

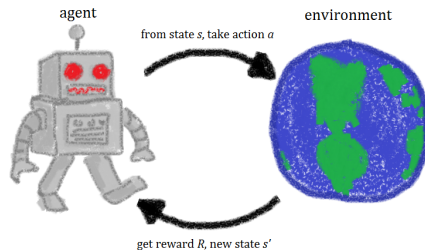
Nonparametric Stochastic Compositional Gradient Descent for Q-Learning in Continuous Markov Decision Problems

Ekaterina Tolstaya^{*}, Alec Koppel[†], Ethan Stump[†], Alejandro Ribeiro^{*}

^{*} University of Pennsylvania

[†] U.S. Army Research Laboratory

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- ▶ At time t , agent is in **state** s_t , select **action** a_t .
- ▶ Transition from **state** s_t to s_{t+1} , with $s_{t+1} \sim \mathbb{P}(\cdot \mid s_t, a_t)$
 - ▶ Reward $r_t := r(s_t, a_t, s_{t+1})$
- ▶ Markov Decision Process (MDP): $(\mathcal{S}, \mathcal{A}, \mathbb{P}, r, \gamma)$
 - ▶ State space \mathcal{S} , action space \mathcal{A} , discount factor $\gamma \in (0, 1)$
- ▶ Goal: find a policy $\pi \in \mathcal{S} \rightarrow \mathcal{A}$, a map from states to actions,
 - ▶ That maximizes the **long-term reward accumulation**

Goal: choose actions to maximize infinite discounted **reward** accumulation

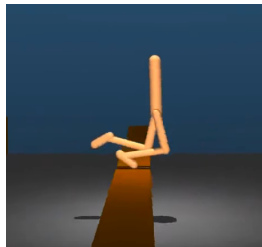
$$\max_{\{a_t\}} \sum_{t=0}^{\infty} \gamma^t r(s_t, a_t, s_{t+1})$$

Recent successes

- ▶ AlphaGo Zero (Silver, 2017)
- ▶ Bipedal walker on terrain (Heess, 2017)
- ▶ Personalized web services (Theocharous, 2015)

Remaining challenges in **infinite** spaces

- ▶ Reproducibility
- ▶ Lack of guarantees for function approx.

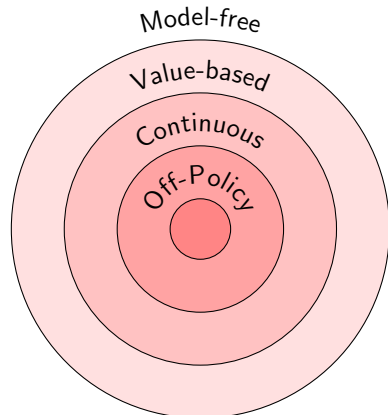


We develop the KQ-Learning algorithm:

- ▶ Formulate a stochastic program for off-policy Bellman loss
- ▶ Compute stochastic gradient
- ▶ Update the kernel model
- ▶ Sparsify the model

Our results provide:

- ▶ Convergence guarantees
- ▶ Experimental validation
- ▶ Low complexity solutions



- ▶ Value function, expected reward accumulation given initial \mathbf{s} :
 - ▶ While following **policy** π

$$V^\pi(\mathbf{s}) := \mathbb{E}_{\mathbf{s}'_t} \left[\sum_{t=0}^{\infty} \gamma^t r(\mathbf{s}_t, \mathbf{a}_t, \mathbf{s}'_t) \mid \mathbf{s}_0 = \mathbf{s}, \mathbf{a}_t = \pi(\mathbf{s}_t) \right] \quad (1)$$

- ▶ Action-value function, the reward accumulation given initial \mathbf{s}, \mathbf{a}

$$Q^\pi(\mathbf{s}, \mathbf{a}) := \mathbb{E}_{\mathbf{s}'_t} \left[\sum_{t=0}^{\infty} \gamma^t r(\mathbf{s}_t, \mathbf{a}_t, \mathbf{s}'_t) \mid \mathbf{s}_0 = \mathbf{s}, \mathbf{a}_0 = \mathbf{a}, \mathbf{a}_t = \pi(\mathbf{s}_t) \right] \quad (2)$$

