

Theory and Algorithms for Forecasting Non-Stationary Time Series

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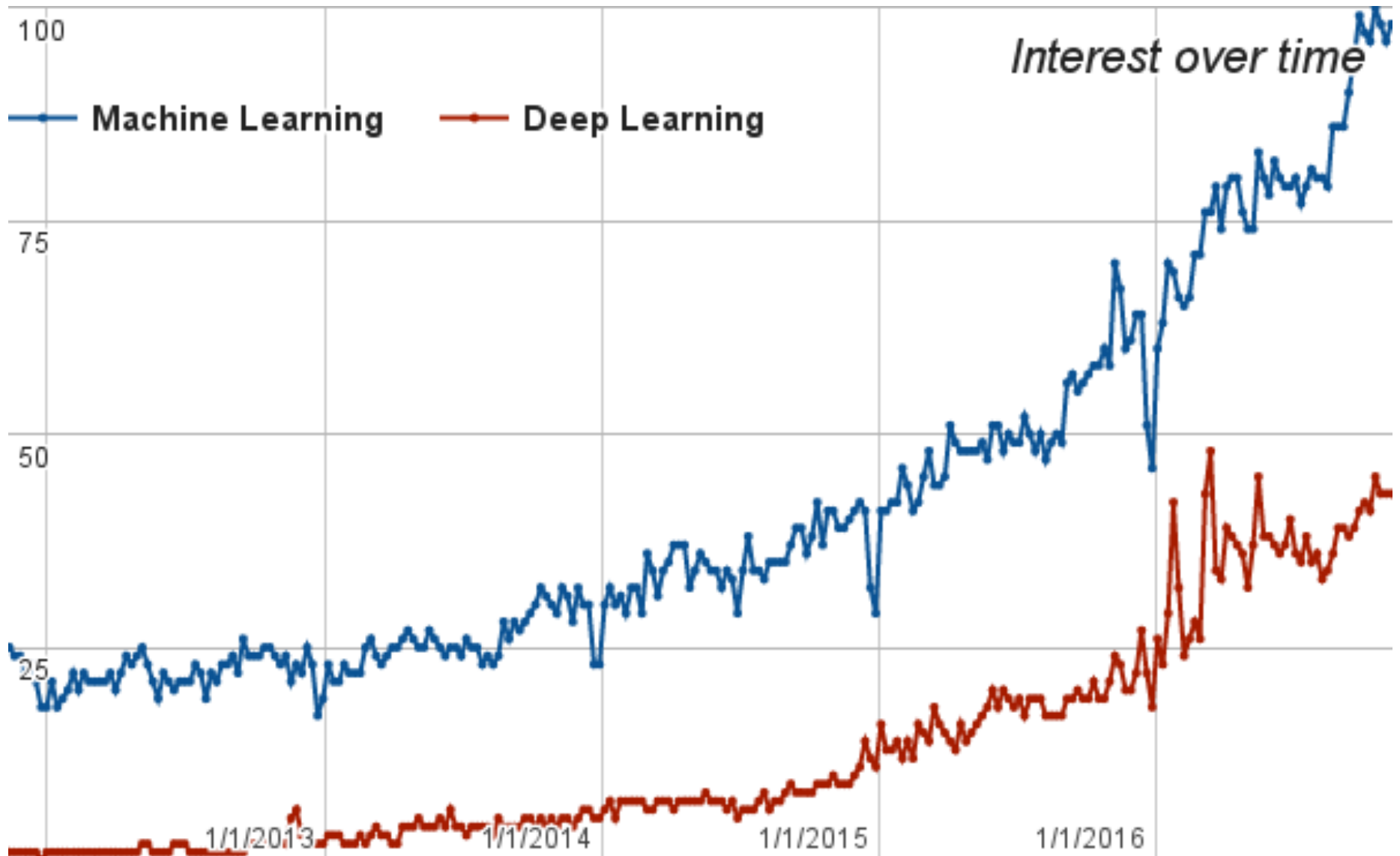
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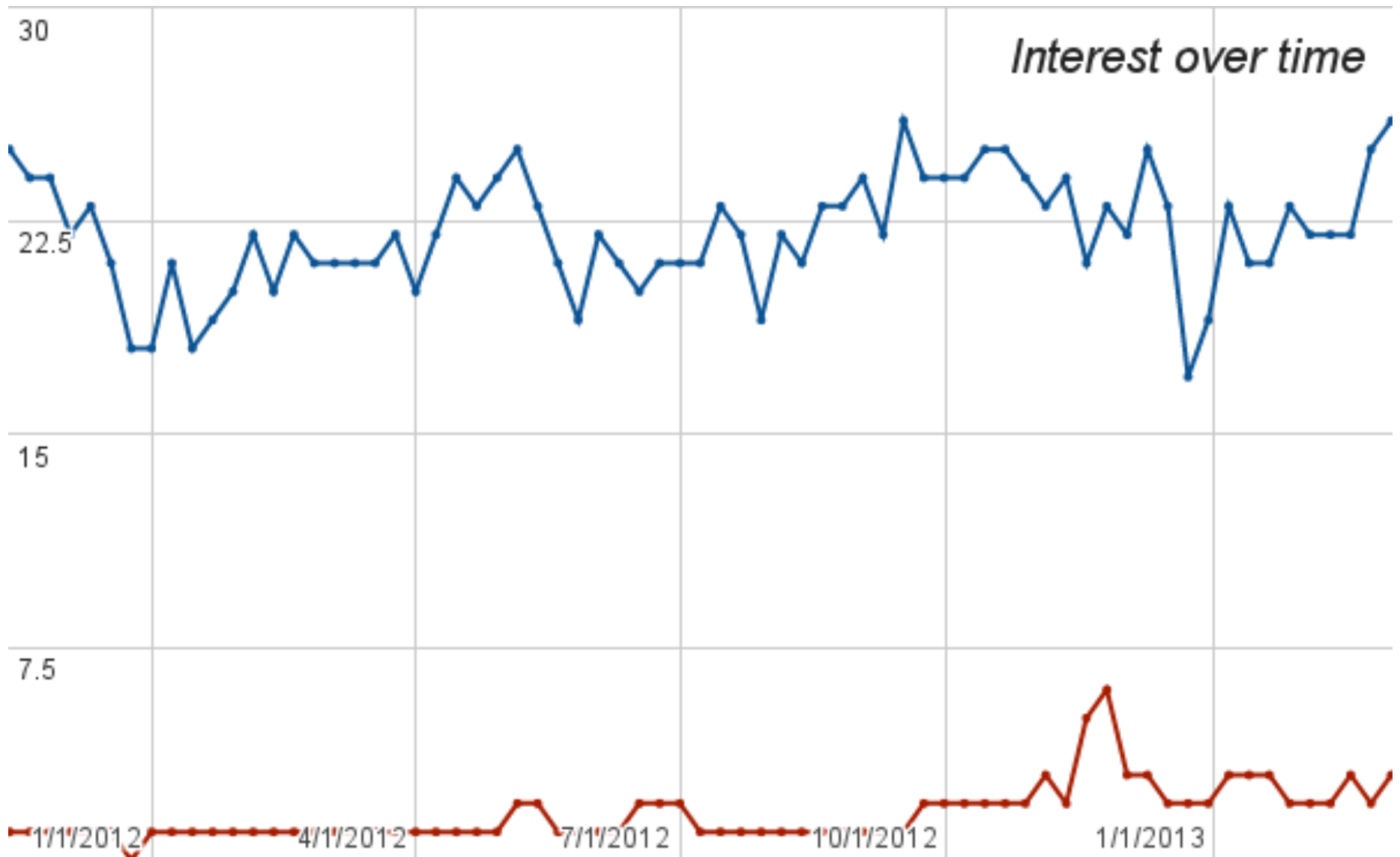
Motivation

- Time series prediction:
 - stock values.
 - economic variables.
 - weather: e.g., local and global temperature.
 - sensors: Internet-of-Things.
 - earthquakes.
 - energy demand.
 - signal processing.
 - sales forecasting.

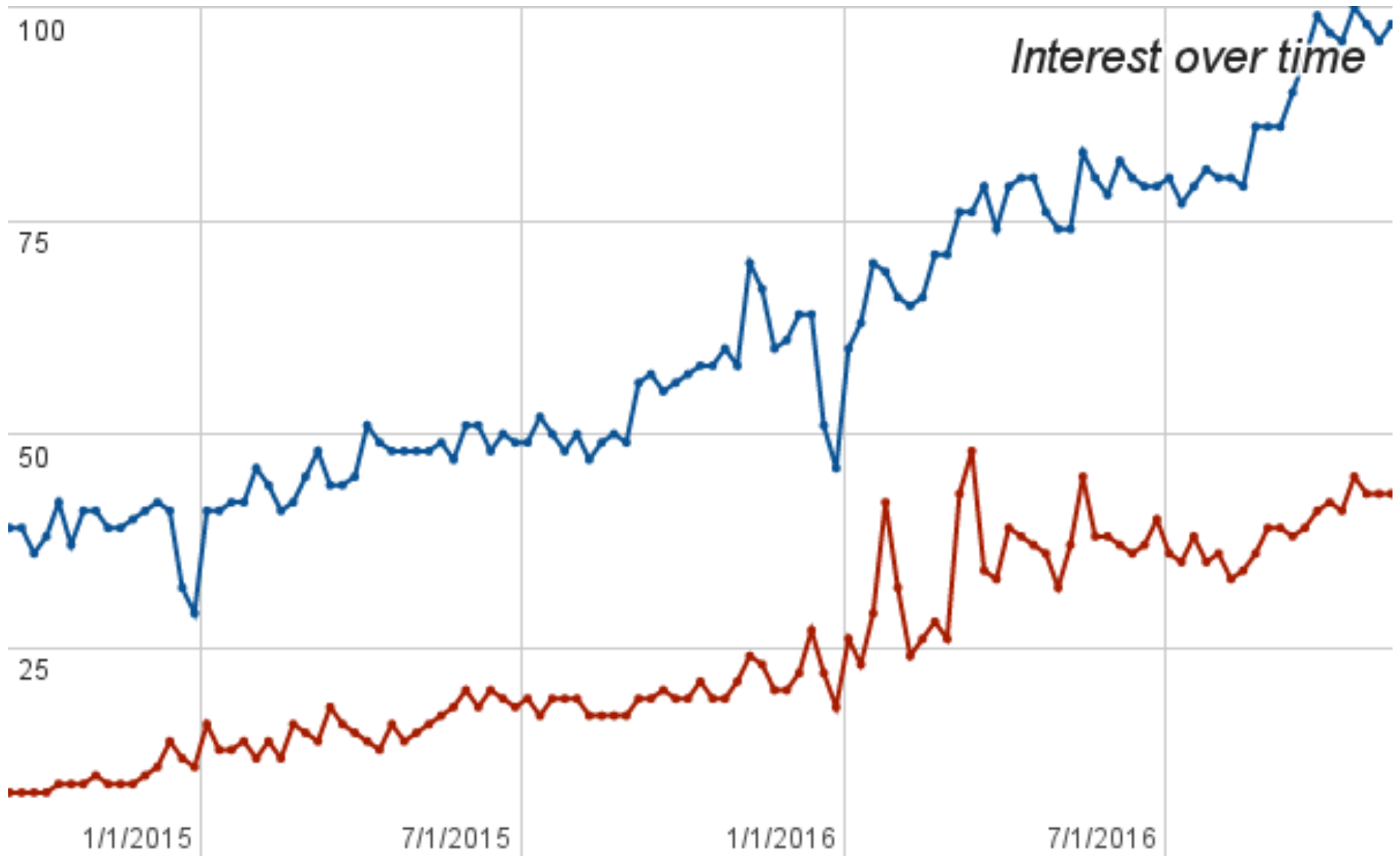
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Challenges

- Standard Supervised Learning:
 - IID assumption.
 - Same distribution for training and test data.
 - Distributions fixed over time (stationarity).
- none of these assumptions holds for time series!

Outline

- Introduction to time series analysis.
- Learning theory for forecasting non-stationary time series.
- Algorithms for forecasting non-stationary time series.
- Time series prediction and on-line learning.

Introduction to Time Series Analysis

Classical Framework

- Postulate a particular form of a parametric model that is assumed to generate data.
- Use given sample to estimate unknown parameters of the model.
- Use estimated model to make predictions.

Autoregressive (AR) Models

- **Definition:** AR(p) model is a linear generative model based on the p th order Markov assumption:

$$\forall t, Y_t = \sum_{i=1}^p a_i Y_{t-i} + \epsilon_t$$

where

- ϵ_t s are zero mean uncorrelated random variables with variance σ .
- a_1, \dots, a_p are autoregressive coefficients.
- Y_t is observed stochastic process.

