PAC-Bayesian Bound for Gaussian Process Regression and Multiple Kernel Additive Model

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Taiji Suzuki: PAC-Bayesian Bound for Gaussian Process Regression and Multiple Kernel Additive Model.
Conference on Learning Theory (COLT2012), *JMLR Workshop and Conference Proceedings 23*, pp. 8.1 – 8.20, 2012.

Taiji Suzuki, and Masashi Sugiyama: Fast learning rate of multiple kernel learning: trade-off between sparsity and smoothness.
The Annals of Statistics, vol. 41, number 3, pp. 1381-1405, 2013.

Taiji Suzuki: Unifying Framework for Fast Learning Rate of Non-Sparse Multiple Kernel Learning.
Advances in Neural Information Processing Systems 24 (NIPS2011). pp.1575–1583.

Outline

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Sparse estimation [Lasso]

Design matrix $X = (X_{ij}) \in \mathbb{R}^{n \times p}$. p (dimension) $\gg n$ (# of samples).
True coefficients $\beta^* \in \mathbb{R}^p$: only $d(< p)$ elements are non-zeros (d-sparse).

$$\text{Model}: \quad Y = X\beta^* + \boldsymbol{\xi}.$$

$$\hat{\beta} \leftarrow \underset{\beta \in \mathbb{R}^p}{\arg\min} \frac{1}{n} \|X\beta - Y\|_2^2 + \lambda_n \|\beta\|_1.$$

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Theorem (Lasso's convergence rate (Bickel et al., 2009; Zhang, 2009))

If the design matrix satisfies "Restricted eigenvalue condition", $\max_{i,j} |X_{ij}| \leq 1$, and the noise satisfy $\mathrm{E}[e^{\tau \xi_i}] \leq e^{\sigma^2 \tau^2 / 2}$ $(\forall \tau > 0)$, then we have, with probability $1 - \delta$,

$$\|\hat{\beta} - \beta^*\|_2^2 \leq C \frac{d \log(p/\delta)}{n}.$$

- p's effect is just $\log(p)$, the effective dimension d is dominant .

Restricted eigenvalue condition (Bickel et al., 2009; Zha g, 2009)

$$\phi_b(I) := \sup \left\{ \phi \geq 0 \mid \phi \leq \frac{\beta^\top X^\top X \beta / n}{\sum_{j \in I} \beta_j^2}, \right.$$
$$\left. \forall \beta \in \mathbb{R}^p \text{ such that } b \sum_{j \in I} |\beta_j| \geq \sum_{j \notin I} |\beta_j| \right\}.$$

Restricted Eigenvalue Condition

There exists a constant $0 < C$ such that

$$0 < C < \min_{I : I_0 \subset I, |I| \leq 2d} \phi_3(I).$$

Motivation: Is there any estimator which does not require this condition to achieve a similar convergence rate?
$\rightarrow$ Bayesian estimator

Goal of this talk

- Change the risk criterion:

$$\|\hat{\beta} - \beta\|_2^2 \quad \longrightarrow \quad \frac{1}{n}\|X(\hat{\beta} - \beta^*)\|_2^2$$

- We generalize the model to non-parametric (sparse) additive model:

$$f(x) = \sum_{j=1}^{p} x_j \beta_j \quad \longrightarrow \quad f(x) = \sum_{m=1}^{M} f_m(x^{(m)})$$

- Finally, we will derive a risk bound of Bayesian sparse estimator:

$$\|\hat{f} - f^*\|_n^2 \leq ?$$

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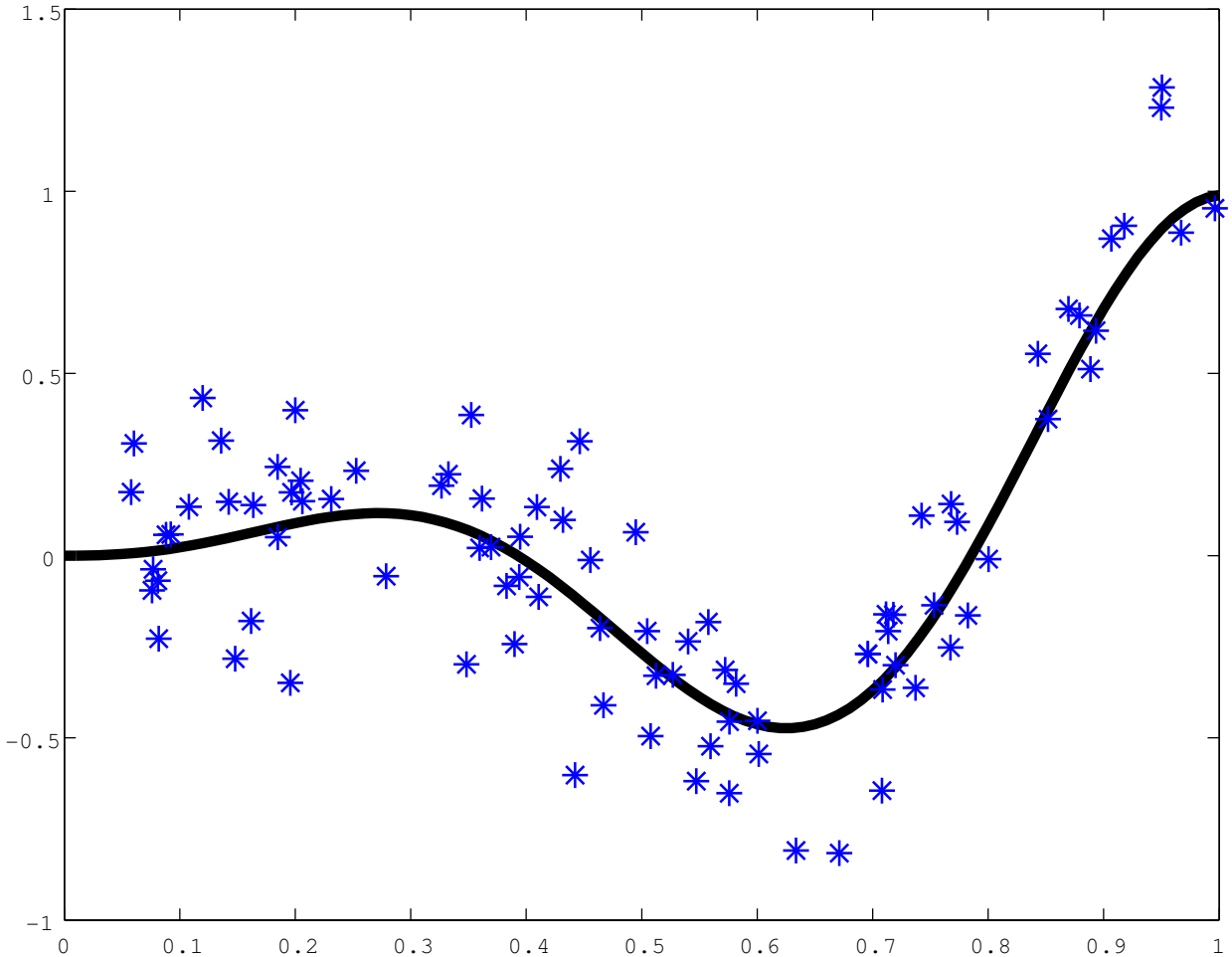
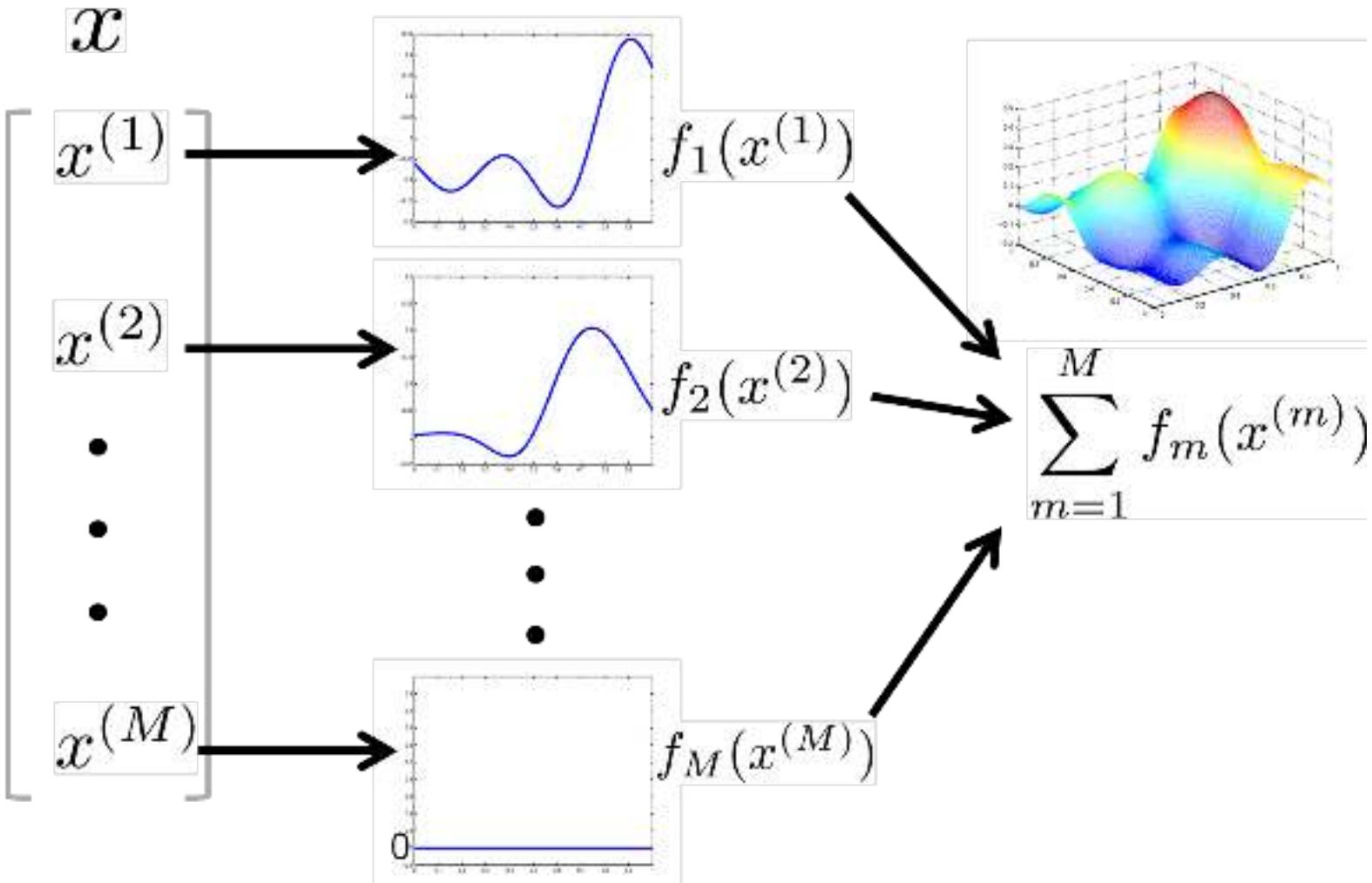
- Finally, we will derive a risk bound of Bayesian sparse estimator:

$$\|\hat{f} - f^*\|_n^2 \leq \sum_{m \in I_0} n^{-\frac{1}{1+s_m}} + \frac{d \log(p/d)}{n}$$