- ▶ Instead, learn the **optimal** action-value function
 - ▶ Satisfying the Bellman optimality equation

$$Q^*(\mathbf{s}, \mathbf{a}) = \mathbb{E}_{\mathbf{s}'_t} [r(\mathbf{s}, \mathbf{a}, \mathbf{s}'_t) + \gamma \max_{\mathbf{a}'} Q^*(\mathbf{s}'_t, \mathbf{a}') \mid \mathbf{s}_0 = \mathbf{s}, \mathbf{a}_0 = \mathbf{a}] \quad (3)$$

- ▶ Q-learning is an **off-policy** approach
- ▶ Given Q^* , can evaluate the optimal policy:
 $\pi^*(\mathbf{s}) = \arg \max_{\mathbf{a}} Q^*(\mathbf{s}, \mathbf{a})$

- ▶ Tabular Q-Learning (Dayan, 1992)
 - ▶ **Off-policy** observations in discrete state and action spaces
 - ▶ Convergence w.p. 1 when all states, actions observed i.o.
- ▶ Policy **evaluation** (Tsitsiklis, 1997)
 - ▶ Continuous state space with **linear** function approximation
 - ▶ Convergence a.s.
- ▶ Gradient Temporal Difference (Sutton, 2009)
 - ▶ **Off-policy** updates with **linear** function approximation
 - ▶ Convergence w.p. 1
- ▶ Policy **evaluation** (Koppel, 2017)
 - ▶ Continuous state space with **non-parametric kernel methods**
 - ▶ Convergence to the Bellman fixed point w.p. 1

- ▶ Bellman optimality equation (Bertsekas, 2004)

$$Q^*(\mathbf{s}, \mathbf{a}) = \mathbb{E}_{\mathbf{s}'} [r(\mathbf{s}, \mathbf{a}, \mathbf{s}') + \gamma \max_{\mathbf{a}'} Q^*(\mathbf{s}', \mathbf{a}')] \quad (4)$$

- ▶ Temporal difference for an observation $(\mathbf{s}, \mathbf{a}, \mathbf{s}')$:

$$\delta := r(\mathbf{s}, \mathbf{a}, \mathbf{s}') + \gamma \max_{\mathbf{a}'} Q(\mathbf{s}', \mathbf{a}') - Q(\mathbf{s}, \mathbf{a}) \quad (5)$$

- ▶ Define an auxiliary function for the expected temporal difference:

$$f(Q; \mathbf{s}, \mathbf{a}) := \mathbb{E}_{\mathbf{s}'} \delta = \mathbb{E}_{\mathbf{s}'} [r(\mathbf{s}, \mathbf{a}, \mathbf{s}') + \gamma \max_{\mathbf{a}'} Q(\mathbf{s}', \mathbf{a}') - Q(\mathbf{s}, \mathbf{a}) \mid \mathbf{s}, \mathbf{a}]$$

- ▶ Reformulate Bellman optimality equation as comp. stochastic prog:

$$L(Q) = \frac{1}{2} \mathbb{E}_{\mathbf{s}, \mathbf{a}} [f^2(Q; \mathbf{s}, \mathbf{a})]. \quad (6)$$

- ▶ Q^* is a function that satisfies $f(Q; \mathbf{s}, \mathbf{a}) = 0$ for all (\mathbf{s}, \mathbf{a}) .
 - ▶ A solution to the **non-convex** optimization problem

- ▶ We restrict $Q \in \mathcal{H}$, a **Reproducing Kernel Hilbert space**
- ▶ An RKHS over $\mathcal{S} \times \mathcal{A}$ is equipped with a **reproducing kernel** (Norkin, 2009; Argyriou, 2009)
 - ▶ An **inner product-like map**, $\kappa : (\mathcal{S} \times \mathcal{A}) \times (\mathcal{S} \times \mathcal{A}) \rightarrow \mathbb{R}$:

$$(i) \langle Q, \kappa((\mathbf{s}, \mathbf{a}), \cdot) \rangle_{\mathcal{H}} = Q((\mathbf{s}, \mathbf{a})), \quad (ii) \mathcal{H} = \text{span}\{\kappa((\mathbf{s}, \mathbf{a}), \cdot)\} \quad (7)$$