Moving Averages (MA)

- **Definition:** MA(q) model is a linear generative model for the noise term based on the q th order Markov assumption:

$$\forall t, Y_t = \epsilon_t + \sum_{j=1}^q b_j \epsilon_{t-j}$$

where

- b_1, \dots, b_q are moving average coefficients.

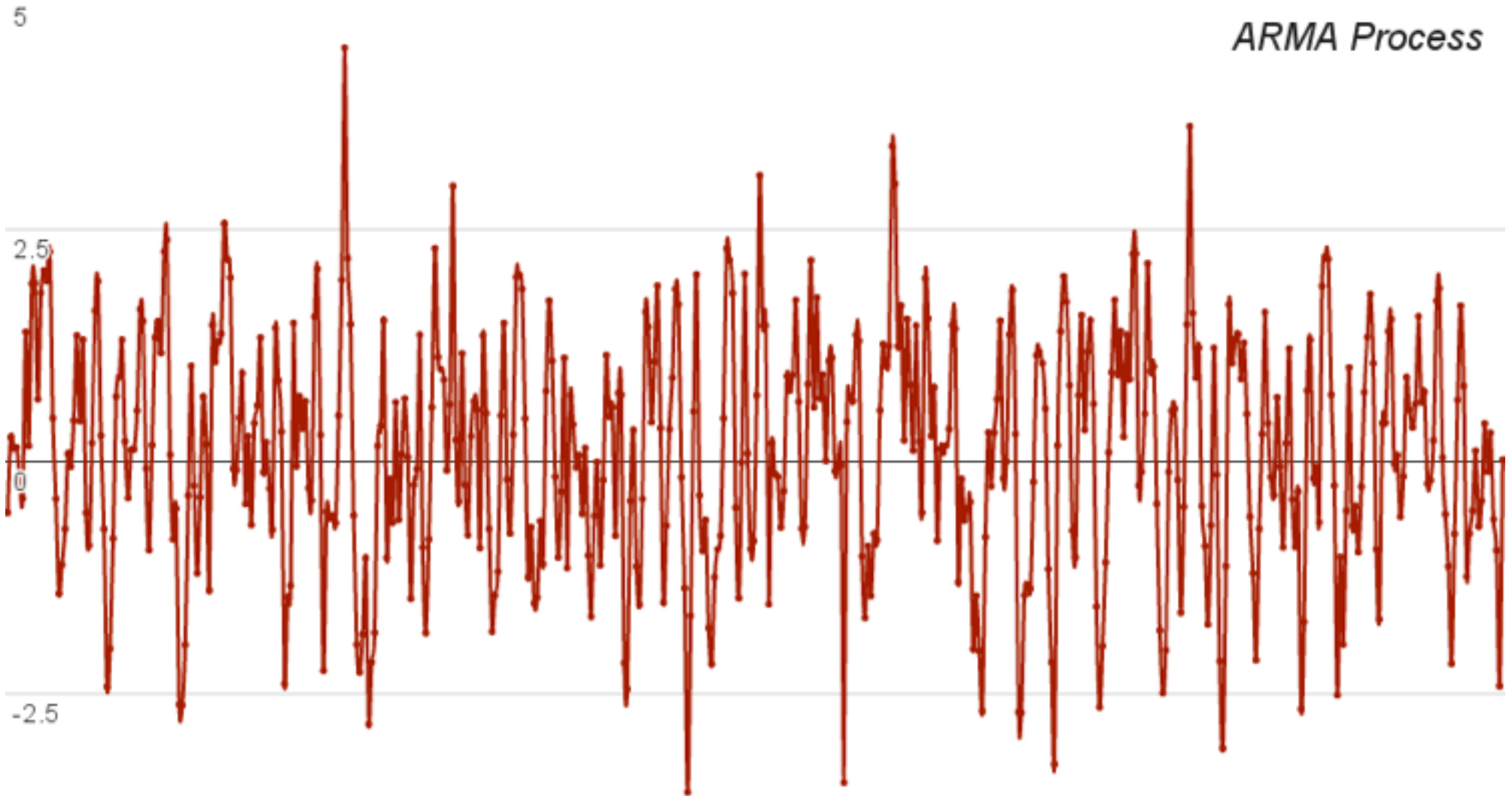
ARMA model

(Whittle, 1951; Box & Jenkins, 1971)

- **Definition:** ARMA(p, q) model is a generative linear model that combines AR(p) and MA(q) models:

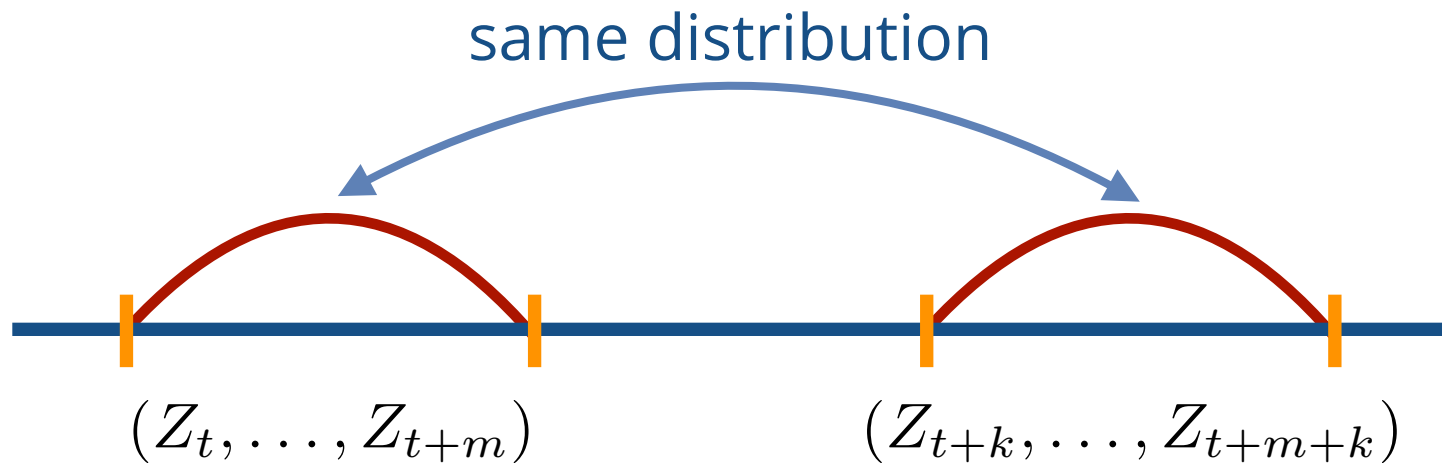
$$\forall t, Y_t = \sum_{i=1}^p a_i Y_{t-i} + \epsilon_t + \sum_{j=1}^q b_j \epsilon_{t-j}.$$

ARMA



Stationarity

- **Definition:** a sequence of random variables $\mathbf{Z} = \{Z_t\}_{-\infty}^{+\infty}$ is **stationary** if its distribution is invariant to shifting in time.



Weak Stationarity

- **Definition:** a sequence of random variables $\mathbf{Z} = \{Z_t\}_{-\infty}^{+\infty}$ is **weakly stationary** if its first and second moments are invariant to shifting in time, that is,
 - $\mathbb{E}[Z_t]$ is independent of t .
 - $\mathbb{E}[Z_t Z_{t-j}] = f(j)$ for some function f .

Lag Operator

- Lag operator \mathcal{L} is defined by $\mathcal{L}Y_t = Y_{t-1}$.
- ARMA model in terms of the lag operator:

$$\left(1 - \sum_{i=1}^p a_i \mathcal{L}^i\right) Y_t = \left(1 + \sum_{j=1}^q b_j \mathcal{L}^j\right) \epsilon_t$$

- Characteristic polynomial

$$P(z) = 1 - \sum_{i=1}^p a_i z^i$$

can be used to study properties of this stochastic process.

Weak Stationarity of ARMA

- **Theorem:** an ARMA(p, q) process is weakly stationary if the roots of the characteristic polynomial $P(z)$ are outside the unit circle.

Proof

- If roots of the characteristic polynomial are outside the unit circle then:

$$\begin{aligned} P(z) &= 1 - \sum_{i=1}^p a_i z^i = c(\psi_1 - z) \cdots (\psi_p - z) \\ &= c'(1 - \psi_1^{-1} z) \cdots (1 - \psi_p^{-1} z) \end{aligned}$$

where $|\psi_i| > 1$ for all $i = 1, \dots, p$ and c, c' are constants.

Proof

- Therefore, the ARMA(p, q) process

$$\left(1 - \sum_{i=1}^p a_i \mathcal{L}^i\right) Y_t = \left(1 + \sum_{j=1}^q b_j \mathcal{L}^j\right) \epsilon_t$$

admits MA(∞) representation:

$$Y_t = \left(1 - \psi_1^{-1} \mathcal{L}\right)^{-1} \cdots \left(1 - \psi_p^{-1} \mathcal{L}\right)^{-1} \left(1 + \sum_{j=1}^q b_j \mathcal{L}^j\right) \epsilon_t$$

where

$$\left(1 - \psi_i^{-1} \mathcal{L}\right)^{-1} = \sum_{k=0}^{\infty} \left(-\psi_i^{-1} \mathcal{L}\right)^k$$

is well-defined since $|\psi_i^{-1}| < 1$.

Proof

- Therefore, it suffices to show that

$$Y_t = \sum_{j=0}^{\infty} \phi_j \epsilon_{t-j}$$

is weakly stationary.

- The mean is constant

$$\mathbb{E}[Y_t] = \sum_{j=0}^{\infty} \phi_j \mathbb{E}[\epsilon_{t-j}] = 0.$$

- Covariance function $\mathbb{E}[Y_t Y_{t-l}]$ only depends on the lag l :

$$\mathbb{E}[Y_t Y_{t-l}] = \sum_{k=0}^{\infty} \sum_{j=0}^{\infty} \phi_k \phi_j \mathbb{E}[\epsilon_{t-j} \epsilon_{t-l-k}] = \sum_{j=0}^{\infty} \phi_j \phi_{j+l}.$$

ARIMA

- Non-stationary processes can be modeled using processes whose characteristic polynomial has unit roots.
- Characteristic polynomial with unit roots can be factored:

$$P(z) = R(z)(1 - z)^D$$

where $R(z)$ has no unit roots.

- **Definition:** ARIMA(p, D, q) model is an ARMA(p, q) model for $(1 - \mathcal{L})^D Y_t$:

$$\left(1 - \sum_{i=1}^p a_i \mathcal{L}^i\right) \left(1 - \mathcal{L}\right)^D Y_t = \left(1 + \sum_{j=1}^q b_j \mathcal{L}^j\right) \epsilon_t.$$

ARIMA

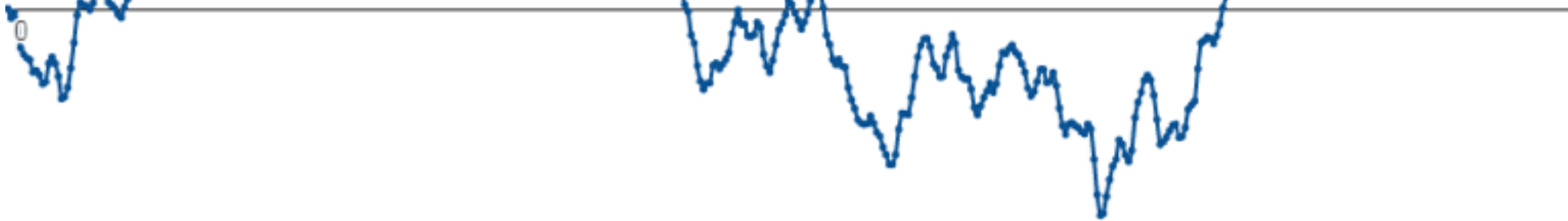
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ARIMA Process

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25

0



Other Extensions

- Further variants:
 - models with seasonal components (SARIMA).
 - models with side information (ARIMAX).
 - models with long-memory (ARFIMA).
 - multi-variate time series models (VAR).
 - models with time-varying coefficients.
 - other non-linear models.

