

Towards Qualitative System Identification Through Optimization

SIOPT23 | MS330 Data-Driven Optimization: Algorithms and Theoretical Guarantees

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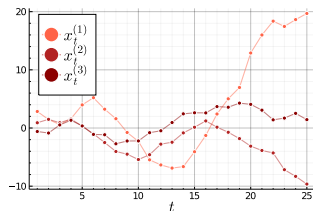
Stability under noisy measurements

Consider a discrete-time system on \mathbb{R}^n

$$x_{t+1} = \theta x_t + w_t, \quad w_t \stackrel{i.i.d.}{\sim} \text{distr}(0, S_w \succ 0) \quad (1)$$

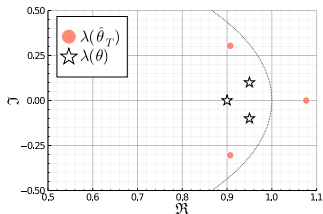
with **unknown** $\theta \in \mathbb{R}^{n \times n}$, being **asymptotically stable** ($\rho(\theta) < 1$). Given measurements $(\hat{x}_t)_{t \geq 0}$ of (1), consider the LS estimator of θ :

$$\hat{\theta}_T = \left(\sum_{t=1}^T \hat{x}_t \hat{x}_{t-1}^T \right) \left(\sum_{t=1}^T \hat{x}_{t-1} \hat{x}_{t-1}^T \right)^{-1} \quad (T \geq n). \quad (2)$$



Collect single trajectory $\subset \mathbb{R}^3$

least squares
estimation of θ ,
denoted $(\hat{\theta}_T)$
 \rightsquigarrow



Estimate $\hat{\theta}_T$ is unstable?

But we understand the process $(\hat{\theta}_t)_{t \geq 0}$ very well?

Outstanding work¹ on LS **statistical** identification of

$$x_{t+1} = \theta x_t + w_t \quad (3)$$

that is, bounds like $\mathbb{P}(\|\hat{\theta}_t - \theta\|_p \leq \delta) \geq 1 - \beta$ for $t \geq T$.

At a lower level we first like to understand **qualitative behaviour**, that is, $\mathbb{P}(\hat{\theta}_T$ qualitatively the same as θ)?

Observation: ℓ_p -norms not appropriate for stability.

$$\text{Let } \theta = \begin{pmatrix} \lambda & C \\ 0 & \lambda \end{pmatrix} \text{ for } \lambda \in (-1, 1), C \gg 1 \text{ and } \hat{\theta}_T = \begin{pmatrix} \lambda & C \\ \epsilon_T & \lambda \end{pmatrix} \text{ for } \epsilon_T > 0.$$

Then, $\|\theta - \hat{\theta}_T\|_2 = \epsilon_T$ yet $\lambda(\hat{\theta}_T) = \{\lambda \pm \sqrt{C\epsilon_T}\}$ [$\rho(\cdot)$ not a norm].

¹Substantial body of work on (sub-)optimal finite-sample concentration bounds for linear systems identified via least squares estimation [Sim+18; JP19; SR19; JP20; SRD21].

Perhaps we can truncate the Jordan normal form?

Naïve method to (asymptotically) stabilize $\theta' \notin \Theta := \{\theta \in \mathbb{R}^{n \times n} : \rho(\theta) < 1\}$:
scale its unstable eigenvalues into $\mathbb{C}_{|z| < 1}$. Consider the matrices

$$\theta' = \begin{bmatrix} 1.01 & 10 \\ 0.01 & 1 \end{bmatrix}, \theta'_a = \begin{bmatrix} 0.84 & 4.77 \\ 0.005 & 0.84 \end{bmatrix}, \theta'_b = \begin{bmatrix} 0.99 & 10 \\ 0 & 0.99 \end{bmatrix}.$$

Clipping off the unstable eigenvalues of θ' at $|\lambda| = 0.99$ yields
 θ'_a with $\rho(\theta'_a) = 0.99$ and $\|\theta' - \theta'_a\|_2 = 5.24$.

However, θ'_b also has $\rho(\theta'_b) = 0.99$ but with $\|\theta' - \theta'_b\|_2 = 0.02!$

Problem is non-trivial, lots of related work

Towards a solution: early work by Maciejowski [Mac95], used in Sys. Id. [VD96] (*distorted*).

