
Supplementary Materials for Generative Adversarial Networks for Markovian Temporal Dynamics

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1. Mathematical Backgrounds

1.1. Notations

In this paper, a time-dependent system is defined on probability space $(\mathbb{R}^d, \mathcal{F}, \mathbb{P})$ with filtration \mathcal{F}_t . We assume that generated process X_t is \mathcal{F}_t -adapted for all t .

1.2. Assumptions

For rigorous technical results, we assume the following conditions for both generator and discriminator networks.

Assumptions for Generator Network.

- **G-H1:**
$$\|f^\theta(t, x) - f^\theta(t, y)\|^2 \vee \|\sigma(x, \theta) - \sigma(y, \theta)\|^2 \vee \mathbf{Tr}[\sigma(x, \theta)^T \sigma(x, \theta)] \leq K, \quad \forall x, y \in \mathbb{R}^d. \quad (1)$$
- **G-H2:** The infinitesimal generator of the parameterized Fokker-Planck equation induces the curvature-dimension condition: $CD(\kappa, \infty)$ (Villani, 2008; Bakry & Émery).

Assumptions for Discriminator Network.

- **D-H1:** The discriminator network is p -Lipschitz on \mathcal{T} , and q -Lipschitz on \mathbb{R}^d in a global sense:

$$|D(\cdot, t_1) - D(\cdot, t_2)| \leq p |t_1 - t_2|, \quad |D(X_1, \cdot) - D(X_2, \cdot)| \leq q \|X_1 - X_2\| \quad (2)$$

for all $t_1 \neq t_2 \in \mathcal{T}$ and $X_1 \neq X_2 \in \mathbb{R}^d$.

- **D-H2:** The norm of second derivatives for the discriminator network is always bounded for some value \hat{q} : *i.e.*, $\sup_{i,j} \|\partial_i \partial_j D(x, \cdot)\| \leq \hat{q}$.

1.3. Stochastic Differential Equations

In the main paper, we use the integral formulation, but it is generally written as *Itô's diffusion*:

$$dX_t = f^\theta(X_t, t)dt + \sigma(X_t)dW_t, \quad (3)$$

where $X_t \in \mathbb{R}^d$ and $f : \mathbb{R}^d \times \mathbf{U} \rightarrow \mathbb{R}^d$ is a neural network parameterized by θ .

By the Lipschitz continuity (*i.e.*, **G-H1**) of both drift and diffusion functions, the solution to (3), X_t , is always a Markov process (Øksendal, 2003).

2. Proofs

Proposition 1. (*Controlled Stability of Discriminator*) Let $G(X_0, s) = X_s$ be a generated sample obtained by the generator G . For simple analysis, let us consider $\sigma(X) := \sigma$ for some positive scalar $\sigma > 0$.¹ Then, the following probability

¹The result of this proposition can be easily extended to general measurable $\sigma(\cdot)$, if we clarify the explicit condition on σ .

inequality is satisfied:

$$\mathbb{P} \left[\sup_{0 \leq s \leq t} \|D(X_s, s) - D(X_0, 0)\| \geq \epsilon \right] \leq \frac{2}{3\epsilon} \left\{ (p \vee q) \mathbb{E} \|X_t - X_0\| + tC \right\}, \quad (4)$$

where the numerical constant C is linearly dependent on σ . In other words, $C \propto \sigma$.

Proof. It is difficult to directly analyse the time-inhomogeneous Feller process, X_t , without appropriate and complicated assumptions on f^θ . Because using a time-variable is to generate high-dimensional and complex data, we transform the time-inhomogeneous Markov process, X_t , into a desirable form and analyze probabilistic properties of X_t . Let $\tilde{X}_t = (X_t, t)$ be a time-augmented stochastic process suggested in (Bossy & Champagnat, 2010; Böttcher, 2014), it is easily shown that the aforementioned time-augmented Markov semigroup can be defined. Let $\mathcal{F}_t = \sigma(X_s; s \leq t)$ be a canonical filtration of X_t . Let $\mu \in \mathcal{P}(\mathbb{R}^d)$ be a probability measure and define $\mathbb{P} := \mathbb{P}^\mu(X_0 \in A) \otimes \mathcal{T}(t_0 \in T)$ for all $A \in \Sigma(\mathbb{R}^d \times \mathcal{T})$.