Modeling Variance

(Engle, 1982; Bollerslev, 1986)

- **Definition:** the generalized autoregressive conditional heteroscedasticity GARCH(p, q) model is an ARMA(p, q) model for the variance σ_t of the noise term ϵ_t :

$$\forall t, \sigma_{t+1}^2 = \omega + \sum_{i=0}^{p-1} \alpha_i \sigma_{t-i}^2 + \sum_{j=0}^{q-1} \beta_j \epsilon_{t-j}^2$$

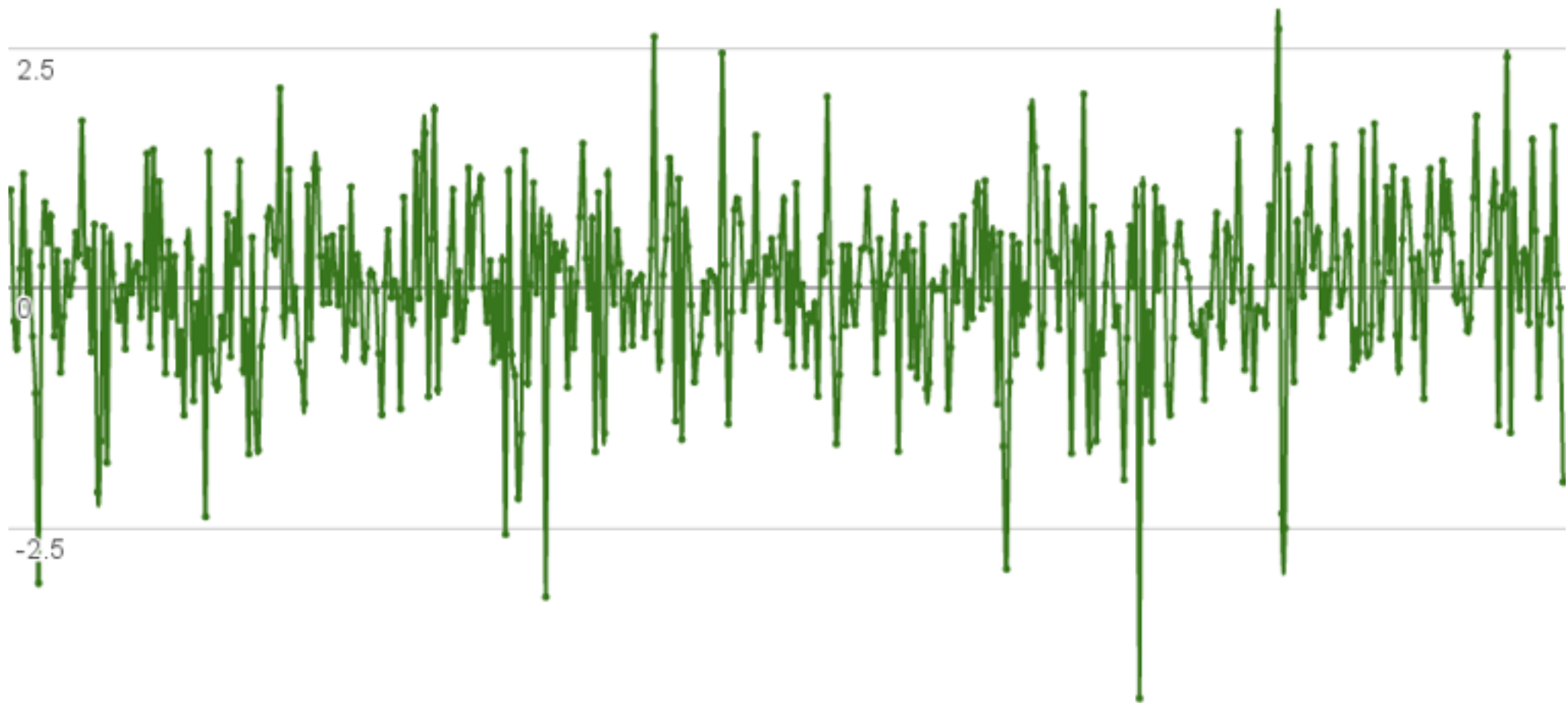
where

- ϵ_t s are zero mean Gaussian random variables with variance σ_t conditioned on $\{Y_{t-1}, Y_{t-2}, \dots\}$.
- $\omega > 0$ is the mean parameter.

GARCH Process

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GARCH Process



State-Space Models

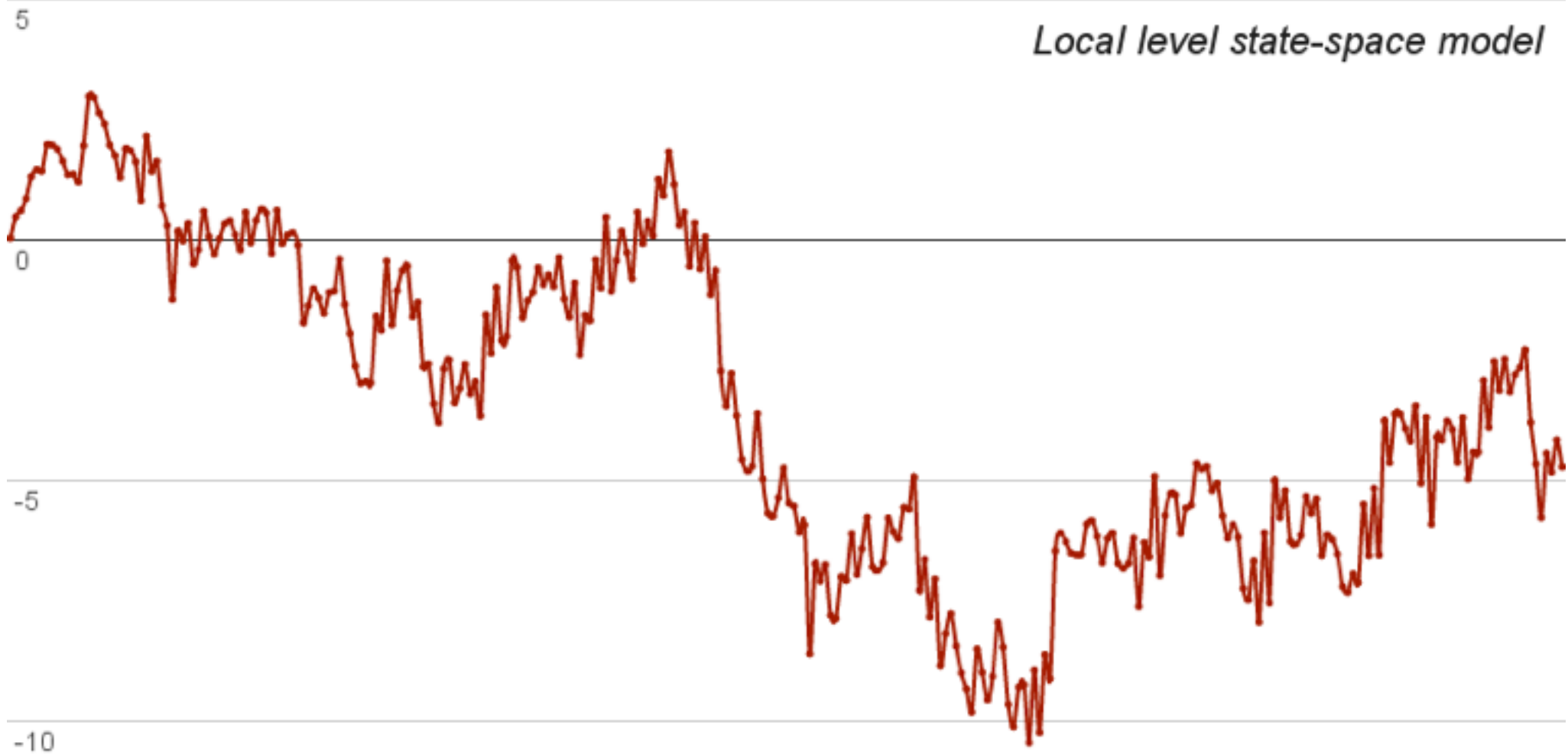
- Continuous state space version of Hidden Markov Models:

$$\begin{aligned}\mathbf{X}_{t+1} &= \mathbf{B}\mathbf{X}_t + \mathbf{U}_t, \\ Y_t &= \mathbf{A}\mathbf{X}_t + \epsilon_t\end{aligned}$$

where

- \mathbf{X}_t is an n -dimensional state vector.
- Y_t is an observed stochastic process.
- \mathbf{A} and \mathbf{B} are model parameters.
- \mathbf{U}_t and ϵ_t are noise terms.

State-Space Models



Estimation

- Different methods for estimating model parameters:
 - Maximum likelihood estimation:
 - Requires further parametric assumptions on the noise distribution (e.g. Gaussian).
 - Method of moments (Yule-Walker estimator).
 - Conditional and unconditional least square estimation.
 - Restricted to certain models.

Invertibility of ARMA

- **Definition:** an ARMA(p, q) process is invertible if the roots of the polynomial

$$Q(z) = 1 + \sum_{j=1}^q b_j z^j$$

are outside the unit circle.

Learning guarantee

- **Theorem:** assume $Y_t \sim \text{ARMA}(p, q)$ is weakly stationary and invertible. Let $\hat{\mathbf{a}}_T$ denote the least square estimate of $\mathbf{a} = (a_1, \dots, a_p)$ and assume that p is known. Then, $\|\hat{\mathbf{a}}_T - \mathbf{a}\|$ converges in probability to zero.
- Similar results hold for other estimators and other models.

Notes

- Many other generative models exist.
- Learning guarantees are asymptotic.
- Model needs to be correctly specified.
- Non-stationarity needs to be modeled explicitly.

Theory

Time Series Forecasting

- **Training data:** finite sample realization of some stochastic process,

$$(X_1, Y_1), \dots, (X_T, Y_T) \in \mathcal{Z} = \mathcal{X} \times \mathcal{Y}.$$

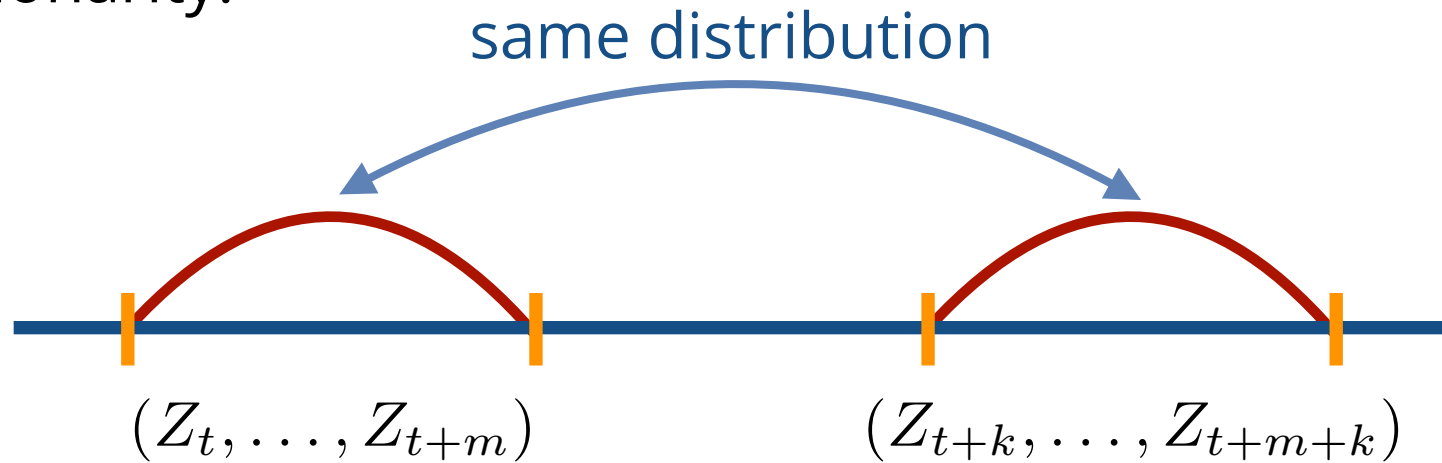
- **Loss function:** $L: H \times \mathcal{Z} \rightarrow [0, 1]$, where H is a hypothesis set of functions mapping from \mathcal{X} to \mathcal{Y} .