Lacy and Bernstein [LB02] **approximate** Θ by $\{\theta \in \mathbb{R}^{n \times n} : \|\theta\|_2 < 1\}$ (*convex, but conservative*), related: [LB03; BGS08; Tur+13] (*conservative/expensive*), regularization [Van+00; Van+01] (*tuning*), MLE approach [Ume+18] (*expensive*), more..

Related to the ***nearest stable matrix problem***

$$\Pi_{\Theta}(\theta') \in \arg \min_{\theta \in \text{cl } \Theta} \|\theta' - \theta\|^2, \quad (4)$$

Solutions: *successive convex approximations* [ONV13], *low-rank matrix differential equations* [GL17], *elegant reparametrization* of $\tilde{\Theta}$ [GKS19; CGS20], Nesterov and Protasov [NP20] solve (4) for *polyhedral norms* and *non-negative* θ' .

Projection problem (4) is mathematically beautiful but perhaps practically not ideal: Given that $\theta \in \Theta$ yet $\hat{\theta}_T \notin \Theta$, do we want to project to *the boundary* $\partial\Theta$ [VD96, pp. 53–60, 125–129]?

Differently: one could try to design a *LQR problem* whose optimal feedback gain $K^* \in \mathbb{R}^{n \times n}$ renders $\hat{\theta}_T + K^*$ stable.

Overlooked but early work: Tanaka and Katayama [TK05] propose a LQR objective that is *inversely proportional* to S_w (clear relation to $\partial\Theta$), yet, without all the analysis.

Additional benefit of LQR: well-understood [BLW91; LR95], fast and scalable ($n \approx 1000$), *structure preserving* [JK21], e.g., $\ker(\hat{\theta}_T) = \ker(\hat{\theta}_T + K^*)$.

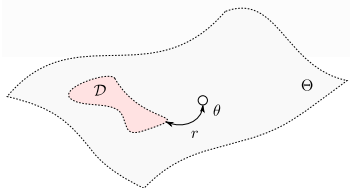
Step 1: understand $(\hat{\theta}_t)_{t \geq 0}$ beyond $\mathbb{P}(\|\theta - \hat{\theta}_t\|_p \geq \delta) (1/2)$

Moderate scale: $(a_T)_T$ such that $\lim_{T \rightarrow \infty} a_T = \infty$ yet $\lim_{T \rightarrow \infty} \frac{a_T}{T} = 0$.

Definition (Moderate Deviation Principle (MDP) [DZ09])

A sequence $(\hat{\theta}_T)_T$ satisfies a MDP if there is a rate (“distance”) function $I(\theta', \theta)$ such that for any Borel set $\mathcal{D} \subseteq \mathbb{R}^{n \times n}$:

$$\begin{aligned} \underbrace{- \inf_{\theta' \in \text{int} \mathcal{D}} I(\theta', \theta)}_{\bar{I}} &\leq \liminf_{T \rightarrow \infty} \frac{1}{a_T} \log \mathbb{P}_\theta (\hat{\theta}_T \in \mathcal{D}) \\ &\leq \limsup_{T \rightarrow \infty} \frac{1}{a_T} \log \mathbb{P}_\theta (\hat{\theta}_T \in \mathcal{D}) \leq - \underbrace{\inf_{\theta' \in \text{cl} \mathcal{D}} I(\theta', \theta)}_{\bar{I}}. \end{aligned}$$



$$\mathbb{P}_\theta (\hat{\theta}_T \in \mathcal{D}) \leq e^{-\bar{I} \cdot a_T + o(a_T)}$$

Finding $I(\cdot, \cdot)$ can be painful..

Step 1: understand $(\hat{\theta}_t)_{t \geq 0}$ beyond $\mathbb{P}(\|\theta - \hat{\theta}_t\|_p \geq \delta)$ (2/2)

*Skipping technical assumptions, e.g., $w \sim \text{subG}$.

Lemma (Least squares MDP [JSK23])

If $(\hat{\theta}_T)_{T \geq 0}$ is a sequence of **least squares** estimators, then $(\frac{T}{\alpha_T}(\hat{\theta}_T - \theta) + \theta)_T$ satisfies a **MDP** with **rate function**

$$I(\theta', \theta) = \frac{1}{2} \text{tr} \left(S_w^{-1} (\theta' - \theta) S_\theta (\theta' - \theta)^\top \right).$$

for² $S_\theta = \theta S_\theta \theta^\top + S_w = \sum_{k=0}^{\infty} \theta^k S_w (\theta^k)^\top$.

proof: Make the results from [YS09] explicit.