Theorem 1. (Böttcher, 2014) *Let $\mathcal{T} = [0, C]$, assume that X_t is a time-inhomogeneous Feller process and has right-continuous infinitesimal generator A_s^+ . Let $f \in C_\infty(\mathbb{R}^d \times \mathcal{T})$, $\pi_1 \circ f \in C^1(\mathcal{T})$, $\pi_2 \circ f \in \mathcal{D}(A_s^+)$. Then, \tilde{X}_t is a time-homogeneous Feller process with generator \tilde{L} defined as follows:*

$$Lf(\tilde{X}) = \partial_s f(s, x) + A_s^+ f(s, x), \quad (5)$$

where $A_s^+ f(s, \cdot) = \frac{\sigma}{2} \sum_i^d \nabla_i^2 f(s, \cdot) + \nabla^T f(s, \cdot)$.

Based on the tools above, we reveal the impact to the probabilistic bound of perturbation according to varying magnitudes of σ in our SDE model. Let us first define the stochastic process $M_t^D : \mathbb{R}^d \times \mathcal{T} \rightarrow \mathbb{R}$ as follows:

$$M_t^D = D(\hat{X}_t) - D(\hat{X}_0) - \int_0^t (\partial_u + A_u^+) D(X_u, u) du. \quad (6)$$

This form is the time-inhomogeneous type of martingale formulation (Bossy & Champagnat, 2010) for itô's formula over discriminator D , i.e., $\mathbb{E}[M_t^D | \mathcal{F}_s] = M_s^D$. In this form, the distortions induced by inhomogeneity are compensated by differential operator ∂_s . As M_t^D is martingale, one can induce the following probability inequality by applying Doob's maximal martingale inequality (Øksendal, 2003) to M_t^D :

$$\mathbb{P} \left[\sup_{0 \leq s \leq t} \|M_s^D\|_2 \geq \epsilon \right] \leq \frac{1}{\epsilon^2} \mathbb{E} [\|M_t^D\|]. \quad (7)$$

From (7), we can obtain the following inequality:

$$\begin{aligned} \epsilon &\leq \sup_{0 \leq s \leq t} \|M_s^D\|_2 \leq \sup_{0 \leq s \leq t} \left[\|D(X_s, s) - D(X_{s=0}, s=0)\|_2 + \left\| \int_0^t -\partial_u D(X_u, u) du \right\|_2 + \left\| \int_0^t -A_u^+ D(X_u, u) du \right\|_2 \right] \\ &\leq \sup_{0 \leq s \leq t} \|D(X_s, s) - D(X_{s=0}, s=0)\|_2 + \sup_{0 \leq s \leq t} \int_0^t \|\partial_u D(X_u, u)\|_2 du + \sup_{0 \leq s \leq t} \int_0^t \|A_u^+ D(X_u, u)\|_2 du. \end{aligned} \quad (8)$$

The second inequality is induced by applying Jensen's inequality to Lebesgue measure du with convex function $\|\cdot\|_2$, and the inequality $\sup_s [A(s) + B(s) + C(s)] \leq \sup_s A(s) + \sup_s B(s) + \sup_s C(s)$.

$$\begin{aligned} \frac{1}{\epsilon^2} \mathbb{E} [\|M_t^D\|] &\geq \mathbb{P} \left[\epsilon \leq \sup_{0 \leq s \leq t} \|M_s^D\|_2 \right] \geq \mathbb{P} \left[\frac{\epsilon}{3} \leq \sup_{0 \leq s \leq t} \|D(X_s, s) - D(X_0, 0)\|_2 \right] \\ &\quad + \mathbb{P} \left[\frac{\epsilon}{3} \leq \sup_{0 \leq s \leq t} B(t) \right] + \mathbb{P} \left[\frac{\epsilon}{3} \leq \sup_{0 \leq s \leq t} C(t) \right]. \end{aligned} \quad (9)$$

By rewriting inequality above using $\mathbb{P}(A^c) = 1 - \mathbb{P}(A)$, $\forall A \in \Sigma$, and rescaling dummy variable $\epsilon \rightarrow 3\epsilon$, we get

$$\mathbb{P} \left[\epsilon \leq \sup_{0 \leq s \leq t} \|D(\tilde{X}_s) - D(\tilde{X}_0)\|_2 \right] \leq \frac{1}{3\epsilon} \mathbb{E} [\|M_t^D\|] + \mathbb{P} \left[\epsilon \geq \sup_{0 \leq s \leq t} B(t) \right] + \mathbb{P} \left[\epsilon \geq \sup_{0 \leq s \leq t} C(t) \right] - 2. \quad (10)$$