Non-parametric Regression



Sparse Additive Model



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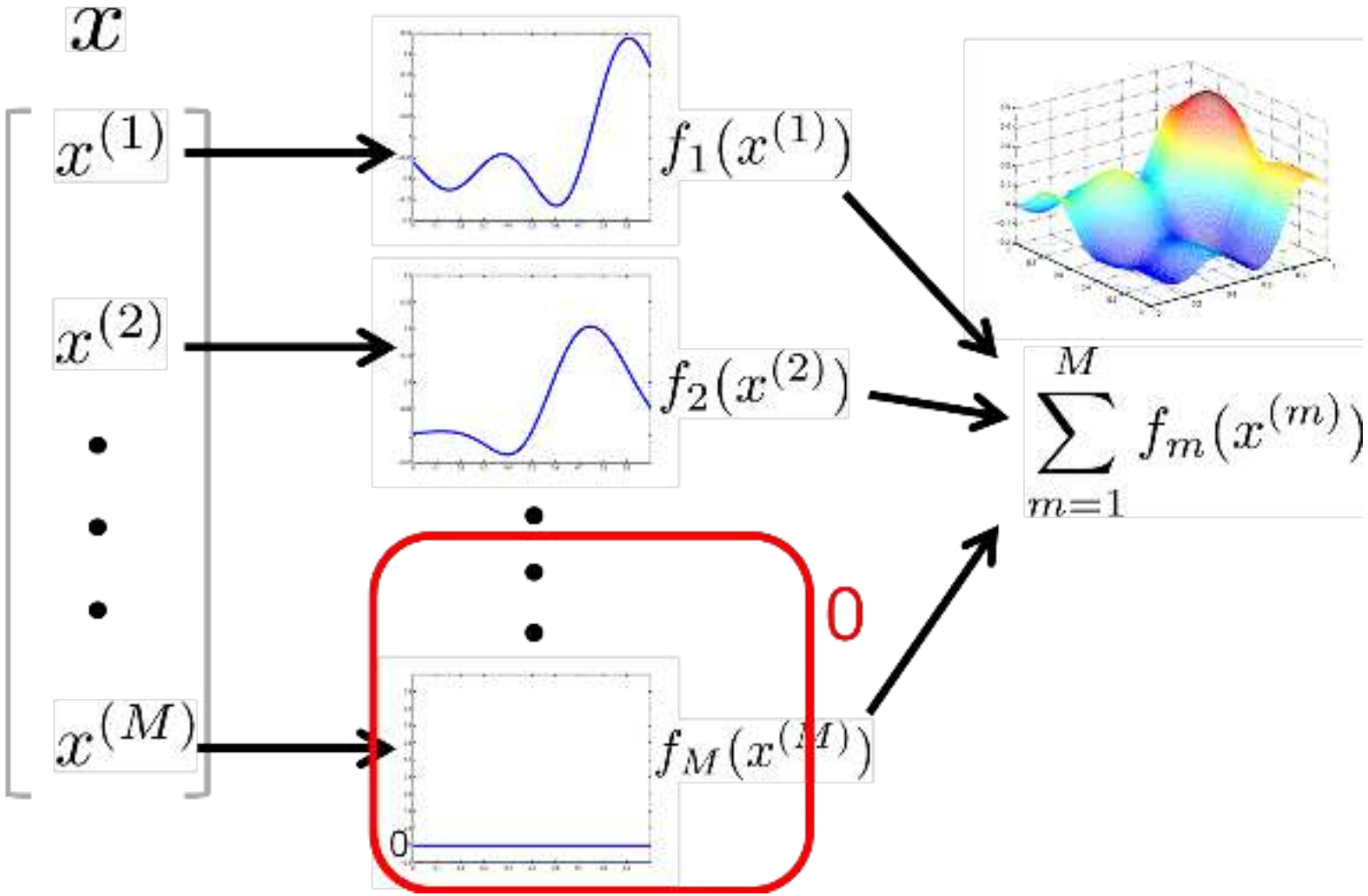

Problem Setting

$$y_i = f^{\mathrm{o}}(x_i) + \xi_i, \quad (i = 1, \ldots, n),$$

where f^{o} is the true function such that $\mathrm{E}[Y|X] = f^{\mathrm{o}}(X)$.

f^{o} is well approximated by a function f^* with a sparse representation:

$$f^{\mathrm{o}}(x) \simeq f^*(x) = \sum_{m=1}^{M} f_m^*(x^{(m)}),$$

where only a few components of $\{f_m^*\}_{m=1}^M$ are non-zero.

Outline

Multiple Kernel Learning

$$\min_{f_m \in \mathcal{H}_m} \quad \frac{1}{n} \sum_{i=1}^{n} \left(y_i - \sum_{m=1}^{M} f_m(x_i^{(m)}) \right)^2 + C \sum_{m=1}^{M} \|f_m\|_{\mathcal{H}_m}$$

($\mathcal{H}_m$: Reproducing Kernel Hilbert Space (RKHS), explained later)

- Extension of Group Lasso: each group is infinite dimensional
- Sparse solution
- Reduced to finite dimensional optimization problem by the representer theorem (Sonnenburg et al., 2006; Rakotomamonjy et al., 2008; Suzuki & Tomioka, 2009)

Various types of regularization

- L_1-MKL (Lanckriet et al., 2004; Bach et al., 2004) : **Sparse**

$$\min_{f_m \in \mathcal{H}_m} \quad L\left(\sum_{m=1}^{M} f_m\right) + C \sum_{m=1}^{M} \|f_m\|_{\mathcal{H}_m}$$