Complication: $I(\theta', \theta)$ non-convex in $\theta \in \Theta$.

²System: $x_{t+1} = \theta x_t + w_t$, State covariance: $S_\theta = \lim_{t \rightarrow \infty} \mathbb{E}_\theta [x_t x_t^\top]$, noise covariance: $S_w = \mathbb{E}[w_t w_t^\top]$.

Step 2: enforcing stability of $\hat{\theta}_T$ (1/2)

Motivated by the MDP-related optimality results³, we construct [JSK23] a *reverse I-projection* defined through

$$\mathcal{P}(\theta') \in \arg \min_{\theta \in \Theta} I(\theta', \theta) \text{ for } I(\theta', \theta) = \frac{1}{2} \text{tr} \left(S_w^{-1} (\theta' - \theta) S_\theta (\theta' - \theta)^\top \right). \quad (5)$$

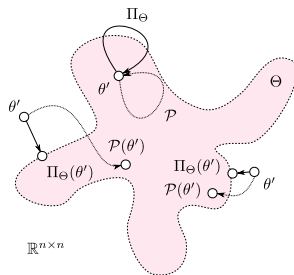


Figure 1: Schematic visualization of $\Pi_\Theta(\theta') \in \arg \min_{\theta \in \text{cl}\Theta} \|\theta' - \theta\|^2$ and $\mathcal{P}(\theta')$ for different estimator realizations θ' inside and outside of Θ .

³VMK21; SVK20; BV21.

Step 2: enforcing stability of $\hat{\theta}_T$ (2/2)

Observations regarding $\mathcal{P}(\theta') \in \arg \min_{\theta \in \Theta} l(\theta', \theta)$:

- (i) $l(\theta', \theta)$ trades off *distance* (weighted $\|\cdot\|_F$) against *stability* (S_θ);
- (ii) By exploiting that $l(\hat{\theta}_T, \theta) = (a_T/T)l(\sqrt{T/a_T}(\hat{\theta}_T - \theta) + \theta, \theta)$, one can show that the PDF $\varrho_{\theta, T}$ of $\hat{\theta}_T$ satisfies

$$\varrho_{\theta, T}(\hat{\theta}_T) \approx \exp(-l(\hat{\theta}_T, \theta) \cdot T). \quad (6)$$

Thus, $\mathcal{P}(\hat{\theta}_T)$ maximizes the RHS of (6) across all $\theta \in \Theta$ (**MLE-like**).

In addition, by using ideas due to Jedra and Proutiere [JP20], one can show that for Gaussian noise, $l(\theta', \theta)$ can be interpreted as the long-run average expected log-likelihood ratio between observations generated under \mathbb{P}_θ and $\mathbb{P}_{\theta'}$.

On an intuitive level, we can motivate

$$\mathcal{P}(\theta') \in \arg \min_{\theta \in \Theta} l(\theta', \theta) \text{ for } l(\theta', \theta) = \frac{1}{2} \text{tr} \left(S_w^{-1} (\theta' - \theta) S_\theta (\theta' - \theta)^\top \right).$$

but can we formalize this?

Better yet, can we work with this operator?

Theorem (Efficient identification with stability guarantees [JSK23])

For any $\theta \in \Theta$, the reverse l -projection has the following properties.

- (i) **Asymptotic consistency.** $\lim_{T \rightarrow \infty} \mathcal{P}(\hat{\theta}_T) = \theta$ \mathbb{P}_θ -a.s.
- (ii) **Finite sample guarantee.** There are constants $\tau \geq 0$ and $\rho \in (0, 1)$ that depend only on θ such that

$$\mathbb{P}_\theta \left(\|\theta - \mathcal{P}(\hat{\theta}_T)\|_2 \leq \kappa(S_w) 2\epsilon n^{\frac{1}{2}} \tau (1 - \rho^2)^{-\frac{1}{2}} \right) \geq 1 - \beta$$

for all $\beta, \epsilon \in (0, 1)$ and $T \geq \kappa(S_w) \tilde{O}(n) \log(1/\beta) / \epsilon^2$.