- **Problem:** find $h \in H$ with small path-dependent expected loss,

$$\mathcal{L}(h, \mathbf{Z}_1^T) = \mathbb{E}_{Z_{T+1}} [L(h, Z_{T+1}) | \mathbf{Z}_1^T].$$

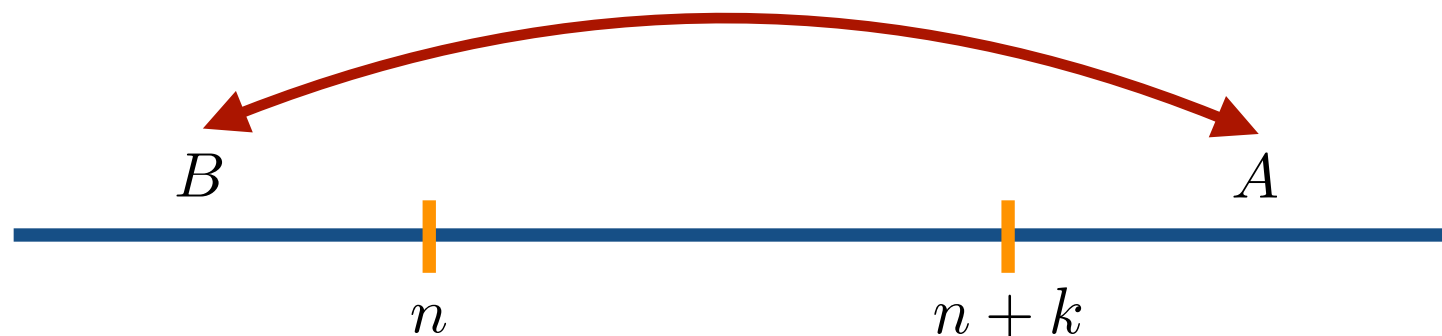
Standard Assumptions

■ Stationarity:



■ Mixing:

dependence between events decaying with k .



Learning Theory

- Stationary and β -mixing process: generalization bounds.
 - PAC-learning preserved in that setting (Vidyasagar, 1997).
 - VC-dimension bounds for binary classification (Yu, 1994).
 - covering number bounds for regression (Meir, 2000).
 - Rademacher complexity bounds for general loss functions (MM and Rostamizadeh, 2000).
 - PAC-Bayesian bounds (Alquier et al., 2014).

Learning Theory

- Stationarity and mixing: algorithm-dependent bounds.
 - AdaBoost (Lozano et al., 1997).
 - general stability bounds (MM and Rostamizadeh, 2010).
 - regularized ERM (Steinwart and Christmann, 2009).
 - stable on-line algorithms (Agarwal and Duchi, 2013).

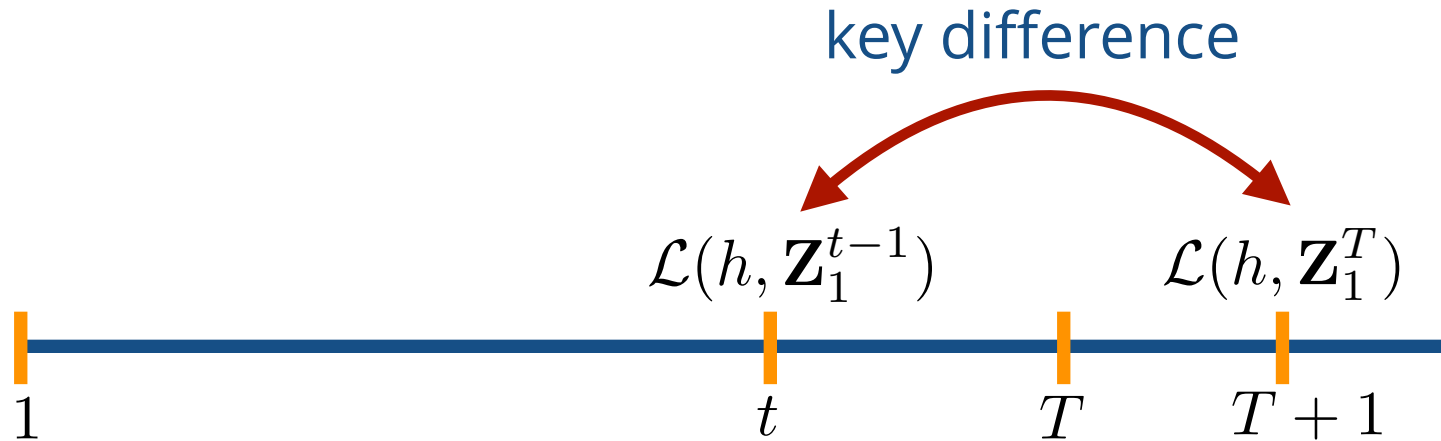
Problem

- Stationarity and mixing assumptions:
 - often do not hold (think trend or periodic signals).
 - not testable.
 - estimating mixing parameters can be hard, even if general functional form known.
 - hypothesis set and loss function ignored.

Questions

- Is learning with general (non-stationary, non-mixing) stochastic processes possible?
- Can we design algorithms with theoretical guarantees?
→ need a new tool for the analysis.

Key Quantity - Fixed h



→ Key average quantity: $\left| \frac{1}{T} \sum_{t=1}^T \left[\mathcal{L}(h, \mathbf{Z}_1^T) - \mathcal{L}(h, \mathbf{Z}_1^{t-1}) \right] \right|.$

Discrepancy

■ Definition:

$$\Delta = \sup_{h \in H} \left| \mathcal{L}(h, \mathbf{Z}_1^T) - \frac{1}{T} \sum_{t=1}^T \mathcal{L}(h, \mathbf{Z}_1^{t-1}) \right|.$$

- captures hypothesis set and loss function.
- can be estimated from data, under mild assumptions.
- $\Delta = 0$ in IID case or for weakly stationary processes with linear hypotheses and squared loss (K and MM, 2014).

Weighted Discrepancy

- **Definition:** extension to weights $(q_1, \dots, q_T) = \mathbf{q}$.

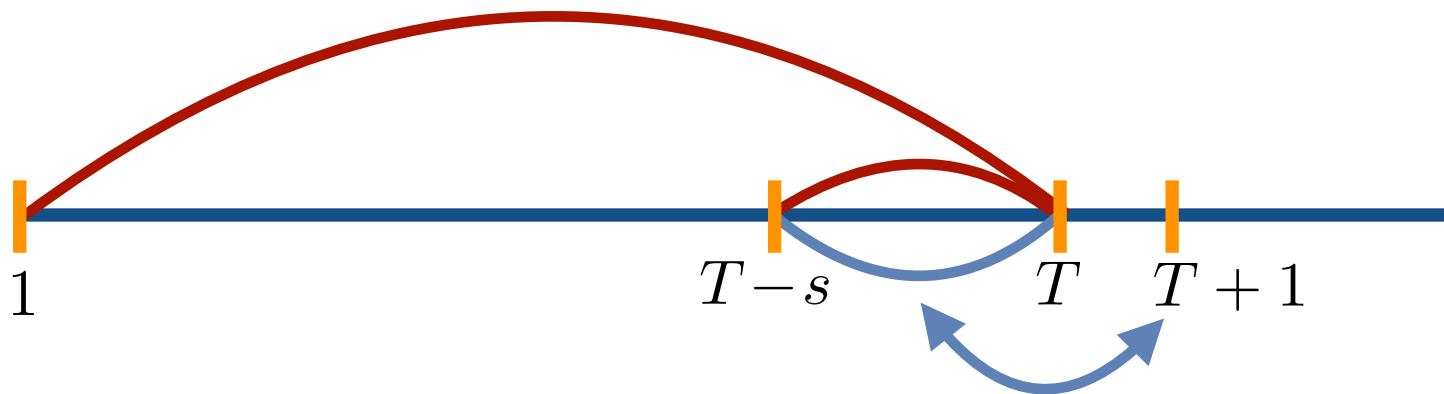
$$\Delta(\mathbf{q}) = \sup_{h \in H} \left| \mathcal{L}(h, \mathbf{Z}_1^T) - \sum_{t=1}^T q_t \mathcal{L}(h, \mathbf{Z}_1^{t-1}) \right|.$$

- strictly extends discrepancy definition in drifting (MM and Muñoz Medina, 2012) or domain adaptation (Mansour, MM, Rostamizadeh 2009; Cortes and MM 2011, 2014); or for binary loss (Devroye et al., 1996; Ben-David et al., 2007).
- admits upper bounds in terms of relative entropy, or in terms of ϕ -mixing coefficients of asymptotic stationarity for an asymptotically stationary process.

Estimation

- Decomposition: $\Delta(\mathbf{q}) \leq \Delta_0(\mathbf{q}) + \Delta_s$.

$$\Delta(\mathbf{q}) \leq \sup_{h \in H} \left(\frac{1}{s} \sum_{t=T-s+1}^T \mathcal{L}(h, \mathbf{Z}_1^{t-1}) - \sum_{t=1}^T q_t \mathcal{L}(h, \mathbf{Z}_1^{t-1}) \right) \\ + \sup_{h \in H} \left(\mathcal{L}(h, \mathbf{Z}_1^T) - \frac{1}{s} \sum_{t=T-s+1}^T \mathcal{L}(h, \mathbf{Z}_1^{t-1}) \right).$$



Learning Guarantee

- **Theorem:** for any $\delta > 0$, with probability at least $1 - \delta$, for all $h \in H$ and $\alpha > 0$,

$$\mathcal{L}(h, \mathbf{Z}_1^T) \leq \sum_{t=1}^T q_t L(h, Z_t) + \Delta(\mathbf{q}) + 2\alpha + \|\mathbf{q}\|_2 \sqrt{2 \log \frac{\mathbb{E}[\mathcal{N}_1(\alpha, \mathcal{G}, \mathbf{z})]}{\delta}},$$

where $\mathcal{G} = \{z \mapsto L(h, z) : h \in H\}$.

Bound with Emp. Discrepancy

- **Corollary:** for any $\delta > 0$, with probability at least $1 - \delta$, for all $h \in H$ and $\alpha > 0$,

$$\mathcal{L}(h, \mathbf{Z}_1^T) \leq \sum_{t=1}^T q_t L(h, Z_t) + \hat{\Delta}(\mathbf{q}) + \Delta_s + 4\alpha + \left[\|\mathbf{q}\|_2 + \|\mathbf{q} - \mathbf{u}_s\|_2 \right] \sqrt{2 \log \frac{2 \mathbb{E} [\mathcal{N}_1(\alpha, \mathcal{G}, \mathbf{z})]}{\delta}},$$

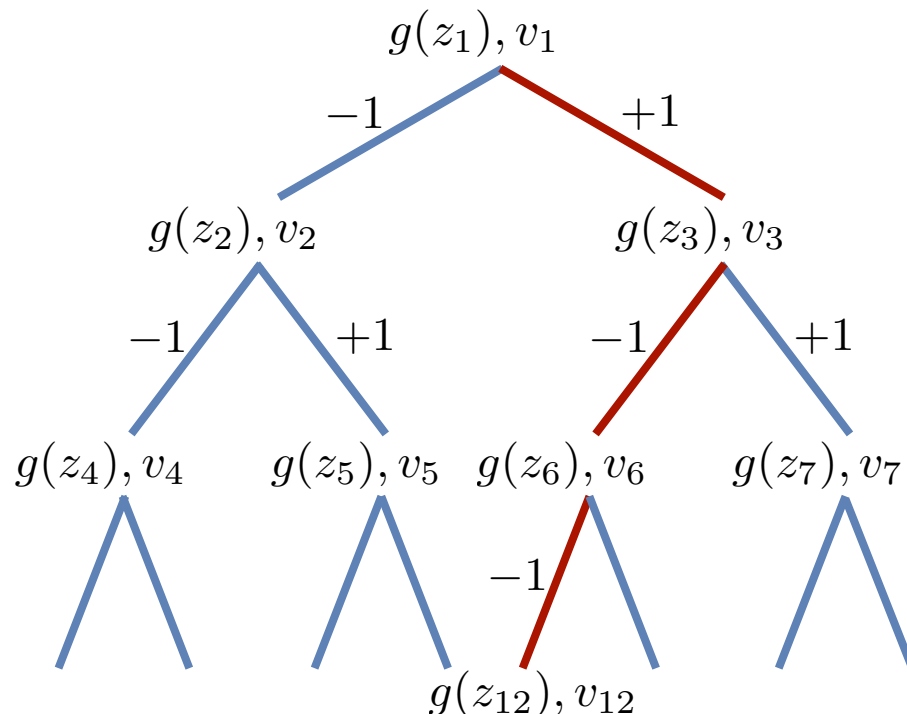
$$\text{where } \left\{ \begin{array}{l} \hat{\Delta}(\mathbf{q}) = \sup_{h \in H} \left(\frac{1}{s} \sum_{t=T-s+1}^T L(h, Z_t) - \sum_{t=1}^T q_t L(h, Z_t) \right) \\ \mathbf{u}_s \text{ unif. dist. over } [T-s, T] \\ \mathcal{G} = \{z \mapsto L(h, z) : h \in H\}. \end{array} \right.$$

Weighted Sequential α -Cover

(Rakhlin et al., 2010; K and MM, 2015)