- L_2-MKL : **Dense**

$$\min_{f_m \in \mathcal{H}_m} \quad L\left(\sum_{m=1}^{M} f_m\right) + C \sum_{m=1}^{M} \|f_m\|_{\mathcal{H}_m}^2$$

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$$\min_{f_m \in \mathcal{H}_m} \quad L\left(\sum_{m=1}^{M} f_m\right) + C \sum_{m=1}^{M} \|f_m\|_{\mathcal{H}_m}^2$$

- Elasticnet-MKL (Tomioka & Suzuki, 2009)

$$\min_{f_m \in \mathcal{H}_m} \quad L\left(\sum_{m=1}^{M} f_m\right) + C_1 \sum_{m=1}^{M} \|f_m\|_{\mathcal{H}_m} + C_2 \sum_{m=1}^{M} \|f_m\|_{\mathcal{H}_m}^2$$

- ℓ_p-MKL (Kloft et al., 2009)

$$\min_{f_m \in \mathcal{H}_m} \quad L\left(\sum_{m=1}^{M} f_m\right) + C_1 \left(\sum_{m=1}^{M} \|f_m\|_{\mathcal{H}_m}^p\right)^{\frac{2}{p}}$$

Sparsity VS accuracy

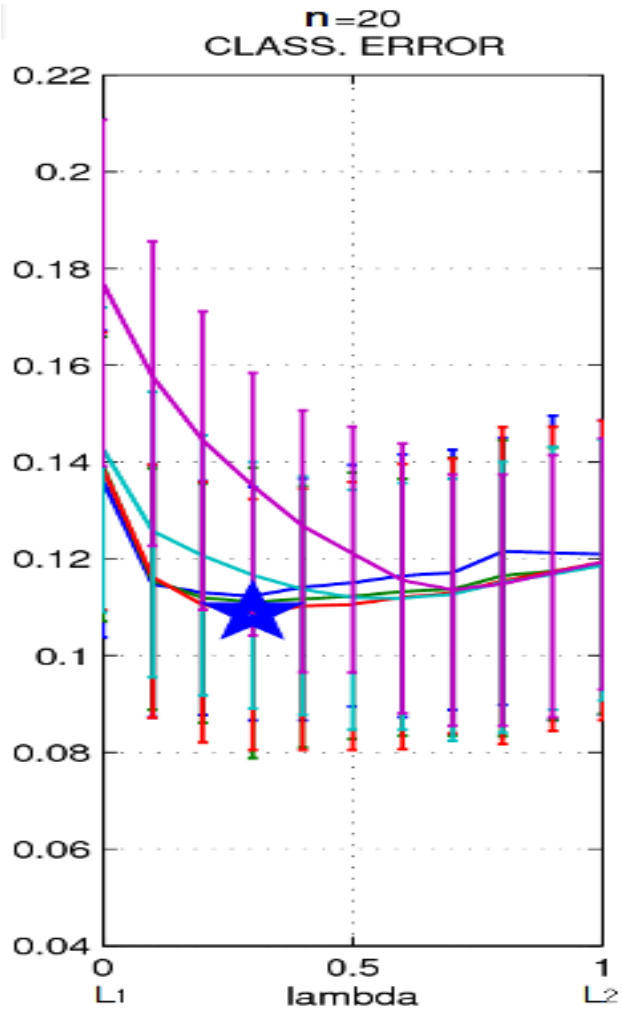


Figure: Relation between accuracy and sparsity of Elasticnet-MKL for caltech 101

Sparsity VS accuracy

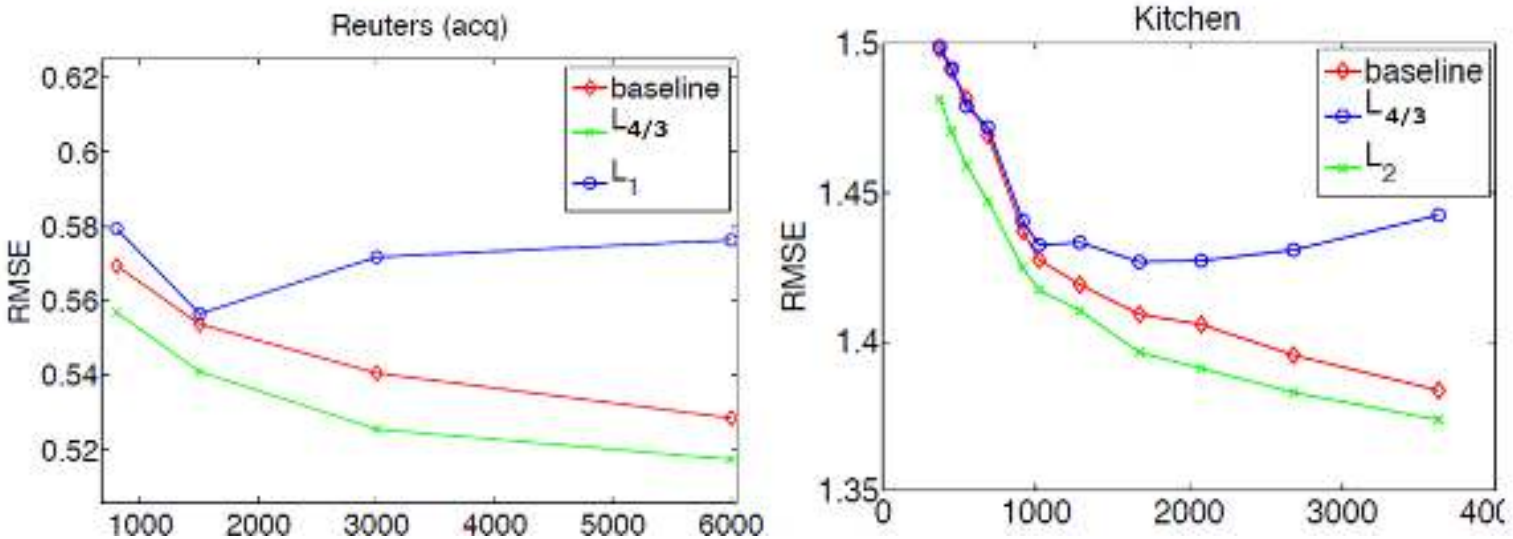


Figure: Relation between accuracy and sparsity of ℓ_p-MKL (Cortes et al., 2009)