- (iii) **Efficient computation.** For any $\theta' \notin \Theta$ and $S_w, Q \succ 0$ there is a $p \geq 1$, such that for all $\delta > 0$ we have that

$$\theta_\delta^* = \theta' + \text{dlqr}(\theta', I_n, Q, (2\delta S_w)^{-1}) \in \Theta \text{ with } \|\mathcal{P}(\theta') - \theta_\delta^*\|_2 \leq O(\delta^p).$$

Main result: comment on (i)

Not particularly surprising since $\mathcal{P}(\theta') = \theta'$ for all $\theta' \in \Theta$.

Formally, this follows readily from continuity, convexity and $\lim_{T \rightarrow \infty} \hat{\theta}_T = \theta$ \mathbb{P}_θ -almost surely [CK98].

In fact, we can prove:

Lemma (Properties of $I(\theta', \theta)$ [JSK23])

The rate function $I(\theta', \theta)$ has the following properties.

- (i) $I(\theta', \theta)$ is analytic in $(\theta', \theta) \in \Theta' \times \Theta$.
- (ii) If $\theta' \in \Theta$, then the sublevel set $\{\theta \in \Theta : I(\theta', \theta) \leq r\}$ is compact for every $r \geq 0$.
- (iii) If $\theta' \in \Theta$, then $I(\theta', \theta)$ tends to infinity as θ approaches the boundary of Θ .

Main result: comment on (ii)

To quantify “where” in Θ the matrix θ lives: we say that the system matrix $\theta \in \Theta$ is (τ, ρ) -stable [KTR19, Def. 1] for some $\tau \geq 1$ and $\rho \in (0, 1)$ if $\|\theta^k\|_2 \leq \tau\rho^k$ for all $k \in \mathbb{N}$.

As θ is (τ, ρ) -stable:

$$\begin{aligned} I(\widehat{\theta}_T, \mathcal{P}(\widehat{\theta}_T)) &\leq I(\widehat{\theta}_T, \theta) = \frac{1}{2} \text{tr} \left(S_w^{-1} (\widehat{\theta}_T - \theta) S_\theta (\widehat{\theta}_T - \theta)^\top \right) \\ &\leq \frac{1}{2} \text{tr}(S_w^{-1}) \|\widehat{\theta}_T - \theta\|_2^2 \|S_\theta\|_2 \\ &\leq \frac{1}{2} n \kappa(S_w) \|\widehat{\theta}_T - \theta\|_2^2 \frac{\tau^2}{1 - \rho^2}, \end{aligned}$$

Combine with a Pinsker-type inequality [JSK23]: for any $\theta' \in \Theta'$ and $\theta \in \Theta$ we have $\|\theta' - \theta\|_2^2 \leq 2\kappa(S_w) I(\theta', \theta)$.

Interestingly, we can get a (similar) probabilistic grip on $\|\widehat{\theta}_T - \theta\|_2$ using the MDP or contemporary identification results [SR19].

Main result: comment on (iii) (1/2)

$\mathcal{P}(\theta') \in \arg \min_{\theta \in \Theta} l(\theta', \theta)$ is *non-convex*, how does that work?

Consider $\min_{\theta \in \Theta} \{\text{tr}(QS_\theta) : l(\theta', \theta) \leq r\}$ for the *smallest* radius $r = \underline{r}$ that preserves feasibility.

Taking a Lagrangian (penalty) viewpoint, equivalent to

$$\begin{aligned} & \min_{\theta \in \Theta} \text{tr}(QS_\theta) + \delta^{-1} l(\theta', \theta) \\ &= \min_{\theta \in \Theta} \lim_{T \rightarrow \infty} T^{-1} \mathbb{E}_\theta \left[\sum_{k=0}^{T-1} x_k^T Q x_k + \frac{1}{2\delta} x_k^T (\theta' - \theta)^T S_w^{-1} (\theta' - \theta) x_k \right] \\ &= \min_{L \in \mathbb{R}^{n \times n}} \lim_{T \rightarrow \infty} T^{-1} \mathbb{E}_{\theta' + L} \left[\sum_{k=0}^{T-1} x_k^T \left(Q + \frac{1}{2\delta} L^T S_w^{-1} L \right) x_k \right], \end{aligned}$$

Here, $\theta = \theta' + L$, with L the *feedback* term.

For $\delta \downarrow 0$, we approach the original problem solution⁴.

⁴If θ' has unimodular eigenvalues, then, approximation is the best we can do.