- Definition:** let \mathbf{z} be a \mathcal{Z} -valued full binary tree of depth T . Then, a set of trees \mathcal{V} is an l_1 -norm \mathbf{q} -weighted α -cover of a function class \mathcal{G} on \mathbf{z} if

$$\forall g \in \mathcal{G}, \forall \boldsymbol{\sigma} \in \{\pm 1\}^T, \exists \mathbf{v} \in \mathcal{V}: \sum_{t=1}^T |v_t(\boldsymbol{\sigma}) - g(z_t(\boldsymbol{\sigma}))| \leq \frac{\alpha}{\|\mathbf{q}\|_\infty}.$$



$$\left\| \begin{bmatrix} v_1 - g(z_1) \\ v_3 - g(z_3) \\ v_6 - g(z_6) \\ v_{12} - g(z_{12}) \end{bmatrix} \right\|_1 \leq \frac{\alpha}{\|\mathbf{q}\|_\infty}.$$

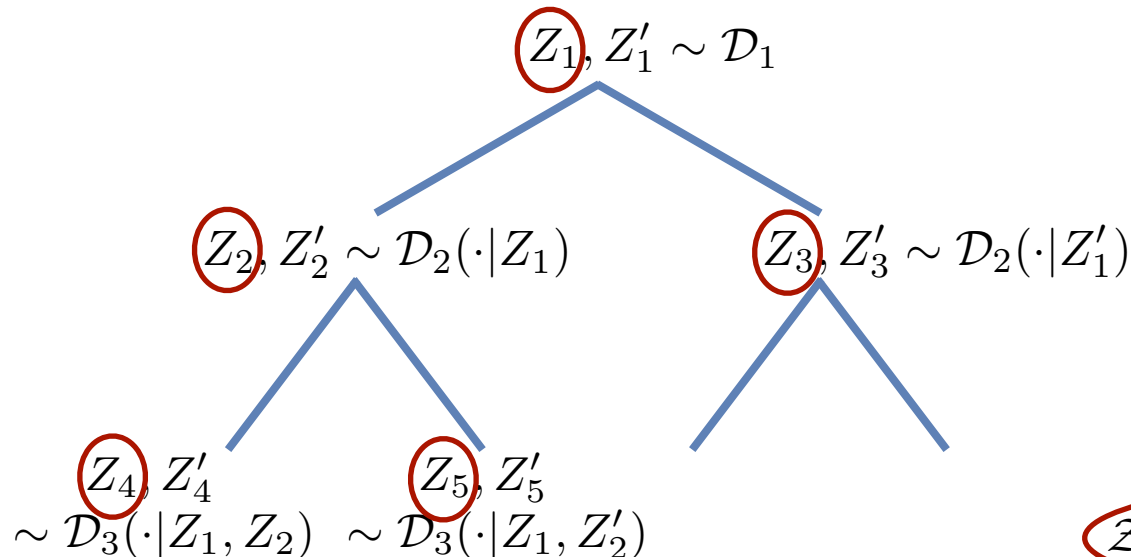
Sequential Covering Numbers

■ Definitions:

- sequential covering number:

$$\mathcal{N}_1(\alpha, \mathcal{G}, \mathbf{z}) = \min\{|\mathcal{V}| : \mathcal{V} \text{ } l_1\text{-norm } \mathbf{q}\text{-weighted } \alpha\text{-cover of } \mathcal{G}\}.$$

- expected sequential covering number: $\mathbb{E}_{\mathbf{z} \sim \mathcal{Z}_T} [\mathcal{N}_1(\alpha, \mathcal{G}, \mathbf{z})]$.



\mathcal{Z}_T : distribution based on Z_t s.

Proof

■ **Key quantities:** $\Phi(\mathbf{Z}_1^T) = \sup_{h \in H} \left(\mathcal{L}(h, Z_T) - \sum_{t=1}^T q_t L(h, Z_t) \right)$

$$\Delta(\mathbf{q}) = \sup_{h \in H} \left| \mathcal{L}(h, \mathbf{Z}_1^T) - \sum_{t=1}^T q_t \mathcal{L}(h, \mathbf{Z}_1^{t-1}) \right|.$$

■ **Chernoff technique:** for any $t > 0$,

$$\begin{aligned} & \mathbb{P} \left[\Phi(\mathbf{Z}_1^T) - \Delta(\mathbf{q}) > \epsilon \right] \\ & \leq \mathbb{P} \left[\sup_{h \in H} \sum_{t=1}^T q_t [\mathcal{L}(h, \mathbf{Z}_1^{t-1}) - L(h, Z_t)] > \epsilon \right] && \text{(sub-add. of sup)} \\ & = \mathbb{P} \left[\exp \left(t \sup_{h \in H} \sum_{t=1}^T q_t [\mathcal{L}(h, \mathbf{Z}_1^{t-1}) - L(h, Z_t)] \right) > e^{t\epsilon} \right] && (t > 0) \\ & \leq e^{-t\epsilon} \mathbb{E} \left[\exp \left(t \sup_{h \in H} \sum_{t=1}^T q_t [\mathcal{L}(h, \mathbf{Z}_1^{t-1}) - L(h, Z_t)] \right) \right]. && \text{(Markov's ineq.)} \end{aligned}$$

Symmetrization

- **Key tool:** decoupled tangent sequence \mathbf{Z}'_1^T associated to \mathbf{Z}_1^T .
 - Z_t and Z'_t i.i.d. given \mathbf{Z}_1^{t-1} .

$$\begin{aligned}
 & \mathbb{P} [\Phi(\mathbf{Z}_1^T) - \Delta(\mathbf{q}) > \epsilon] \\
 & \leq e^{-t\epsilon} \mathbb{E} \left[\exp \left(t \sup_{h \in H} \sum_{t=1}^T q_t [\mathcal{L}(h, \mathbf{Z}_1^{t-1}) - L(h, Z_t)] \right) \right] \\
 & = e^{-t\epsilon} \mathbb{E} \left[\exp \left(t \sup_{h \in H} \sum_{t=1}^T q_t [\mathbb{E}[L(h, Z'_t) | \mathbf{Z}_1^{t-1}] - L(h, Z_t)] \right) \right] \quad (\text{tangent seq.}) \\
 & = e^{-t\epsilon} \mathbb{E} \left[\exp \left(t \sup_{h \in H} \mathbb{E} \left[\sum_{t=1}^T q_t [L(h, Z'_t) - L(h, Z_t)] \mid \mathbf{Z}_1^T \right] \right) \right] \quad (\text{lin. of expectation}) \\
 & \leq e^{-t\epsilon} \mathbb{E} \left[\exp \left(t \sup_{h \in H} \sum_{t=1}^T q_t [L(h, Z'_t) - L(h, Z_t)] \right) \right]. \quad (\text{Jensen's ineq.})
 \end{aligned}$$

Symmetrization

$$\begin{aligned}
 & \mathbb{P} [\Phi(\mathbf{Z}_1^T) - \Delta(\mathbf{q}) > \epsilon] \\
 & \leq e^{-t\epsilon} \mathbb{E} \left[\exp \left(t \sup_{h \in H} \sum_{t=1}^T q_t [L(h, Z'_t) - L(h, Z_t)] \right) \right] \\
 & = e^{-t\epsilon} \mathbb{E}_{(\mathbf{z}, \mathbf{z}')} \mathbb{E}_{\boldsymbol{\sigma}} \left[\exp \left(t \sup_{h \in H} \sum_{t=1}^T q_t \sigma_t [L(h, z'_t(\boldsymbol{\sigma})) - L(h, z_t(\boldsymbol{\sigma}))] \right) \right] \quad (\text{tangent seq. prop.}) \\
 & = e^{-t\epsilon} \mathbb{E}_{(\mathbf{z}, \mathbf{z}')} \mathbb{E}_{\boldsymbol{\sigma}} \left[\exp \left(t \sup_{h \in H} \sum_{t=1}^T q_t \sigma_t L(h, z'_t(\boldsymbol{\sigma})) + t \sup_{h \in H} \sum_{t=1}^T q_t \sigma_t L(h, z_t(\boldsymbol{\sigma})) \right) \right] \quad (\text{sub-add. of sup}) \\
 & \leq e^{-t\epsilon} \mathbb{E}_{(\mathbf{z}, \mathbf{z}')} \mathbb{E}_{\boldsymbol{\sigma}} \left[\frac{1}{2} \exp \left(2t \sup_{h \in H} \sum_{t=1}^T q_t \sigma_t L(h, z'_t(\boldsymbol{\sigma})) \right) \right. \\
 & \quad \left. + \frac{1}{2} \exp \left(2t \sup_{h \in H} \sum_{t=1}^T q_t \sigma_t L(h, z_t(\boldsymbol{\sigma})) \right) \right] \quad (\text{convexity. of exp}) \\
 & = e^{-t\epsilon} \mathbb{E}_{\mathbf{z}} \mathbb{E}_{\boldsymbol{\sigma}} \left[\exp \left(2t \sup_{h \in H} \sum_{t=1}^T q_t \sigma_t L(h, z_t(\boldsymbol{\sigma})) \right) \right].
 \end{aligned}$$

Covering Number

$$\begin{aligned}
 & \mathbb{P} [\Phi(\mathbf{z}_1^T - \Delta(\mathbf{q}) > \epsilon)] \\
 & \leq e^{-t\epsilon} \mathbb{E}_{\mathbf{z}} \mathbb{E}_{\boldsymbol{\sigma}} \left[\exp \left(2t \sup_{h \in H} \sum_{t=1}^T q_t \sigma_t L(h, z_t(\boldsymbol{\sigma})) \right) \right] \\
 & \leq e^{-t\epsilon} \mathbb{E}_{\mathbf{z}} \mathbb{E}_{\boldsymbol{\sigma}} \left[\exp \left(2t \left[\max_{\mathbf{v} \in \mathcal{V}} \sum_{t=1}^T q_t \sigma_t v_t(\boldsymbol{\sigma}) + \alpha \right] \right) \right] && (\alpha\text{-covering}) \\
 & \leq e^{-t(\epsilon-2\alpha)} \mathbb{E}_{\mathbf{z}} \left[\sum_{\mathbf{v} \in \mathcal{V}} \mathbb{E}_{\boldsymbol{\sigma}} \left[\exp \left(2t \sum_{t=1}^T q_t \sigma_t v_t(\boldsymbol{\sigma}) \right) \right] \right] && (\text{monotonicity of exp}) \\
 & \leq e^{-t(\epsilon-2\alpha)} \mathbb{E}_{\mathbf{z}} \left[\sum_{\mathbf{v} \in \mathcal{V}} \exp \left(\frac{t^2 \|\mathbf{q}\|^2}{2} \right) \right] && (\text{Hoeffding's ineq.}) \\
 & \leq \mathbb{E}_{\mathbf{z}} \left[\mathcal{N}_1(\alpha, \mathcal{G}, \mathbf{z}) \right] \exp \left[-t(\epsilon - 2\alpha) + \frac{t^2 \|\mathbf{q}\|^2}{2} \right].
 \end{aligned}$$

Algorithms

Review

- **Theorem:** for any $\delta > 0$, with probability at least $1 - \delta$, for all $h \in H$ and $\alpha > 0$,

$$\mathcal{L}(h, \mathbf{Z}_1^T) \leq \sum_{t=1}^T q_t L(h, Z_t) + \hat{\Delta}(\mathbf{q}) + \Delta_s + 4\alpha \\ + \left[\|\mathbf{q}\|_2 + \|\mathbf{q} - \mathbf{u}_s\|_2 \right] \sqrt{2 \log \frac{2 \mathbb{E}_{\mathbf{z}} [\mathcal{N}_1(\alpha, \mathcal{G}, \mathbf{z})]}{\delta}}.$$

- This bound can be extended to hold uniformly over \mathbf{q} at the price of the additional term:

$$\tilde{O}(\|\mathbf{q} - \mathbf{u}\|_1 \sqrt{\log_2 \log_2 (1 - \|\mathbf{q} - \mathbf{u}\|)}^{-1}).$$

- Data-dependent learning guarantee.

Discrepancy-Risk Minimization

- **Key Idea:** directly optimize the upper bound on generalization over q and h .
- This problem can be solved efficiently for some L and H .