Then, we use the assumptions to remove second and third term in (10). While we assume that D is global p -Lipschitz continuous on \mathcal{T} , the following inequality is induced by **D-H1**.

$$\mathbb{P}\left[|D(X, t_1) - D(X, t_2)| \leq p \|(X, t_1) - (X, t_2)\| = p|t_1 - t_2|\right] = 1. \quad (11)$$

Let us assume $\epsilon \leq pt$. As the inequality in (11) is equivalent to $\|\partial_u D\| \leq p$ iff D is p -Lipschitz continuous, the second term in right-hand side of (10) is naturally bounded above with the following inequality because we assume that $\epsilon \leq pt$. Subsequently, we get followings:

$$\begin{aligned} \mathbb{P}\left[\sup_{0 \leq s \leq t} B(t) \leq \epsilon\right] &\leq \mathbb{P}\left[\sup_{0 \leq s \leq t} \int_0^t \|\partial_u D(G(X_0, u), u)\| du \leq \sup_{0 \leq s \leq t} \int_0^t pdu = pt\right] \\ &\leq \mathbb{P}\left[\sup_{0 \leq s \leq t} \int_0^t \|\partial_u D(X_u, u)\| du \leq pt\right] = 1. \end{aligned} \quad (12)$$

As our discriminator is assumed to be q -Lipschitz on data dimension, the following inequality is naturally induced. The probability densities, P and Q induced by both $d\mathbb{P}_t = p_t(x)d\mathcal{L}(x)$, $d\mathbb{Q}_t = q_t(x)d\mathcal{L}(x)$ for Lebesgue measure $\mathcal{L}(x)$ with respect to \mathbb{R}^d , and $U_{P,Q} := \text{supp}(p_t) \cup \text{supp}(q_t) \subset \mathbb{R}^d$. Based on the assumption that $D(\cdot, t)$ is global p -Lipschitz continuous for any $t \in \mathcal{T}$, we can induce the following set inclusion:

$$\{w : D[G(X_0, t)(w), t] \in \text{Lip}_p(U_{P,Q})\} \subset \{w : D(Y(w), t) \in \text{Lip}_p(\mathbb{R}^d), \forall Y \in \mathbb{R}^d\}. \quad (13)$$

Assume that $D(\cdot, t)$ vanishes outside of $\text{supp}(p_t)$. Then, in probability, we can induce

$$\mathbb{P}[D[G(X(w), t), t] \in \text{Lip}_p(\text{supp}(P))] \leq \mathbb{P}[D(X, t) \in \text{Lip}_p(\mathbb{R}^d)] = \mathbb{P}[\|\nabla_i D(X, t)\| \leq q] = 1. \quad (14)$$

$$\|A_s^+ D(X_s, s)\| \leq \frac{\sigma}{2} \underbrace{\left\| \sum_i^d \nabla_i^2 D(X_s, s) \right\|}_{\text{bounded second derivative}} + \underbrace{\left\| \sum_i^d \nabla_i D(X_s, s) \right\|}_{q\text{-Lipschitz on data space}} \leq 2^{-1}\sigma d \sup_{0 \leq i \leq d} \hat{q}_i + q. \quad (15)$$

We denote $\hat{q} = \sup_{0 \leq i \leq d} \hat{q}_i$ for simplicity. The following equality is naturally induced by the assumption **D-H2**.

$$\mathbb{P}[\|A_s^+ D(X_s, s)\| \leq 2^{-1}\sigma d \hat{q} + q] = 1, \forall 0 \leq s \leq t. \quad (16)$$

If $\epsilon \leq 2^{-1}\sigma d \hat{q} + q$, this naturally induces the following probability inequality:

$$\mathbb{P}\left[\sup_{0 \leq s \leq t} C(t) \leq \epsilon\right] \leq \mathbb{P}\left[\sup_{0 \leq s \leq t} \int_0^t \|A_u^+ D(X_u, u)\| du \leq (2^{-1}\sigma d \hat{q} + q)t\right] = 1. \quad (17)$$