Main result: comment on (iii) (2/2)

Let $P_\delta \succ 0$ be a fixed point of $P_\delta = Q + \theta'^T P_\delta \theta' - \theta'^T P_\delta (P_\delta + (2\delta S_w)^{-1})^{-1} P_\delta \theta'$, then

$$\begin{aligned}\theta_\delta^* &= \theta' + \text{dlqr}(\theta', I_n, Q, (2\delta S_w)^{-1}) \\ &= \Lambda_\delta^{-1} \theta' \text{ for } \Lambda_\delta = (I_n + 2\delta S_w P_\delta) \text{ (topological ramifications).}\end{aligned}$$

Observe that $\theta_\delta^* \in \Theta$ for any δ !

By using [Pol86, Lem. 3.2], one can show that P_δ and consequently also θ_δ^* are real-analytic (C^ω) in $\delta > 0$.

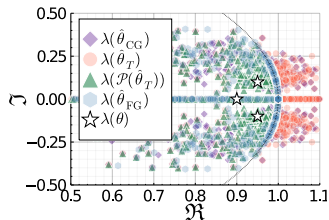


Figure 2: Comparison to CG [BGS08] and FG [GKS19] methods.

We compute

$$\mathcal{P}(\theta') \in \arg \min_{\theta \in \Theta} l(\theta', \theta) \text{ for } l(\theta', \theta) = \frac{1}{2} \text{tr} \left(S_w^{-1} (\theta' - \theta) S_\theta (\theta' - \theta)^\top \right).$$

(approximately) through

$$\theta_\delta^* = \theta' + \text{dlqr}(\theta', I_n, Q, (2\delta S_w)^{-1}) \text{ for "small" } \delta,$$

$\text{dlqr}(\cdot)$ standard routine in MATLAB, Julia, Python and so forth,
but how to pick $Q \succ 0$ and does $\delta \downarrow 0$ not look problematic?

The *algebraic Riccati equation* (ARE)

$$P_\delta = Q + \theta'^T P_\delta (I_n + 2\delta S_w P_\delta)^{-1} \theta' \quad (7)$$

is well-understood [BLW91; LR95]. Fixed-point (DP) schemes can be unstable, elegant solution proposed in the 80s.

To start, define the pair of matrices $S_1, S_2 \in \mathbb{R}^{2n \times 2n}$ by

$$S = \{S_1, S_2\} = \left\{ \begin{pmatrix} \theta' & 0_{n \times n} \\ -Q & I_n \end{pmatrix}, \begin{pmatrix} I_n & 2\delta S_w \\ 0_{n \times n} & \theta'^T \end{pmatrix} \right\}. \quad (8)$$

Now, consider the *generalized eigenvalue* problem

$$S_1 x = \lambda S_2 x, \quad x \in \mathbb{C}^{2n} \quad \lambda \in \mathbb{C}. \quad (9)$$

Unroll $S_1X = S_2XJ$ as

$$\begin{pmatrix} \theta' & 0_{n \times n} \\ -Q & I_n \end{pmatrix} \begin{pmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{pmatrix} = \begin{pmatrix} I_n & 2\delta S_w \\ 0_{n \times n} & \theta'^T \end{pmatrix} \begin{pmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{pmatrix} \begin{pmatrix} J^s & 0_{n \times n} \\ 0_{n \times n} & J^u \end{pmatrix}$$

Eigenvalues come in reciprocal pairs, so without unimodular λ we have a *stable* and *unstable* subspace.

Lemma (Structure of ARE solutions [PLS80, Lem. 1])

Let P_δ be a solution to (7) and let $X^s = [X_{11}^H \ X_{21}^H]^H \in \mathbb{C}^{2n \times n}$ denote a basis for the stable eigenspace. Then, $P_\delta = X_{21}X_{11}^{-1}$ and $\theta_\delta^* = X_{11}J^sX_{11}^{-1} \in \Theta$.

Follows by direct computation (inspired by the maximum principle).

Symplectic perspective on the computation (3/5)

Eigenvector decomposition is not continuous [Lax07; Kat95].. so? One can show that $\text{fl}(T^{-1}AT) = T^{-1}AT + E$ for $\|E\|_2 \lesssim \mu\kappa_2(T)\|A\|_2$ [GL13].

So, ideally we find $T \in \arg \min_{T \in \text{GL}(n, \mathbb{R})} \kappa_2(T)$, e.g., $T \in O(n, \mathbb{R})$. We cannot simply assume symmetry, instead we use:

Lemma (Gen. real Schur decomposition [GL13, Thm. 7.7.2])

For any $A, B \in \mathbb{R}^{n \times n}$ there exist $Q, Z \in O(n, \mathbb{R})$ such that $Q^T A Z$ is upper quasi-triangular and $Q^T B Z$ is upper triangular.