Kernel-Based Regression

■ Squared loss function: $L(y, y') = (y - y')^2$

■ Hypothesis set: for PDS kernel K ,

$$H = \left\{ x \mapsto \mathbf{w} \cdot \Phi_K(x) : \|\mathbf{w}\|_{\mathbb{H}} \leq \Lambda \right\}.$$

■ Complexity term can be bounded by

$$O\left((\log^{3/2} T) \Lambda \sup_x K(x, x) \|\mathbf{q}\|_2\right).$$

Instantaneous Discrepancy

- Empirical discrepancy can be further upper bounded in terms of instantaneous discrepancies:

$$\widehat{\Delta}(\mathbf{q}) \leq \sum_{t=1}^T q_t d_t + M \|\mathbf{q} - \mathbf{u}\|_1$$

where $M = \sup_{y, y'} L(y, y')$ and

$$d_t = \sup_{h \in H} \left(\frac{1}{s} \sum_{t=T-s+1}^T L(h, Z_t) - L(h, Z_t) \right).$$

Proof

- By sub-additivity of supremum

$$\begin{aligned}\widehat{\Delta}(\mathbf{q}) &= \sup_{h \in H} \left\{ \frac{1}{s} \sum_{t=T-s+1}^T L(h, Z_t) - \sum_{t=1}^T q_t L(h, Z_t) \right\} \\ &= \sup_{h \in H} \left\{ \sum_{t=1}^T q_t \left(\frac{1}{s} \sum_{t=T-s+1}^T L(h, Z_t) - L(h, Z_t) \right) \right. \\ &\quad \left. + \sum_{t=1}^T \left(\frac{1}{T} - q_t \right) \frac{1}{s} \sum_{t=T-s+1}^T L(h, Z_t) \right\} \\ &\leq \sum_{t=1}^T q_t \sup_{h \in H} \left(\frac{1}{s} \sum_{t=T-s+1}^T L(h, Z_t) - q_t L(h, Z_t) \right) + M \|\mathbf{u} - \mathbf{q}\|_1.\end{aligned}$$

Computing Discrepancies

- Instantaneous discrepancy for kernel-based hypothesis with squared loss:

$$d_t = \sup_{\|\mathbf{w}'\| \leq \Lambda} \left(\sum_{s=1}^T u_s (\mathbf{w}' \cdot \Phi_K(x_s) - y_s)^2 - (\mathbf{w}' \cdot \Phi_K(x_t) - y_t)^2 \right).$$

- Difference of convex (DC) functions.
- Global optimum via DC-programming: (Tao and Ahn, 1998).

Discrepancy-Based Forecasting

- **Theorem:** for any $\delta > 0$, with probability at least $1 - \delta$, for all kernel-based hypothesis $h \in H$ and all $0 < \|\mathbf{q} - \mathbf{u}\|_1 \leq 1$

$$\begin{aligned} \mathcal{L}(h, \mathbf{Z}_1^T) &\leq \sum_{t=1}^T q_t L(h, Z_t) + \widehat{\Delta}(\mathbf{q}) + \Delta_s \\ &\quad + \tilde{O}\left(\log^{3/2} T \sup_x K(x, x) \Lambda + \|\mathbf{q} - \mathbf{u}\|_1\right). \end{aligned}$$

- Corresponding optimization problem:

$$\min_{\mathbf{q} \in [0,1]^T, \mathbf{w}} \left\{ \sum_{t=1}^T q_t (\mathbf{w} \cdot \Psi_K(x_t) - y_t)^2 + \lambda_1 \sum_{t=1}^T q_t d_t + \lambda_2 \|\mathbf{w}\|_{\mathbb{H}} + \lambda_3 \|\mathbf{q} - \mathbf{u}\|_1 \right\}.$$

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Discrepancy-Based Forecasting

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Convex Problem

- Change of variable: $r_t = 1/q_t$.
- Upper bound: $|r_t^{-1} - 1/T| \leq T^{-1}|r_t - T|$.

$$\min_{\mathbf{r} \in \mathcal{D}, \mathbf{w}} \left\{ \sum_{t=1}^T \frac{(\mathbf{w} \cdot \Psi_K(x_t) - y_t)^2 + \lambda_1 d_t}{r_t} + \lambda_2 \|\mathbf{w}\|_{\mathbb{H}} + \lambda_3 \sum_{t=1}^T |r_t - T| \right\}.$$

- where $\mathcal{D} = \{\mathbf{r} : r_t \geq 1\}$.
- convex optimization problem.

Two-Stage Algorithm

- Minimize empirical discrepancy $\hat{\Delta}(\mathbf{q})$ over \mathbf{q} (convex optimization).
- Solve (weighted) kernel-ridge regression problem:

$$\min_{\mathbf{w}} \left\{ \sum_{t=1}^T q_t^* (\mathbf{w} \cdot \Psi_K(x_t) - y_t)^2 + \lambda \|\mathbf{w}\|_{\mathbb{H}} \right\}$$

where q^* is the solution to discrepancy minimization problem.

Preliminary Experiments

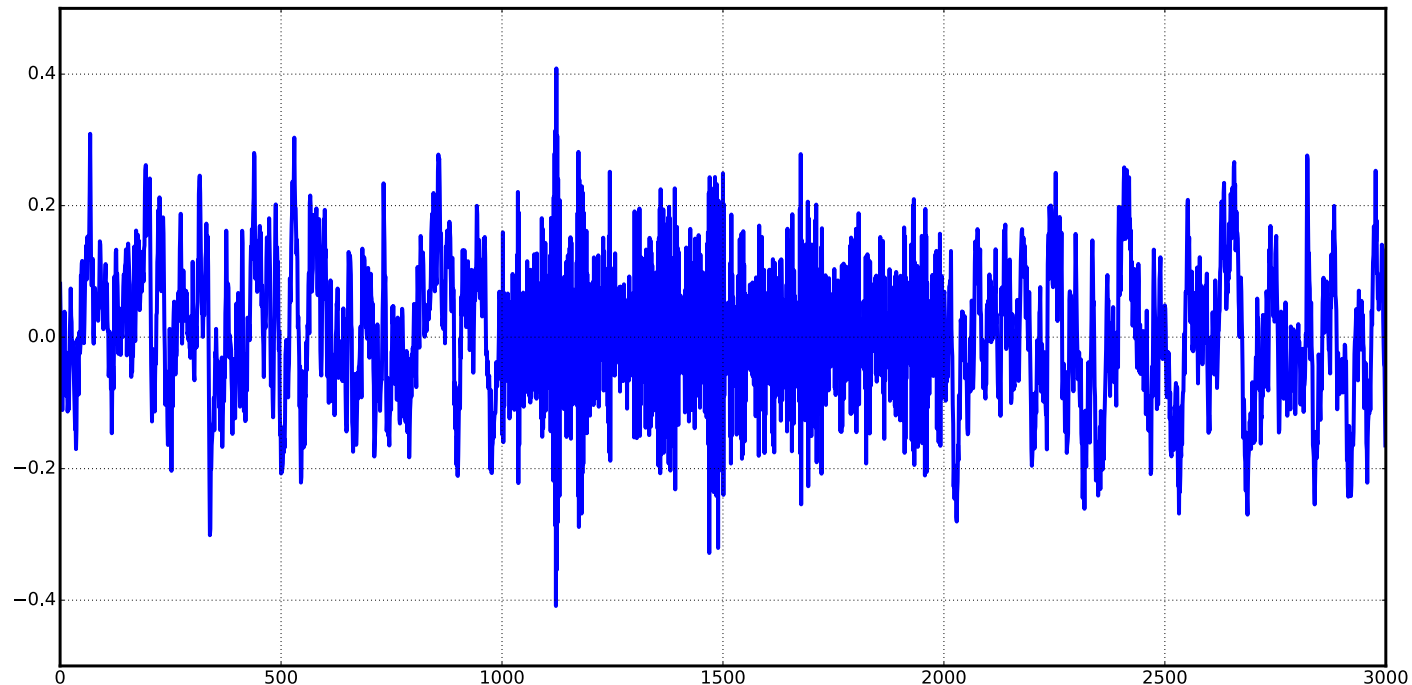
■ Artificial data sets:

ads1: $Y_t = \alpha_t Y_{t-1} + \epsilon_t$, $\alpha_t = -0.9$ if $t \in [1000, 2000]$ and 0.9 otherwise,

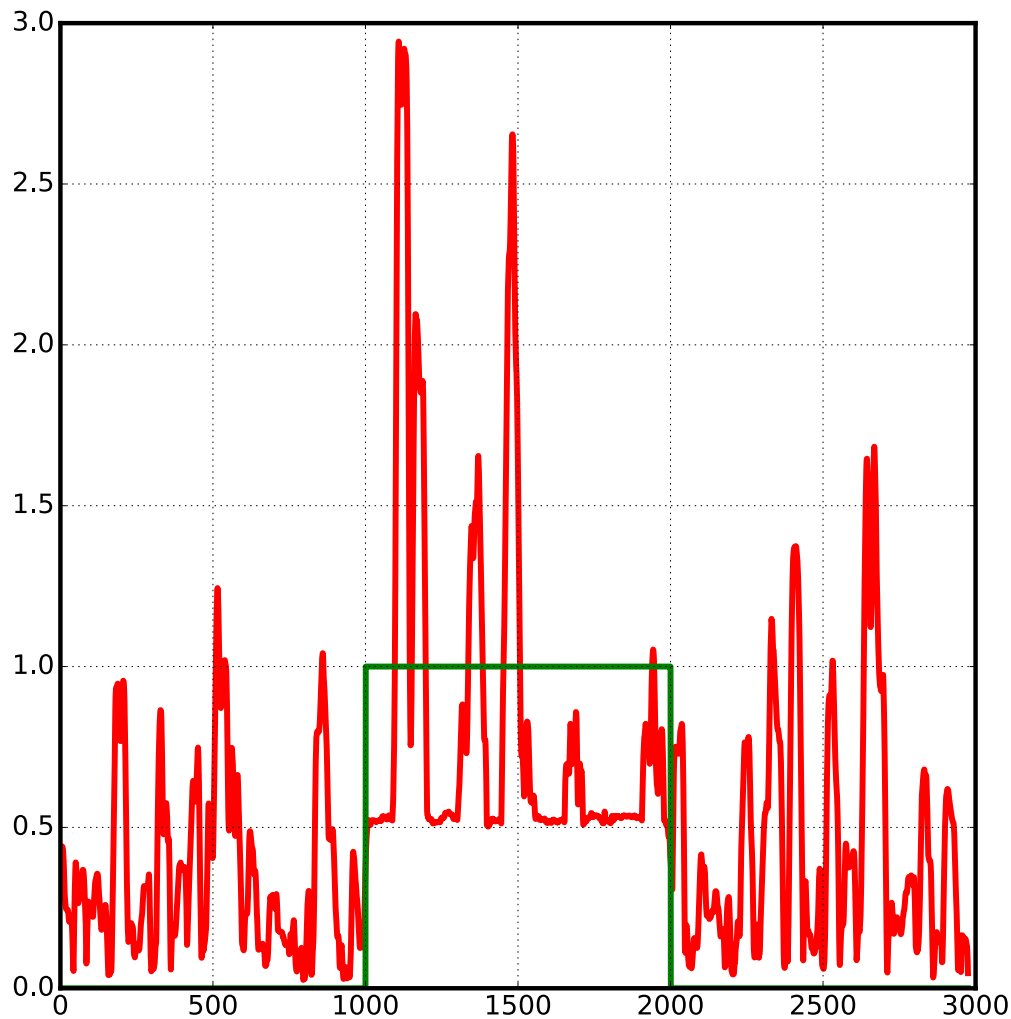
ads2: $Y_t = \alpha_t Y_{t-1} + \epsilon_t$, $\alpha_t = 1 - (t/1500)$,

ads3: $Y_t = \alpha_{i(t)} Y_{t-1} + \epsilon_t$, $\alpha_1 = -0.5$ and $\alpha_2 = 0.9$,