- ▶ A continuous function over a compact set may be approx. uniformly
 - ▶ In an RKHS equipped with a **universal kernel** (Michelli, 2006)
- ▶ We solve the regularized problem:

$$Q^* = \arg \min_{Q \in \mathcal{H}} J(Q) = \arg \min_{Q \in \mathcal{H}} L(Q) + \frac{\lambda}{2} \|Q\|_{\mathcal{H}}^2. \quad (8)$$

- ▶ Goal: optimize $J(Q)$ over \mathcal{H} given samples $(\mathbf{s}_t, \mathbf{a}_t, r_t, \mathbf{s}'_t)$
- ▶ First, differentiate $J(Q)$ w.r.t. Q . (Koppel, 2017)

$$\nabla_Q J(Q_t) = \mathbb{E}_{\mathbf{s}_t, \mathbf{a}_t} \left[f(Q_t; \mathbf{s}_t, \mathbf{a}_t) \times \nabla_Q f(Q_t; \mathbf{s}_t, \mathbf{a}_t) \right] + \lambda Q_t. \quad (9)$$

- ▶ Stoch. grad. unusable since $\nabla_Q J(Q)$ has **two expectations**
- ▶ **Coupled descent**: estimate both terms in product-of-expectations
- ▶ Construct total mean of $\hat{\nabla}_Q f = [\gamma \kappa((\mathbf{s}'_t, \mathbf{a}'_t), \cdot) - \kappa((\mathbf{s}_t, \mathbf{a}_t), \cdot)]?$
 - ▶ Infinite complexity!
- ▶ Instead: build up **expectation** of scalar **temporal difference** δ

- ▶ Goal: extend gradient temporal diff. (Sutton, 2009) to infinite MDPs
- ▶ Define a scalar fixed pt. recursion z_t to estimate average TD $\bar{\delta}$

$$\delta_t = r(\mathbf{s}_t, \mathbf{a}_t, \mathbf{s}') + \gamma \max_{\mathbf{a}'} Q(\mathbf{s}'_t, \mathbf{a}') - Q_t(\mathbf{s}_t, \mathbf{a}_t),$$

$$z_{t+1} = (1 - \beta_t)z_t + \beta_t \delta_t$$

- ▶ $\delta_t \Rightarrow$ temporal difference; $\beta_t \in (0, 1) \Rightarrow$ step-size.
- ▶ $\mathbf{a}'_t = \arg \max_{\mathbf{a}'} Q(\mathbf{s}'_t, \mathbf{a}')$ can be replaced with a softmax
 - ▶ In practice, evaluated via simulated annealing
- ▶ Stoch. descent step: replace 1st term in expectation w/ **estimate**
 - ▶ $[\gamma \kappa((\mathbf{s}'_t, \mathbf{a}'_t), \cdot) - \kappa((\mathbf{s}_t, \mathbf{a}_t), \cdot)]$, evaluated at $(\mathbf{s}_t, \mathbf{a}_t, \mathbf{s}'_t, \mathbf{a}'_t)$
 - ▶ replace δ_t by $z_{t+1} \Rightarrow$ stoch. quasi-gradient (Ermoliev '83)

$$\hat{Q}_{t+1} = (1 - \alpha_t \lambda) \hat{Q}_t - \alpha_t z_{t+1} [\gamma \kappa((\mathbf{s}'_t, \mathbf{a}'_t), \cdot) - \kappa((\mathbf{s}_t, \mathbf{a}_t), \cdot)]$$

- ▶ α_t is a second step-size

- ▶ If $Q_0 = 0 \in \mathcal{H}$, inductively applying Representer Thm. yields

$$Q_t(\mathbf{s}, \mathbf{a}) = \sum_{n=1}^{2(t-1)} w_n \kappa((\mathbf{s}_n, \mathbf{a}_n), (\mathbf{s}, \mathbf{a})) = \mathbf{w}_t^T \kappa_{\mathbf{X}_t}((\mathbf{s}, \mathbf{a})) \quad (10)$$

$$\begin{aligned} \mathbf{w}_t &= [w_1, \dots, w_{2(t-1)}], \\ \mathbf{X}_t &= [(\mathbf{s}_1, \mathbf{a}_1), (\mathbf{s}'_1, \mathbf{a}'_1), \dots, (\mathbf{s}_{t-1}, \mathbf{a}_{t-1}), (\mathbf{s}'_{t-1}, \mathbf{a}'_{t-1})], \end{aligned} \quad (11)$$