Lemma (QZ alg. [PLS80, Thm. 8a], know since the 70s [Fat69; Wil71]!)

Consider for the pair (S_1, S_2) its gen. real Schur decomposition as proposed above, then, all ARE solutions are of the form $P = U_{21} U_{11}^{-1}$, for U :

$$U = \begin{pmatrix} U_{11} \\ U_{21} \end{pmatrix} = Z \begin{pmatrix} I_n \\ 0_{n \times n} \end{pmatrix} = \begin{pmatrix} Z_{11} \\ Z_{21} \end{pmatrix}. \quad (10)$$

Symplectic perspective on the computation (4/5)

If $\theta' \in \text{GL}(n, \mathbb{R})$ (a.s.), then $S_1x = \lambda S_2x \rightarrow S_2^{-1}S_1x = \lambda x$, but $S_2^{-1}S_1 \in \text{Sp}(2n, \mathbb{R}) = \{M \in \mathbb{R}^{2n \times 2n} : M^T \Omega M = \Omega\}$ (**unlock structure**). Specifically, we can define the curve $M : \mathbb{R} \rightarrow \text{Sp}(2n, \mathbb{R})$ by

$$\delta \mapsto M(\delta) = S_2^{-1}S_1 = \begin{pmatrix} \theta' + 2\delta S_w \theta'^{-T} Q & -2\delta S_w \theta'^{-T} \\ -\theta'^{-T} Q & \theta'^{-T} \end{pmatrix}. \quad (11)$$

Use (11) to compute “optimal” pair $(\delta, Q(\delta))$.

Lemma (Approximately geodesic [Jon22])

For $Q(\delta) = 2\delta \theta'^T S_w \theta'$ and $\delta(t) = \delta_0 - t$, $t \in [0, \delta_0)$ then $t \mapsto M(\delta(t)) \approx \exp(tX)M(\delta_0)$ is δ -approximately geodesic.

Exploit Lie group structure and define a *left-invariant* metric g via

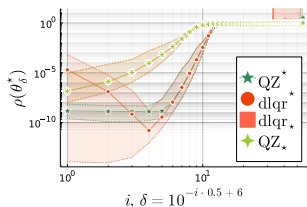
$$g_g(X, Y) = \langle X, Y \rangle_g = \langle d(L_{g^{-1}})_g(X), d(L_{g^{-1}})_g(Y) \rangle_e, \quad X, Y \in T_g \text{Sp}(n, \mathbb{R}).$$

We have $\mathcal{L}_X g = 0$ (Killing), leads to bounds.

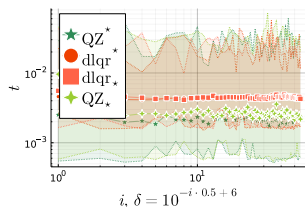
Symplectic perspective on the computation (5/5)

Original QZ algorithm due to Moler and Stewart [MS73] (so Mathworks `dlqr(·)` not bad).

Shorthand notation: $Q^* = 2^{-1}\delta^2\theta'^T(2S_w)^{-1}\theta'$ (damped) and $Q_* = 2\delta\theta'^T S_w\theta'$ (approx. geodesic).



(a) Convergence for $n = 10$



(b) Time to compute θ_δ^* for $n = 10$

Figure 3: Numerical experiments (250 per δ), computing θ_δ^* by means of the QZ algorithm or Julia's `dlqr(·)` routine, for $\text{vec}(\theta') \sim \mathcal{N}(0, I_{n^2})$ under different choices of Q and $S_w = (1/n^2)I_n$. Each figure displays all available data.

Take away:

- (I) LDPs allow for probabilistic results adapted to the process;
- (II) Steady-state covariances can be linked to optimal control;
- (III) Geometric thinking pays off towards fast and reliable algorithms.

Further topics:

(i) (Topological identification [JSK22]): for $\theta \in \Theta \cap GL(n, \mathbb{R})$ we have

$$\mathbb{P}(\mathcal{P}(\hat{\theta}_T) \not\approx \theta) \lesssim e^{-\mathcal{O}(\sigma_{\min}(\theta)^2 a_T)}.$$

(ii) Hyperbolic nonlinear systems and Lyapunov exponents.

Thank you! Questions?

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