Lemma 1. *The discriminator network D is $2(p \vee q)$ -Lipschitz on $\mathbb{R}^d \times \mathcal{T}$.*

Proof. The proof is trivial by the triangle inequality.

$$\begin{aligned} |D(X_1, t_1) - D(X_2, t_2)| &\leq |D(X_1, t_1) - D(X_1, t_2)| + |D(X_1, t_2) - D(X_2, t_2)| \\ &\leq p|t_1 - t_2| + q\|X_1 - X_2\| \\ &\leq 2(p \vee q)[|t_1 - t_2| + \|X_1 - X_2\|] = 2(p \vee q)\|(X_1, t_1) - (X_2, t_2)\|. \end{aligned} \quad (18)$$

□

By integrating inequalities in (17) and (12) into (10), we can obtain the following inequality:

$$\begin{aligned} \mathbb{P}\left[\sup_{0 \leq s \leq t} \|D(X_s, s) - D(X_0, 0)\| \geq \epsilon\right] &\leq \frac{1}{3\epsilon} \mathbb{E}[\|M_t^D\|] \leq \frac{1}{3\epsilon} \left\{ \mathbb{E}\|D(X_t, t) - D(X_0, 0)\| + t[p + q + 2^{-1}\sigma d \hat{q}] \right\} \\ &\leq \frac{2}{3\epsilon} \left\{ (p \vee q) \mathbb{E}\|X_t - X_0\| + t[2(p \vee q) + 4^{-1}\sigma d \hat{q}] \right\}, \end{aligned} \quad (19)$$

where $\epsilon = [p \wedge (2^{-1}\sigma d\hat{q} + q)]t$. The second inequality induced by the fact that D is global $2(p \vee q)$ -Lipschitz continuous by Lemma 1, and the metric on $\mathbb{R}^d \times \mathcal{T}$ can be decomposed into metrics on \mathbb{R}^d and \mathcal{T} .

$$\|\mathbb{E}[D(X_t, t) - D(X_0, 0)]\| \leq \mathbb{E}\|D(X_t, t) - D(X_0, 0)\| \leq 2(p \vee q)\mathbb{E}\|\hat{X}_t - \hat{X}_0\| \leq 2(p \vee q)(\mathbb{E}\|X_t - X_0\| + t). \quad (20)$$

The proof is completed by setting $C(p, q, \sigma, d, \|\nabla^2 D\|) = 2(p \vee q) + 4^{-1}\sigma d\hat{q}$. Please note that this numerical constant is linearly dependent on σ . \square

Proposition 2. (Controlled Stability of Wasserstein distance) *Let us define the spatial-temporal gradient operator as $\tilde{\nabla}_{x,t} = \nabla_x + \partial_t$. Then, the expectation norm of the spatial-temporal gradient for the conditional distance is bounded as follows:*

$$\mathbb{E}\left[\left\|\tilde{\nabla}_{x,t}\mathcal{W}^\varphi(\mathbb{P}_t|x, \mathbb{Q}_t)\right\|\right] \leq C + (p \vee q)(1 + e^{-\kappa t}) \quad (21)$$

for some numerical constants $\kappa, C > 0$.

Proof. The left-hand side of inequality in (21) can be divided into two terms as follows:

$$\mathbb{E}\left[\left\|\tilde{\nabla}_{x,t}\mathcal{W}^\varphi(\mathbb{P}_t|x, \mathbb{Q}_t)\right\|\right] \leq \mathbb{E}\left[\left\|\nabla\mathcal{W}^\varphi(\mathbb{P}_t|x, \mathbb{Q}_t)\right\|\right] + \left\|\partial_t\mathcal{W}^\varphi(\mathbb{P}_t|x, \mathbb{Q}_t)\right\|. \quad (22)$$