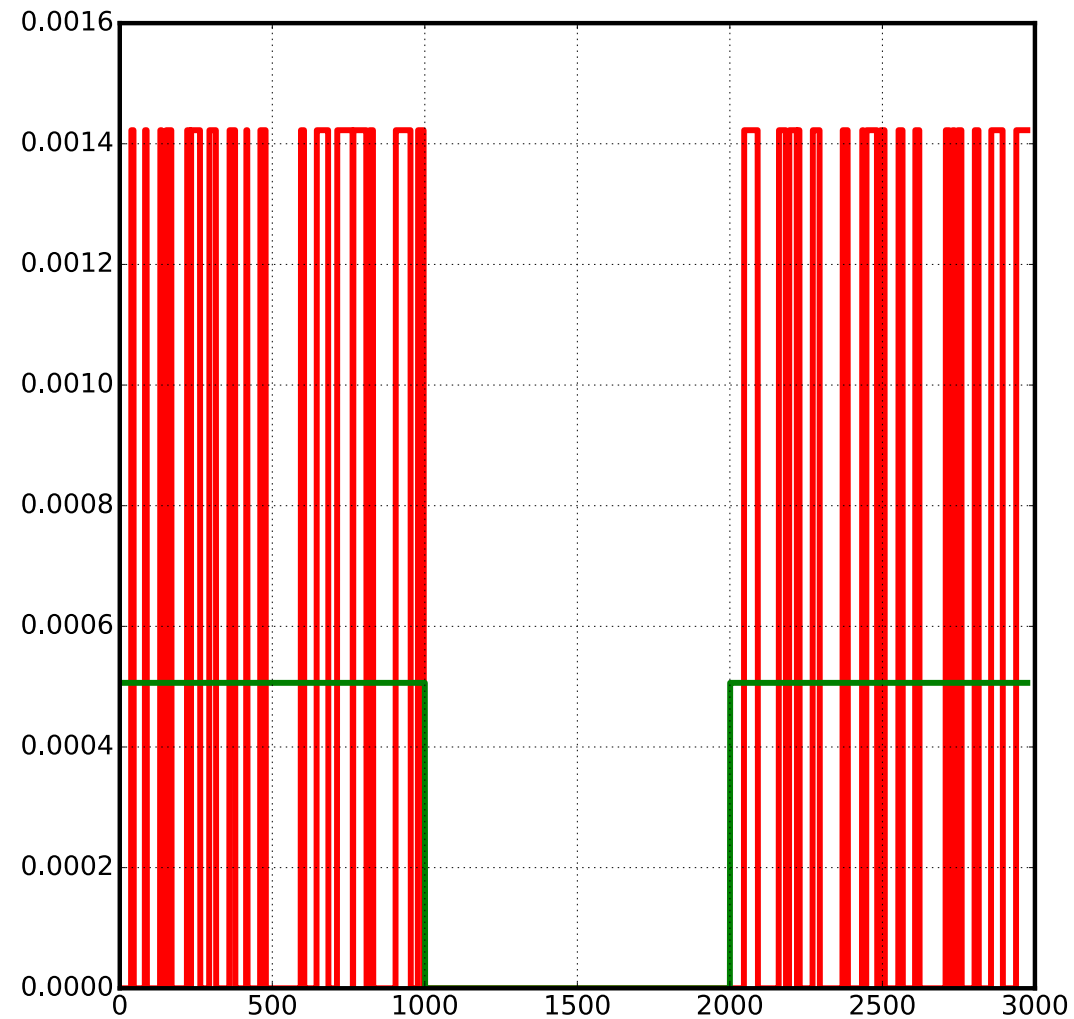
ads4: $Y_t = -0.5 Y_{t-1} + \epsilon_t$,



True vs. Empirical Discrepancies

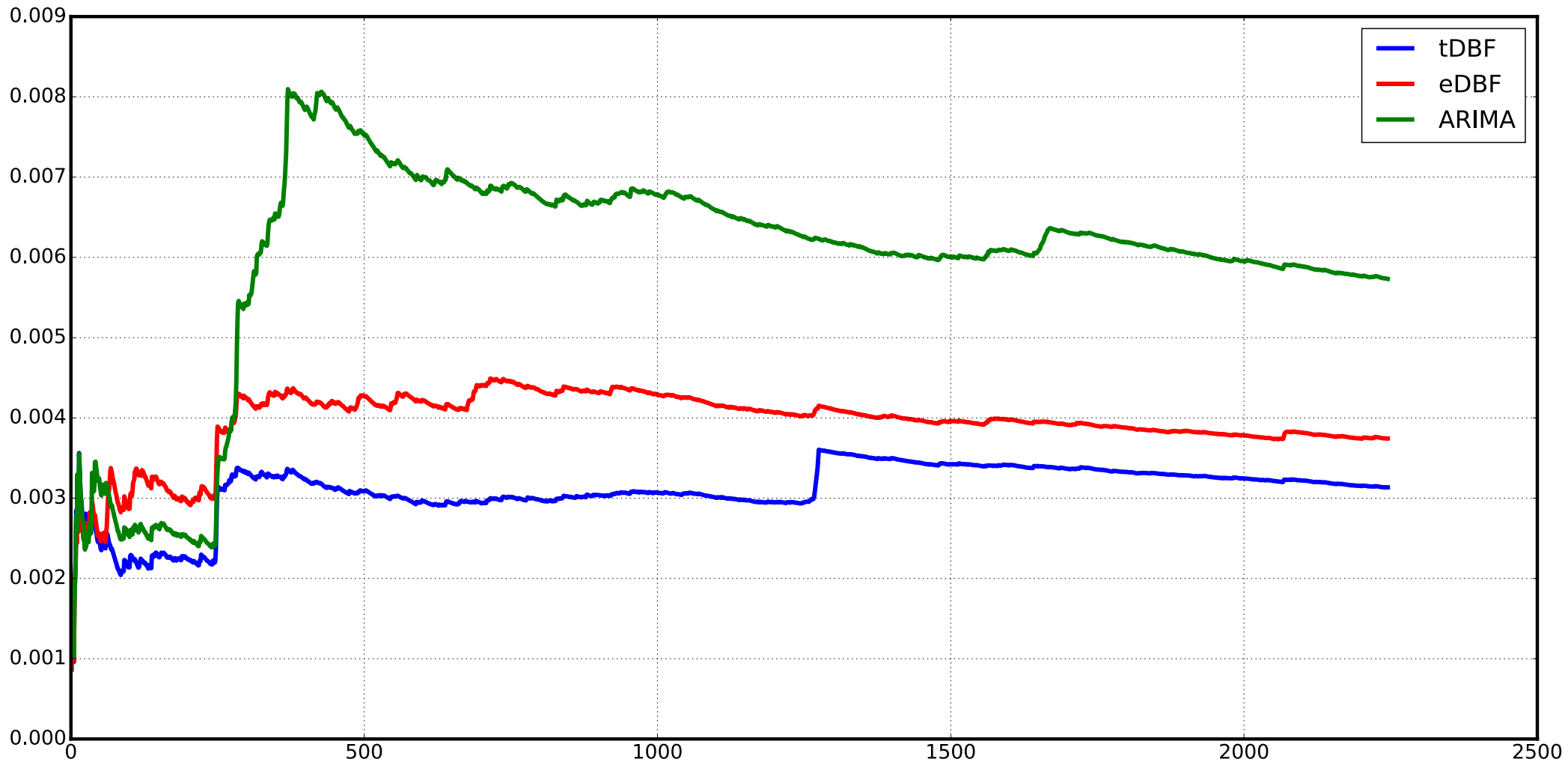


Discrepancies



Weights

Running MSE



Real-world Data

- Commodity prices, exchange rates, temperatures & climate.

Dataset	DBF	ARIMA
bitcoin	4.400×10^{-3} (26.500×10^{-3})	4.900×10^{-3} (29.990×10^{-3})
coffee	3.080×10^{-3} (6.570×10^{-3})	3.260×10^{-3} (6.390×10^{-3})
eur/jpy	7.100×10^{-5} (16.900×10^{-5})	7.800×10^{-5} (24.200×10^{-5})
jpy/usd	9.770×10^{-1} (25.893×10^{-1})	10.004×10^{-1} (27.531×10^{-1})
mso	32.876×10^0 (55.586×10^0)	32.193×10^0 (51.109×10^0)
silver	7.640×10^{-4} (46.65×10^{-4})	34.180×10^{-4} (158.090×10^{-4})
soy	5.071×10^{-2} (9.938×10^{-2})	5.003×10^{-2} (10.097×10^{-2})
temp	6.418×10^0 (9.958×10^0)	6.461×10^0 (10.324×10^0)

Time Series Prediction & On-line Learning

Two Learning Scenarios

■ Stochastic scenario:

- distributional assumption.
- performance measure: expected loss.
- guarantees: generalization bounds.

■ On-line scenario:

- no distributional assumption.
- performance measure: regret.
- guarantees: regret bounds.
- active research area: (Cesa-Bianchi and Lugosi, 2006; Anava et al. 2013, 2015, 2016; Bousquet and Warmuth, 2002; Herbster and Warmuth, 1998, 2001; Koolen et al., 2015).

On-Line Learning Setup

- Adversarial setting with hypothesis/action set H .
- For $t = 1$ to T do
 - player receives $x_t \in \mathcal{X}$.
 - player selects $h_t \in H$.
 - adversary selects $y_t \in \mathcal{Y}$.
 - player incurs loss $L(h_t(x_t), y_t)$.
- **Objective:** minimize (external) regret

$$\text{Reg}_T = \sum_{t=1}^T L(h_t(x_t), y_t) - \min_{h \in H^*} \sum_{t=1}^T L(h(x_t), y_t).$$

Example: Exp. Weights (EW)

- Expert set $H^* = \{\mathcal{E}_1, \dots, \mathcal{E}_N\}$, $H = \text{conv}(H^*)$.

EW($\{\mathcal{E}_1, \dots, \mathcal{E}_N\}$)

```
1  for  $i \leftarrow 1$  to  $N$  do
2       $w_{1,i} \leftarrow 1$ 
3  for  $t \leftarrow 1$  to  $T$  do
4      RECEIVE( $x_t$ )
5       $h_t \leftarrow \frac{\sum_{i=1}^N w_{t,i} \mathcal{E}_i}{\sum_{i=1}^N w_{t,i}}$ 
6      RECEIVE( $y_t$ )
7      INCUR-LOSS( $L(h_t(x_t), y_t)$ )
8      for  $i \leftarrow 1$  to  $N$  do
9           $w_{t+1,i} \leftarrow w_{t,i} e^{-\eta L(\mathcal{E}_i(x_t), y_t)}$     ▷ (parameter  $\eta > 0$ )
10 return  $h_T$ 
```

EW Guarantee

- **Theorem:** assume that L is convex in its first argument and takes values in $[0, 1]$. Then, for any $\eta > 0$ and any sequence $y_1, \dots, y_T \in \mathcal{Y}$, the regret of EW at time T satisfies

$$\text{Reg}_T \leq \frac{\log N}{\eta} + \frac{\eta T}{8}.$$

For $\eta = \sqrt{8 \log N / T}$,

$$\text{Reg}_T \leq \sqrt{(T/2) \log N}.$$

$$\frac{\text{Reg}_T}{T} = O\left(\sqrt{\frac{\log N}{T}}\right).$$

EW - Proof

■ **Potential:** $\Phi_t = \log \sum_{i=1}^N w_{t,i}$.

■ **Upper bound:**

$$\begin{aligned}\Phi_t - \Phi_{t-1} &= \log \frac{\sum_{i=1}^N w_{t-1,i} e^{-\eta L(\mathcal{E}_i(x_t), y_t)}}{\sum_{i=1}^N w_{t-1,i}} \\ &= \log \left(\mathbb{E}_{w_{t-1}} [e^{-\eta L(\mathcal{E}_i(x_t), y_t)}] \right) \\ &= \log \left(\mathbb{E}_{w_{t-1}} \left[\exp \left(-\eta \left(L(\mathcal{E}_i(x_t), y_t) - \mathbb{E}_{w_{t-1}} [L(\mathcal{E}_i(x_t), y_t)] \right) - \eta \mathbb{E}_{w_{t-1}} [L(\mathcal{E}_i(x_t), y_t)] \right) \right] \right) \\ &\leq -\eta \mathbb{E}_{w_{t-1}} [L(\mathcal{E}_i(x_t), y_t)] + \frac{\eta^2}{8} \quad (\text{Hoeffding's ineq.}) \\ &\leq -\eta L \left(\mathbb{E}_{w_{t-1}} [\mathcal{E}_i(x_t)], y_t \right) + \frac{\eta^2}{8} \quad (\text{convexity of first arg. of } L) \\ &= -\eta L(h_t(x_t), y_t) + \frac{\eta^2}{8}.\end{aligned}$$

EW - Proof

- Upper bound: summing up the inequalities yields

$$\Phi_T - \Phi_0 \leq -\eta \sum_{t=1}^T L(h_t(x_t), y_t) + \frac{\eta^2 T}{8}.$$

- Lower bound:

$$\begin{aligned} \Phi_T - \Phi_0 &= \log \sum_{i=1}^N e^{-\eta \sum_{t=1}^T L(\mathcal{E}_i(x_t), y_t)} - \log N \\ &\geq \log \max_{i=1}^N e^{-\eta \sum_{t=1}^T L(\mathcal{E}_i(x_t), y_t)} - \log N \\ &= -\eta \min_{i=1}^N \sum_{t=1}^T L(\mathcal{E}_i(x_t), y_t) - \log N. \end{aligned}$$

- Comparison:

$$\sum_{t=1}^T L(h_t(x_t), y_t) - \min_{i=1}^N \sum_{t=1}^T L(\mathcal{E}_i(x_t), y_t) \leq \frac{\log N}{\eta} + \frac{\eta T}{8}.$$

Questions

- Can we exploit both batch and on-line to
 - design flexible algorithms for time series prediction with stochastic guarantees?
 - tackle notoriously difficult time series problems e.g., model selection, learning ensembles?

