require kernel bandwidth selection, by adaptively discretizing the treatment space using deep discretization;
- has a better convergence rate for any decision rule of interest, allowing the conditional mean outcome to be either a <u>continuous</u> or piecewise function of the treatment.

# Thank You!