First, We investigate the first term of right-hand side in (22):

$$\begin{aligned} \mathbb{E}_x\|\nabla\mathcal{W}^\varphi(\mathbb{P}_t|x, \mathbb{Q}_t)\| &= \int \|\nabla M_t D^\varphi(x, 0) - \nabla\mathbb{E}_{Y_t \sim \mathbb{Q}_t} D^\varphi(Y_t, t)\| d\mathbb{P}_0(x) \leq \int e^{-\kappa t} \mathbb{E}_x M_t (\|\nabla D(x)\|) d\mathbb{P}_0(x) \\ &= e^{-\kappa t} \int \|\nabla D_1\|(x) p(t, y|0, x) p_0(x) d\mathcal{L}(x) = e^{-\kappa t} \int \|\nabla D_1\| d\mathbb{P}_t = e^{-\kappa t} \mathbb{E}\left[\|\nabla D(X_t)\|\right] \\ &\leq e^{-\kappa t} q. \end{aligned} \quad (23)$$

The first inequality is induced by the assumption **G-H2** on curvature-dimension condition $CD(\kappa, \infty)$ of our parameterized Fokker-Planck equation. By the spatial constraints assumption **D-H2**, The last inequality is induced as $\|\nabla D\| \leq q$, $d\mathbb{P}_t(x)$ -almost surely. Subsequently, we investigate the second term of right-hand side in (22):

$$\begin{aligned} \mathbb{E}_x\|\partial_t\mathcal{W}^\varphi(\mathbb{P}_t|x, \mathbb{Q}_t)\| &= \int \|\partial_t M_t D^\varphi(x, 0) - \partial_t \mathbb{E}_{Y_t \sim \mathbb{Q}_t} D^\varphi(Y_t, t)\| d\mathbb{P}_0(x, 0) \\ &= \int \|M_t L D^\varphi(x, 0) - \mathbb{E}[\partial_t D^\varphi(Y_t, t)]\| d\mathbb{P}_0(x) \\ &\leq \int \|M_t L D^\varphi(x, 0)\| d\mathbb{P}_0(x) + \int \mathbb{E}\left[\|\partial_t D^\varphi(Y_t, t)\|\right] d\mathbb{P}_0(x) \\ &\leq \int M_t \left[\|\partial_t D(x, t)\| + \frac{\sigma}{2} d \sup_{0 \leq i \leq d} \hat{q}_i + \|\nabla D(X)\|\right] d\mathbb{P}_0(x) \\ &= p + \frac{\sigma}{2} d \sup_{0 \leq i \leq d} \hat{q}_i + \mathbb{E}\|\nabla D(X_t)\| \leq p + q + 2^{-1}\sigma d\hat{q}. \end{aligned} \quad (24)$$

The first inequality is induced by the dual identity of Fokker-Planck equation: $\partial_t M_t f = M_t L f$ for Markovian generator L , and we use the fact that $\partial_t \mathbb{E} f(x, t) = \mathbb{E} \partial_t f(x, t)$ for bounded and second differentiable $f(x, t)$. The second inequality is induced by dividing L defined in Theorem 1 into two terms. The third equality holds as $\mathbb{E}_{x_0} M_t \|\nabla D(X_0)\| = \mathbb{E}\|\nabla D(X_t)\|$, which is bounded above q almost surely. Combining these results, it is easy to see that the following inequality is satisfied: $2^{-1}\sigma d\hat{q} + p + (1 + e^{-\kappa t})q \leq 2^{-1}\sigma d\hat{q} + (p \vee q)(1 + e^{-\kappa t})$ where $C = 2^{-1}\sigma d\hat{q}$. By the fact that $\int e^{-\kappa t} dt \leq \frac{1 - e^{-\kappa T}}{\kappa}$, the proof is completed. \square

Proposition 3. *Let V^λ be the function defined above, and x, \hat{x} be two initial states such that $\hat{\mathbb{P}}_t = h_{\#}[\mathbb{P}_t]$. If the generator solves the regularization term in (25), such that*

$$\min_{\theta} \mathbb{E}_{X_t \sim \mathbb{P}_t, Z_t \sim \hat{\mathbb{P}}_t} V^\lambda(\theta, X_t, Z_t) = 0, \quad (25)$$

the following inequality holds:

$$\mathcal{W}_2(\mathbb{P}_t, \hat{\mathbb{P}}_t) \leq \sqrt{A + e^{-2\lambda t} \|h\|_{\mathbf{L}_2(\mathbb{P})}}, \quad (26)$$

where $\|\cdot\|_{\mathbf{L}_2(\mathbb{P})}$ denotes L_2 -norm over probability measure \mathbb{P} , for some $A > 0$.