Convergence rate of MKL

Suzuki (2011) gave a unifying framework to derive convergence rates of various types of regularizations.
Examples:

- ℓ_p-MKL: $\|f\|_\psi = (\sum_{m=1}^M \|f_m\|_{\mathcal{H}_m}^p)^{\frac{1}{p}}$

$$\|\hat{f} - f^*\|_{L_2(\Pi)}^2 = \mathcal{O}_p\left(n^{-\frac{1}{1+s}} M^{1-\frac{2s}{p(1+s)}} R_p^{\frac{2s}{1+s}} + \frac{M\log(M)}{n}\right)$$

- Elasticnet-MKL:
  $\|f\|_\psi = \lambda \sum_{m=1}^M \|f_m\|_{\mathcal{H}_m} + (1-\lambda)(\sum_{m=1}^M \|f_m\|_{\mathcal{H}_m}^2)^{\frac{1}{2}}$

$$\|\hat{f} - f^*\|_{L_2(\Pi)}^2 = \mathcal{O}_p\left(n^{-\frac{1}{1+s}} \frac{M^{1-\frac{s}{1+s}}}{(1-\lambda+\lambda\sqrt{M})^{\frac{2s}{1+s}}} [\lambda\|f^*\|_{\ell_1} + (1-\lambda)\|f^*\|_{\ell_2}]^{\frac{2s}{1+s}} + \frac{M\log(M)}{n}\right)$$

- VSKL: $\|f\|_\psi = \|f\|_{(p,q)} = \left[\sum_{j=1}^{M'} \left(\sum_{k=1}^{M_j} \|f_{j,k}\|_{\mathcal{H}_{j,k}}^p\right)^{\frac{q}{p}}\right]^{\frac{1}{q}}$.

$$\|\hat{f} - f^*\|_{L_2(\Pi)}^2 = \mathcal{O}_p\left(\frac{\left(\sum_{j=1}^{M'} M_j\right)^{\frac{1-s}{1+s}}}{n^{\frac{1}{1+s}}} \left\{\left(\sum_{j=1}^{M'} M_j^{\frac{q^*}{p^*}}\right)^{\frac{1}{q^*}} \left[\sum_{j=1}^{M'} \left(\sum_{k=1}^{M_j} \|f_{j,k}^*\|_{\mathcal{H}_{j,k}}^p\right)^{\frac{q}{p}}\right]^{\frac{1}{q}}\right\}^{\frac{2s}{1+s}} + \frac{M\log(M)}{n}\right)$$

Convergence rate L_1 and elastic-net MKL

$$\min_{f_m \in \mathcal{H}_m} \quad L\left(\sum_{m=1}^{M} f_m\right) + \sum_{m=1}^{M} (\lambda_1^{(n)} \|f_m\|_n + \lambda_2^{(n)} \|f_m\|_{\mathcal{H}_m} + \lambda_3^{(n)} \|f_m\|_{\mathcal{H}_m}^2).$$

Theorem (Convergence rate of Mixed-Norm-Elasticnet-MKL (Suzuki & Sugiyama, 2013))

Under the conditions stated above, for sufficiently large n, for appropriately chosen $\lambda_1^{(n)}$, $\lambda_2^{(n)}$, $\lambda_3^{(n)}$, we have

$$\text{(L1)} \qquad \|\hat{f} - f^*\|_{L_2(\Pi)}^2 \leq C' \left(d^{\frac{1-s}{1+s}} n^{-\frac{1}{1+s}} R_{1,f^*}^{\frac{2s}{1+s}} + \frac{d \log(M)}{n} \right) \eta(t)^2,$$

$$\text{(Elastic)} \quad \|\hat{f} - f^*\|_{L_2(\Pi)}^2 \leq C' \left(d^{\frac{1+q}{1+q+s}} n^{-\frac{1+q}{1+q+s}} R_{2,g^*}^{\frac{2s}{1+q+s}} + \frac{d \log(M)}{n} \right) \eta(t)^2,$$

with probability $1 - e^{-t} - e^{-\zeta_n}$ $(\forall t \geq 1)$.

$\eta(t) := \max(\sqrt{t}, t/\sqrt{n})$ and, R_{1,f^*}, R_{2,g^*} are defined as

$$R_{1,f^*} := \sum_{m=1}^{M} \|f_m^*\|_{\mathcal{H}_m}, \quad R_{2,g^*} := \left(\sum_{m=1}^{M} \|g_m^*\|_{\mathcal{H}_m}^2 \right)^{\frac{1}{2}}.$$

(Generalized) Restricted Eigenvalue Condition

To prove a fast convergence rate of MKL, we utilize the following (generalized) *Restricted Eigenvalue Condition* (Bickel et al., 2009; Koltchinskii & Yuan, 2010; Suzuki, 2011; Suzuki & Sugiyama, 2012).

Restricted Eigenvalue Condition

There exists a constant $0 < C$ such that

$$0 < C < \beta_{\sqrt{d}}(I_0).$$

$$\beta_b(I) := \sup \left\{ \beta \geq 0 \mid \beta \leq \frac{\| \sum_{m=1}^M f_m \|_{L_2(\Pi)}^2}{\sum_{m \in I} \| f_m \|_{L_2(\Pi)}^2}, \right.$$
$$\left. \forall f \text{ such that } b \sum_{m \in I} \| f_m \|_{L_2(\Pi)} \geq \sum_{m \notin I} \| f_m \|_{L_2(\Pi)} \right\}.$$

f_ms are not totally correlated inside I_0 and between I_0 and I_0^c.