- ▶ Kernel expansion + together with FSQG \Rightarrow parametric updates:

$$\begin{aligned} \mathbf{X}_{t+1} &= [\mathbf{X}_t, (\mathbf{s}_t, \mathbf{a}_t), (\mathbf{s}'_t, \mathbf{a}'_t)], \\ \mathbf{w}_{t+1} &= [(1 - \alpha_t \lambda) \mathbf{w}_t, \alpha_t z_{t+1}, -\alpha_t \gamma z_{t+1}] \end{aligned} \quad (12)$$

- ▶ **Intractable complexity** intrinsic to RKHS optimization: $M_t = \mathcal{O}(t)$
- ▶ Solve via **Kernel Orthogonal Matching Pursuit (KOMP)** (Koppel, 2016)

Require: $\{\mathbf{s}_t, \mathbf{a}_t, \mathbf{s}'_t, \alpha_t, \beta_t, \epsilon_t\}_{t=0,1,2,\dots}$
initialize $Q_0(\cdot) = 0, \mathbf{D}_0 = \square, \mathbf{w}_0 = \square, z_0 = 0$
for $t = 0, 1, 2, \dots$ **do**
 Obtain trajectory realization $(\mathbf{s}_t, \mathbf{a}_t, \mathbf{s}'_t)$
 Evaluate instantaneous maximizing action $\mathbf{a}'_t = \arg \max_{\mathbf{a}'} Q(\mathbf{s}'_t, \mathbf{a}')$
 Compute temporal difference
 $\delta_t = r(\mathbf{s}_t, \mathbf{a}_t, \mathbf{s}'_t) + \gamma \max_{\mathbf{a}'} Q_t(\mathbf{s}_t, \mathbf{a}') - Q_t(\mathbf{s}_t, \mathbf{a}_t)$
 Update auxiliary sequence $\mathbf{z}_{t+1} = (1 - \beta_t)\mathbf{z}_t + \beta_t\delta_t$
 Compute functional stochastic quasi-gradient step

$$\hat{Q}_{t+1}(\cdot) = (1 - \alpha_t\lambda)Q_t(\cdot) - \alpha_t\mathbf{z}_{t+1}[\gamma\kappa((\mathbf{s}'_t, \mathbf{a}'_t), \cdot) - \kappa((\mathbf{s}_t, \mathbf{a}_t), \cdot)]$$

 Revise dictionary $\hat{\mathbf{D}}_{t+1} = [\mathbf{D}_t, (\mathbf{s}_t, \mathbf{a}_t), (\mathbf{s}'_t, \mathbf{a}'_t)]$,
 and weights $\hat{\mathbf{w}}_{t+1} = [(1 - \alpha_t\lambda)\mathbf{w}_t, \alpha_t\mathbf{z}_{t+1}, -\alpha_t\gamma\mathbf{z}_{t+1}]$
 Project function $(Q_{t+1}, \mathbf{D}_{t+1}, \mathbf{w}_{t+1}) = \mathbf{KOMP}(\hat{Q}_{t+1}, \hat{\mathbf{D}}_{t+1}, \hat{\mathbf{w}}_{t+1}, \epsilon_t)$
end for

Theorem

Consider the sequence z_t and $\{Q_t\}$ as stated in the KQ-Learning algorithm. Assume the regularizer is positive $\lambda > 0$, Assumptions ??-?? hold, and the step-size conditions hold, with $C > 0$ a positive constant:

$$\sum_{t=1}^{\infty} \alpha_t = \infty, \sum_{t=1}^{\infty} \beta_t = \infty, \sum_{t=1}^{\infty} \alpha_t^2 + \beta_t^2 + \frac{\alpha_t^2}{\beta_t} < \infty, \epsilon_t = C\alpha_t^2 \quad (13)$$

Then $\|\nabla_Q J(Q)\|_{\mathcal{H}}$ **converges to null with probability 1**, and Q_t attains a stationary point of (??).