Proof. Assume that the function V^λ vanishes for some for some fixed x, y and parameter θ^* . That is, $V^\lambda(\theta^*, x, y) := 0$. In this case, (25) indicates the following inequality:

$$(x - y)^T \left[\nabla f_{\alpha x + (1-\alpha)y}^{\theta^*} \right] (x - y) \leq -\lambda(x - y)^T I(x - y), \quad (27)$$

where we simply denote $\nabla f^{\theta^*} = \nabla_x f(\theta^*, x, t)$ for the fixed t . The drift function satisfying the inequality above is called *contraction function*. By the Theorem 2 (Pham et al., 2009), this property gives powerful stochastic contraction for processes X_t^x, X_t^y starting at different initial states $x \sim \mu, y \sim \nu$. In particular, any diffusion Markov process of which drift functions satisfy inequality in (27) can induce the following property:

$$\mathbb{E} \|X_t^x - X_t^y\|^2 \leq \frac{K}{\lambda} + e^{-2\lambda t} \int_{\mathcal{A}} \|x - y\|^2 d(\mu \otimes \nu), \quad (28)$$

where $\mathcal{A} = \text{supp}(\mu_0) \cup \text{supp}(\nu_0) \subset \mathbb{R}^d$. Let us consider $\hat{x} = x + h(x)$ for some measurable h . As the optimal transport between $\mathbb{P}_t^x, \mathbb{P}_t^y$ always exists, which is denoted as $\pi_t^{x,y}$, inducing the followings are straightforward.

We consider the system of SDEs consist of trained drift, diffusion functions $f(\theta^*)$, and $\sigma(\theta^*)$ with different initial states.

$$\begin{cases} dX_t = f(\theta^*, X_t, t) + \sigma(X_t) dW_t^1 \\ d\hat{X}_t = f(\theta^*, \hat{X}_t, t) + \sigma(\hat{X}_t) dW_t^2 \end{cases} \quad (29)$$

with i.i.d Wiener processes W_t^1, W_t^2 . In this case, it is easy to see that $Z_t = (X_t, \hat{X}_t)$ is also a Markov process on $\mathbb{R}^d \times \mathbb{R}^d$. We define $\iota(Z_t) = d^2(X_t, \hat{X}_t)$ for the Euclidean metric d on \mathbb{R}^d and define Π as an optimal transport between initial state measures μ and ν . Expectation of Markov semi-group $M_t \iota$ over π yields followings:

$$\begin{aligned} \int_{\mathcal{A}^2} M_t \iota(z) d\Pi &= \int_{\mathcal{A}^2} \mathbb{E}[\iota(Z_t) | z = (x, y)] d\Pi(x, y) = \int_{\mathcal{A}^2} \mathbb{E} \left[d^2(X_t, \hat{X}_t)^2 \middle| (X_0, \hat{X}_0) = (x, y) \right] d\Pi(x, y) \\ &\leq \frac{K}{\lambda} + e^{-2\lambda t} \int_{\mathcal{A}^2} \int_{\mathcal{A}} \iota(Z_0) d(\mu \otimes \nu) d\Pi(x, y) = \frac{K}{\lambda} + e^{-2\lambda t} \mathcal{W}_2^2(\mu, \nu) = \frac{K}{\lambda} + e^{-2\lambda t} \|h\|_{\mathbf{L}_2(\mu)}^2. \end{aligned} \quad (30)$$

$\Gamma_t = \mathbb{E}_{z \sim \Pi} p(t, z, \cdot)$ denotes a push forward of Π through transition kernel. Then, for the any Z_t ,

$$\mathcal{W}_2^2(\mathbb{P}_t^{x \sim \mu}, \mathbb{P}_t^{\hat{x} \sim \nu}) = \inf_{\Pi_t} \int \iota(Z_t) d\Pi_t(Z_t) \leq \int \iota d\Gamma_t. \quad (31)$$

By combining two inequalities above and the fact that $\mathbb{E}_{\Pi}[M_t \iota] = \mathbb{E}_{\Gamma_t}[\iota]$, we can conclude that $\mathcal{W}_2(\mathbb{P}_t^x, \mathbb{P}_t^{\hat{x}}) \leq \sqrt{\frac{K}{\lambda} + e^{-2\lambda t} \|h\|_{\mathbf{L}_2(\mu)}^2}$, where $A = K\lambda^{-1}$. □

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