Model Selection

- **Problem:** given N time series models, how should we use sample \mathbf{Z}_1^T to select a single best model?
 - in i.i.d. case, cross-validation can be shown to be close to the structural risk minimization solution.
 - but, how do we select a validation set for general stochastic processes?
 - use most recent data?
 - use the most distant data?
 - use various splits?
 - models may have been pre-trained on \mathbf{Z}_1^T .

Learning Ensembles

- **Problem:** given a hypothesis set H and a sample \mathbf{Z}_1^T , find accurate convex combination $h = \sum_{t=1}^T q_t h_t$ with $\mathbf{h} \in H_{\mathcal{A}}$ and $\mathbf{q} \in \Delta$.
- in most general case, hypotheses may have been pre-trained on \mathbf{Z}_1^T .
- ➔ on-line-to-batch conversion for general non-stationary non-mixing processes.

On-Line-to-Batch (OTB)

- **Input:** sequence of hypotheses $\mathbf{h} = (h_1, \dots, h_T)$ returned after T rounds by an on-line algorithm \mathcal{A} minimizing general regret

$$\text{Reg}_T = \sum_{t=1}^T L(h_t, Z_t) - \inf_{\mathbf{h}^* \in \mathbf{H}^*} \sum_{t=1}^T L(\mathbf{h}^*, Z_t).$$

On-Line-to-Batch (OTB)

- **Problem:** use $\mathbf{h} = (h_1, \dots, h_T)$ to derive a hypothesis $h \in H$ with small path-dependent expected loss,

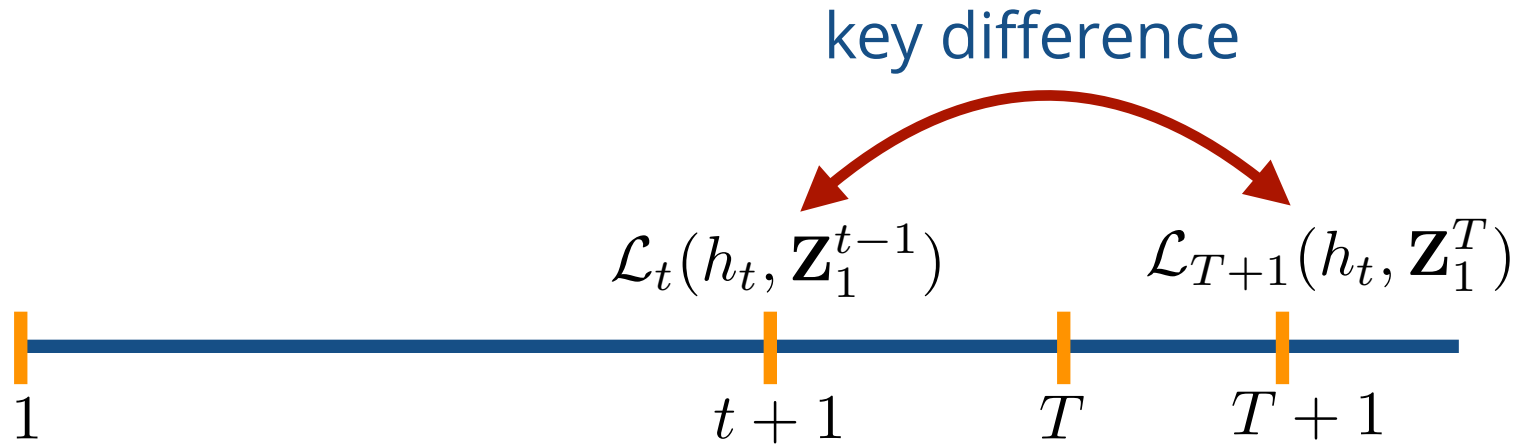
$$\mathcal{L}_{T+1}(h, \mathbf{Z}_1^T) = \mathbb{E}_{Z_{T+1}} [L(h, Z_{T+1}) | \mathbf{Z}_1^T].$$

- i.i.d. problem is standard: (Littlestone, 1989), (Cesa-Bianchi et al., 2004).
- but, how do we design solutions for the general time-series scenario?

Questions

- Is OTB with general (non-stationary, non-mixing) stochastic processes possible?
- Can we design algorithms with theoretical guarantees?
→ need a new tool for the analysis.

Relevant Quantity



→ Average difference: $\frac{1}{T} \sum_{t=1}^T \left[\mathcal{L}_{T+1}(h_t, \mathbf{Z}_1^T) - \mathcal{L}_t(h_t, \mathbf{Z}_1^{t-1}) \right].$

On-line Discrepancy

■ Definition:

$$\text{disc}(\mathbf{q}) = \sup_{\mathbf{h} \in \mathbf{H}_{\mathcal{A}}} \left| \sum_{t=1}^T q_t \left[\mathcal{L}_{T+1}(h_t, \mathbf{Z}_1^T) - \mathcal{L}_t(h_t, \mathbf{Z}_1^{t-1}) \right] \right|.$$

- $\mathbf{H}_{\mathcal{A}}$: sequences that \mathcal{A} can return.
- $\mathbf{q} = (q_1, \dots, q_T)$: arbitrary weight vector.
- natural measure of non-stationarity or dependency.
- captures hypothesis set and loss function.
- can be efficiently estimated under mild assumptions.
- generalization of definition of [\(Kuznetsov and MM, 2015\)](#).

Discrepancy Estimation

- Batch discrepancy estimation method.
- Alternative method:
 - assume that the loss is μ -Lipschitz.
 - assume that there exists an accurate hypothesis h^* :

$$\eta = \inf_{h^*} \mathbb{E} \left[L(Z_{T+1}, h^*(X_{T+1})) | \mathbf{Z}_1^T \right] \ll 1.$$

Discrepancy Estimation

- **Lemma:** fix sequence \mathbf{Z}_1^T in \mathcal{Z} . Then, for any $\delta > 0$, with probability at least $1 - \delta$, the following holds for all $\alpha > 0$:

$$\text{disc}(\mathbf{q}) \leq \widehat{\text{disc}}_{H^T}(\mathbf{q}) + \mu\eta + 2\alpha + M\|\mathbf{q}\|_2 \sqrt{2 \log \frac{\mathbb{E}[\mathcal{N}_1(\alpha, \mathcal{G}, \mathbf{z})]}{\delta}},$$

where

$$\widehat{\text{disc}}_H(\mathbf{q}) = \sup_{h \in H, \mathbf{h} \in H_{\mathcal{A}}} \left| \sum_{t=1}^T q_t \left[L(h_t(X_{T+1}), h(X_{T+1})) - L(h_t, Z_t) \right] \right|.$$

Proof Sketch

$$\begin{aligned}
 \text{disc}(\mathbf{q}) &= \sup_{\mathbf{h} \in \mathbf{H}_{\mathcal{A}}} \left| \sum_{t=1}^T q_t \left[\mathcal{L}_{T+1}(h_t, \mathbf{Z}_1^T) - \mathcal{L}_t(h_t, \mathbf{Z}_1^{t-1}) \right] \right| \\
 &\leq \sup_{\mathbf{h} \in \mathbf{H}_{\mathcal{A}}} \left| \sum_{t=1}^T q_t \left[\mathcal{L}_{T+1}(h_t, \mathbf{Z}_1^T) - \mathbb{E} \left[L(h_t(X_{T+1}), h^*(X_{T+1})) \mid \mathbf{Z}_1^T \right] \right] \right| \\
 &\quad + \sup_{\mathbf{h} \in \mathbf{H}_{\mathcal{A}}} \left| \sum_{t=1}^T q_t \left[\mathbb{E} \left[L(h_t(X_{T+1}), h^*(X_{T+1})) \mid \mathbf{Z}_1^T \right] - \mathcal{L}_t(h_t, \mathbf{Z}_1^{t-1}) \right] \right| \\
 &\leq \mu \sup_{\mathbf{h} \in H_{\mathcal{A}}} \sum_{t=1}^T q_t \mathbb{E} \left[L(h^*(X_{T+1}), Y_{T+1}) \mid \mathbf{Z}_1^T \right] \\
 &\quad + \sup_{\mathbf{h} \in \mathbf{H}_{\mathcal{A}}} \left| \sum_{t=1}^T q_t \left[\mathbb{E} \left[L(h_t(X_{T+1}), h^*(X_{T+1})) \mid \mathbf{Z}_1^T \right] - \mathcal{L}_t(h_t, \mathbf{Z}_1^{t-1}) \right] \right| \\
 &= \mu \sup_{\mathbf{h} \in H_{\mathcal{A}}} \mathbb{E} \left[L(h^*(X_{T+1}), Y_{T+1}) \mid \mathbf{Z}_1^T \right] \\
 &\quad + \sup_{\mathbf{h} \in \mathbf{H}_{\mathcal{A}}} \left| \sum_{t=1}^T q_t \left[\mathbb{E} \left[L(h_t(X_{T+1}), h^*(X_{T+1})) \mid \mathbf{Z}_1^T \right] - \mathcal{L}_t(h_t, \mathbf{Z}_1^{t-1}) \right] \right|.
 \end{aligned}$$

Learning Guarantee

- **Lemma:** let L be a convex loss bounded by M and \mathbf{h}_1^T a hypothesis sequence adapted to \mathbf{Z}_1^T . Fix $\mathbf{q} \in \Delta$. Then, for any $\delta > 0$, the following holds with probability at least $1 - \delta$ for the hypothesis $h = \sum_{t=1}^T q_t h_t$:

$$\mathcal{L}_{T+1}(h, \mathbf{Z}_1^T) \leq \sum_{t=1}^T q_t L(h_t, Z_t) + \text{disc}(\mathbf{q}) + M \|\mathbf{q}\|_2 \sqrt{2 \log \frac{1}{\delta}}.$$

Proof

- By definition of the on-line discrepancy,

$$\sum_{t=1}^T q_t \left[\mathcal{L}_{T+1}(h_t, \mathbf{Z}_1^T) - \mathcal{L}_t(h_t, \mathbf{Z}_1^{t-1}) \right] \leq \text{disc}(\mathbf{q}).$$

- $A_t = q_t \left[\mathcal{L}_t(h_t, \mathbf{Z}_1^{t-1}) - L(h_t, Z_t) \right]$ is a martingale difference, thus by Azuma's inequality, whp,

$$\sum_{t=1}^T q_t \mathcal{L}_t(h_t, \mathbf{Z}_1^{t-1}) \leq \sum_{t=1}^T q_t L(h_t, Z_t) + \|\mathbf{q}\|_2 \sqrt{2 \log \frac{1}{\delta}}.$$

- By convexity of the loss:

$$\mathcal{L}_{T+1}(h, \mathbf{Z}_1^T) \leq \sum_{t=1}^T q_t \mathcal{L}_{T+1}(h_t, \mathbf{Z}_1^T).$$

Learning Guarantee

- **Theorem:** let L be a convex loss bounded by M and \mathbf{H}^* a set of hypothesis sequences adapted to \mathbf{Z}_1^T . Fix $\mathbf{q} \in \Delta$. Then, for any $\delta > 0$, the following holds with probability at least $1 - \delta$ for the hypothesis $h = \sum_{t=1}^T q_t h_t$:

$$\begin{aligned} & \mathcal{L}_{T+1}(h, \mathbf{Z}_1^T) \\ & \leq \inf_{\mathbf{h}^* \in H} \sum_{t=1}^T \mathcal{L}_{T+1}(h^*, \mathbf{Z}_1^T) + 2\text{disc}(\mathbf{q}) + \frac{\text{Reg}_T}{T} \\ & \quad + M\|\mathbf{q} - \mathbf{u}\|_1 + 2M\|\mathbf{q}\|_2 \sqrt{2 \log \frac{2}{\delta}}. \end{aligned}$$

Conclusion

- Time series forecasting:
 - key learning problem in many important tasks.
 - very challenging: theory, algorithms, applications.
 - new and general data-dependent learning guarantees for non-mixing non-stationary processes.
 - algorithms with guarantees.
- Time series prediction and on-line learning:
 - proof for flexible solutions derived via OTB.
 - application to model selection.
 - application to learning ensembles.

Time Series Workshop

**Join us in Room 117
Friday, December 9th.**

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β -Mixing

- **Definition:** a sequence of random variables $\mathbf{Z} = \{Z_t\}_{-\infty}^{+\infty}$ is β -mixing if

$$\beta(k) = \sup_n \mathbb{E} \left[\sup_{B \in \sigma_{-\infty}^n} \left[\sup_{A \in \sigma_{n+k}^{\infty}} \left| \mathbb{P}[A | B] - \mathbb{P}[A] \right| \right] \right] \rightarrow 0.$$

dependence between events decaying with k .