We investigate a Bayesian variant of MKL.

We show a fast learning rate of it **without** conditions on the design such as the restricted eigenvalue condition.

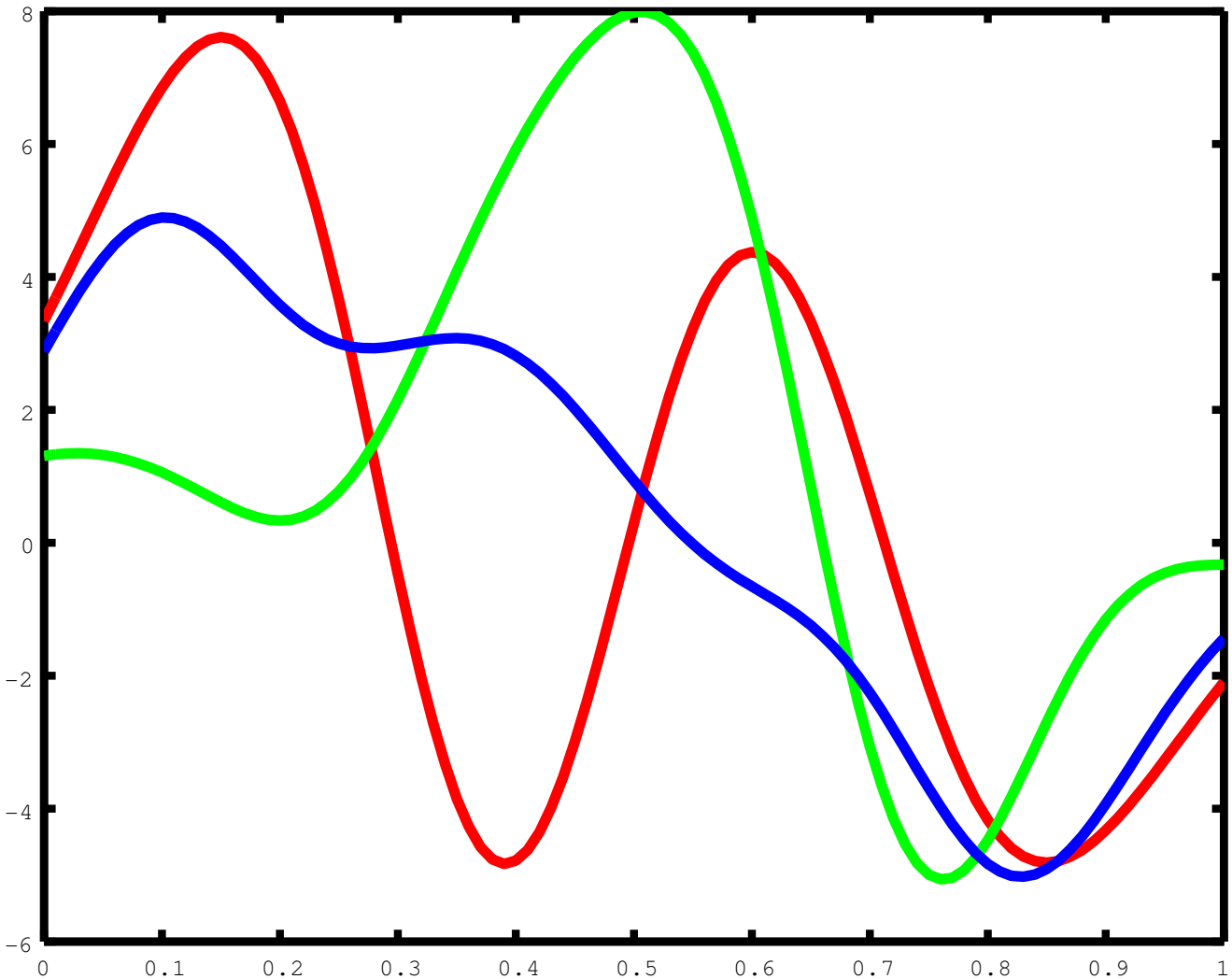
Outline

Our proposal = sparse aggregated estimation + Gaussian process

- Aggregated Estimator, Exponential Screening, Model Averaging (Leung & Barron, 2006; Rigollet & Tsybakov, 2011)
- Gaussian Process Regression (Rasmussen & Williams, 2006; van der Vaart & van Zanten, 2008a; van der Vaart & van Zanten, 2008b; van der Vaart & van Zanten, 2011)

Gaussian Process Regression

Gaussian Process Regression



Gaussian Process Regression

Gaussian process prior: a prior on a functions $f = (f(x) : x \in \mathcal{X})$.

$$f \sim \mathrm{GP}$$

means that each finite subset $(f(x_1), f(x_2), \ldots, f(x_j))$ $(j = 1, 2, \ldots)$ obeys a zero-mean multivariate normal distribution.
We assume that $\sup_x |f(x)| < \infty$ and $f : \Omega \to \ell_\infty(\mathcal{X})$ is tight and Borel measurable.