- ▶ The limit of Q_t achieves a Bellman fixed point in the RKHS.
- ▶ Proof uses existing results for compositional stochastic gradient descent (Wang, 2017)

Theorem

Consider the sequence z_t and $\{Q_t\}$ as stated in the KQ-Learning algorithm. Assume the regularizer is positive $\lambda > 0$, Assumptions ??-?? hold, and the step-sizes are chosen as constant such that $0 < \alpha < \beta < 1$, with $\epsilon = C\alpha^2$ and the parsimony constant $C > 0$ is positive.

Then **Bellman error converges to a neighborhood in expectation**:

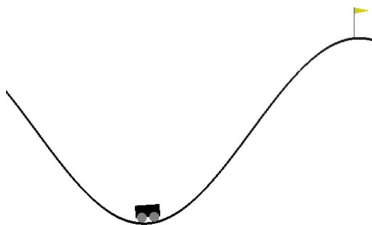
$$\liminf_{t \rightarrow \infty} \mathbb{E}[J(Q_t)] \leq \mathcal{O} \left(\frac{\alpha\beta}{\beta - \alpha} \left[1 + \sqrt{1 + \frac{\beta - \alpha}{\alpha\beta} \left(\frac{1}{\beta} + \frac{\beta^2}{\alpha^2} \right)} \right] \right) \quad (14)$$

	Diminishing	Constant
Learning rate	$\sum_{t=1}^{\infty} \alpha_t^2 + \beta_t^2 + \frac{\alpha_t^2}{\beta_t} < \infty$	$0 < \alpha < \beta < 1$
Compression	$\epsilon_t = \mathcal{O}(\alpha_t^2)$	$\epsilon = \mathcal{O}(\alpha^2)$
Regularization	$0 < \lambda$	$0 < \lambda$
Convergence	$\ \nabla_Q J(Q_t)\ _{\mathcal{H}} \rightarrow 0$ a.s.	$\liminf_t \mathbb{E}[J(Q_t)] = R(\alpha, \beta)$
Model Order	Infinite	Finite

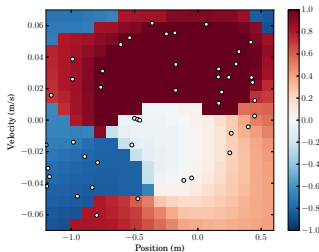
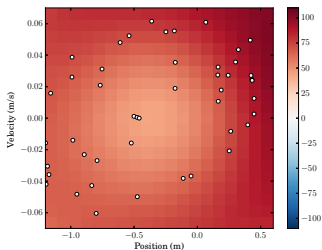
▶ $R(\alpha, \beta) = \mathcal{O} \left(\frac{\alpha\beta}{\beta-\alpha} \left[1 + \sqrt{1 + \frac{\beta-\alpha}{\alpha\beta} \left(\frac{1}{\beta} + \frac{\beta^2}{\alpha^2} \right)} \right] \right)$

- ▶ Exact solution requires infinite memory
- ▶ **Approximate, but accurate solution with finite memory**

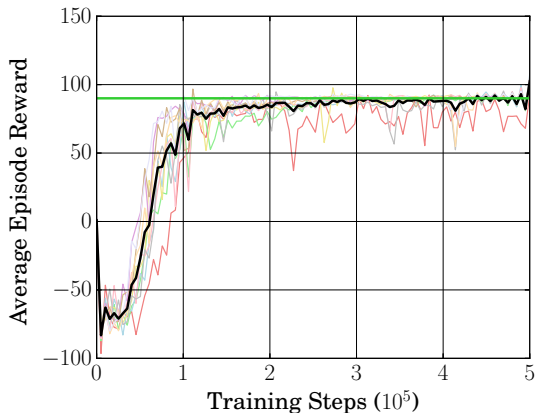
- ▶ Open AI Gym benchmark problem
- ▶ State is 2-dimensional: position and velocity
- ▶ Action is 1-dimensional: force within a continuous interval $[-1, 1]$
- ▶ Reward is 100 at goal position, and $-0.1a^2$ for actions a