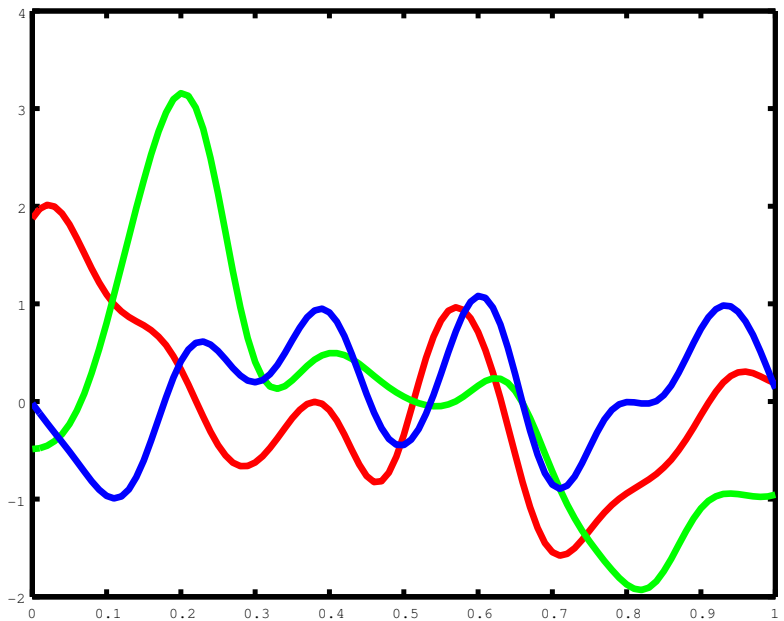
Kernel function:

$$k(x, x') := \mathrm{E}_{f \sim GP}[f(x)f(x')].$$

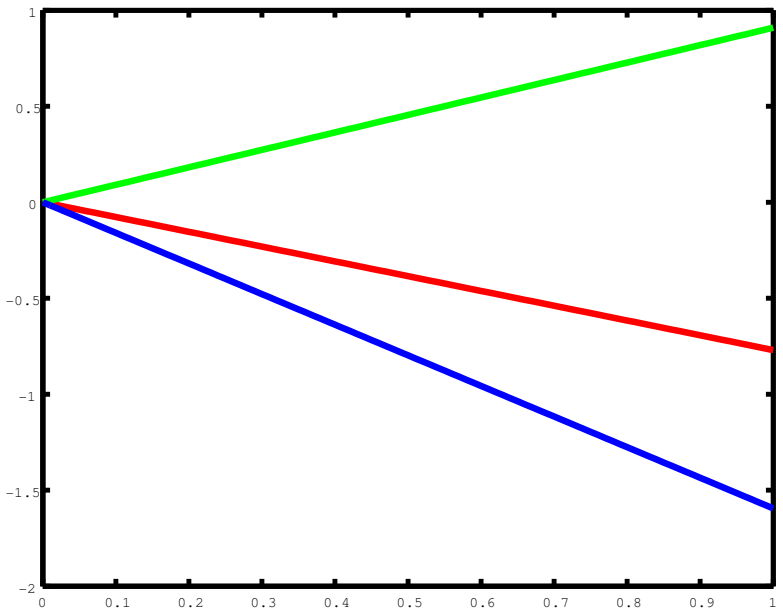
Examples:

- Linear kernel: $k(x, x') = x^\top x'$.
- Gaussian kernel: $k(x, x') = \exp(-\|x - x'\|^2/2\sigma^2)$.
- polynomial kernel: $k(x, x') = (1 + x^\top x')^d$.

Gaussian Process Prior



(a) Gaussian kernel



(b) Linear kernel

Estimation

Suppose $\{y_i\}_{i=1}^n$ are generated from the following model:

$$y_i = f^{\mathrm{o}}(x_i) + \xi_i,$$

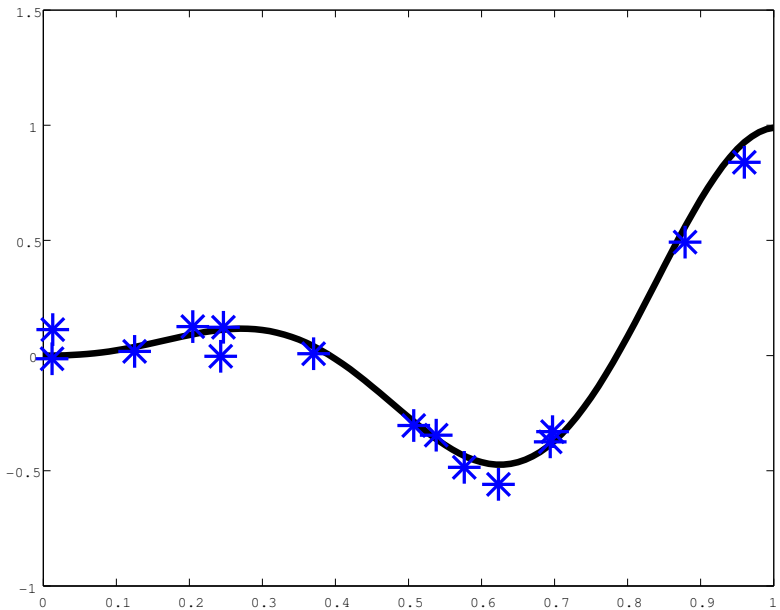
where ξ_i is i.i.d. Gaussian noise $\mathcal{N}(0, \sigma^2)$.
Posterior distribution: let $\mathbf{f} = (f(x_1), \ldots, f(x_n))$, then

$$\begin{aligned} p(\mathbf{f}|D_n) &= \frac{1}{C} \exp\left(-n\frac{\|\mathbf{f} - Y\|_n^2}{2\sigma^2}\right) \exp\left(-\frac{1}{2}\mathbf{f}^\top K^{-1}\mathbf{f}\right) \\ &= \frac{1}{C} \exp\left(-\frac{1}{2}\left\|\mathbf{f} - (K + \sigma^2 I_n)^{-1} KY\right\|^2_{(K^{-1} + I_n/\sigma^2)}\right), \end{aligned}$$