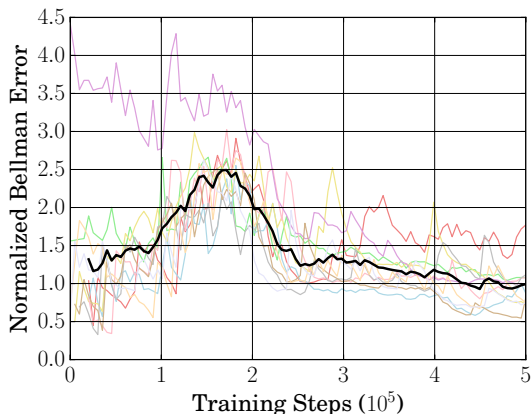
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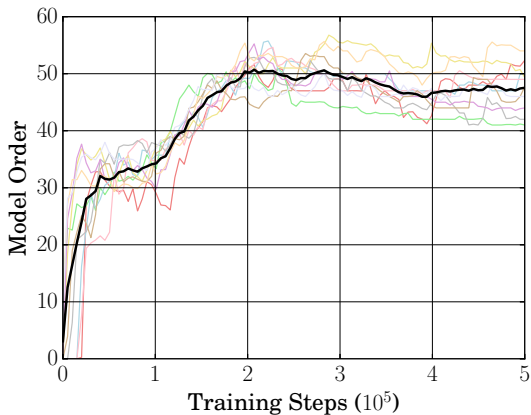
- ▶ Visualization of the learned value function and policy
 - ▶ Grid color - value, policy
 - ▶ White circles - kernel dictionary elements



- ▶ Reward above 90 (green line) is considered solved



- ▶ Corroborated by Q function converging to stationarity
- ▶ Bellman error $J(Q)$ normalized by $\|Q\|_{\mathcal{H}}$








- ▶ This is done with an automatic sparse parameterization of Q
 - ▶ Directly in a continuous space
 - ▶ Model order stabilizes between 45-55



- ▶ Contributions
 - ▶ KQ-learning approach using non-parametric RKHS representations
 - ▶ Convergence guarantees for the KQ-Learning algorithm
- ▶ Demonstration on the Mountain Car benchmark problem
 - ▶ High reproducibility of results
 - ▶ Low complexity of solutions
- ▶ Future work
 - ▶ Applications in higher-dimensional problems
 - ▶ Robotics applications
 - ▶ Policy and actor-critic based approaches

Thank you!

⇒ eig@seas.upenn.edu

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- ▶ The state space $\mathcal{S} \subset \mathbb{R}^p$ and action space $\mathcal{A} \subset \mathbb{R}^q$ are compact.
- ▶ The reproducing kernel map is **bounded**:

$$\sup_{\mathbf{s} \in \mathcal{S}, \mathbf{a} \in \mathcal{A}} \sqrt{\kappa((\mathbf{s}, \mathbf{a}), (\mathbf{s}, \mathbf{a}))} = S < \infty \quad (15)$$

- ▶ The temporal difference δ and z satisfy, for $\bar{\delta} = \mathbb{E}[\delta | \mathbf{s}, \mathbf{a}]$,

$$\mathbb{E}[\delta | \mathbf{s}, \mathbf{a}] = \bar{\delta}, \quad \mathbb{E}[(\delta - \bar{\delta})^2] \leq \sigma_\delta^2, \quad \mathbb{E}[z^2 | \mathbf{s}, \mathbf{a}] \leq G_\delta^2 \quad (16)$$

- ▶ The quasi-gradient is an **unbiased estimate** for $\nabla_Q J(Q)$:

$$\mathbb{E}[(\gamma \kappa((\mathbf{s}'_t, \mathbf{a}'_t), \cdot) - \kappa((\mathbf{s}_t, \mathbf{a}_t), \cdot)) \bar{\delta}] = \nabla_Q J(Q) \quad (17)$$

- ▶ The difference of reproducing kernels has **finite cond. variance**:

$$\mathbb{E}[\|\gamma \kappa((\mathbf{s}'_t, \mathbf{a}'_t), \cdot) - \kappa((\mathbf{s}_t, \mathbf{a}_t), \cdot)\|_{\mathcal{H}}^2 | \mathcal{F}_t] \leq G_Q^2 \quad (18)$$

- ▶ The projected functional gradient has **finite cond. 2nd moments**:

$$\mathbb{E}[\|\tilde{\nabla}_Q J(Q_t z_{t+1}; \mathbf{s}_t, \mathbf{a}_t, \mathbf{s}'_t)\|_{\mathcal{H}}^2 | \mathcal{F}_t] \leq \sigma_Q^2 \quad (19)$$