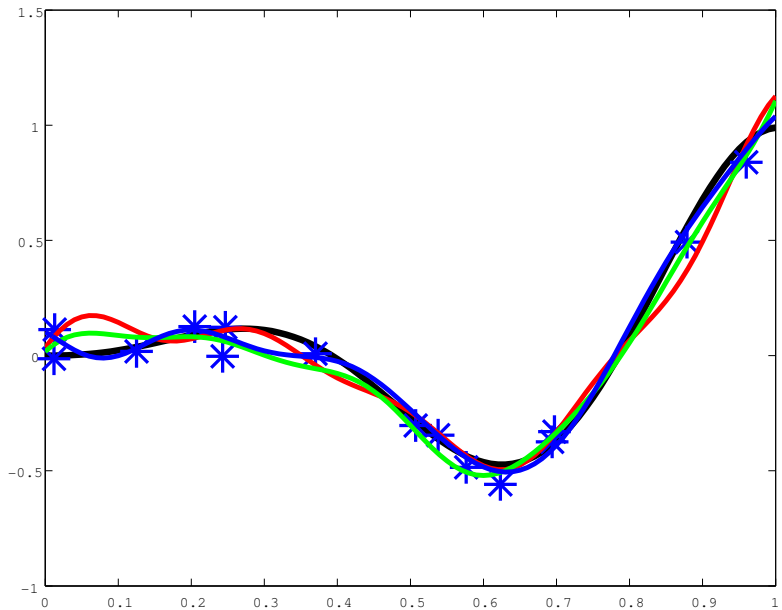
where $K \in \mathbb{R}^{n \times n}$ is the Gram matrix $(K_{i,j} = k(x_i, x_j))$.

- posterior mean: $\hat{\mathbf{f}} = (K + \sigma^2 I_n)^{-1} KY$.
- posterior covariance: $K - K(K + \sigma^2 I_n)^{-1} K$.

Gaussian Process Posterior

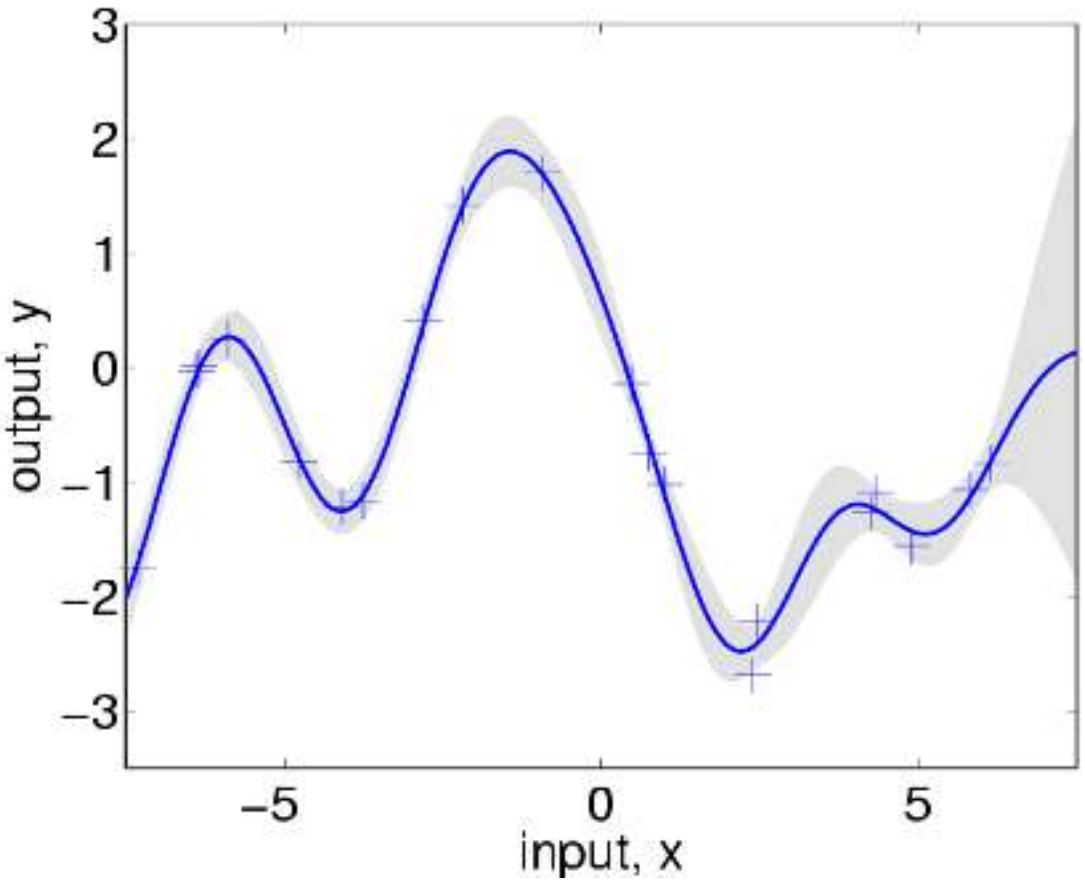


(c) Training Data



(d) Posterior Sample

Gaussian Process Posterior 2



Our interest

How fast does the posterior concentrate around the true?

Reproducing Kernel Hilbert Space (RKHS)

The kernel function defines Reproducing Kernel Hilbert Space (RKHS) $\mathcal{H}$ as a completion of the linear space spanned by all functions

$$x \mapsto \sum_{i=1}^{I} \alpha_i k(x_i, x), \quad (I = 1, 2, \dots)$$

relative to the RKHS norm $\|\cdot\|_{\mathcal{H}}$ induced by the inner product

$$\left\langle \sum_{i=1}^{I} \alpha_i k(x_i, \cdot), \sum_{j=1}^{J} \alpha'_j k(x'_j, \cdot) \right\rangle_{\mathcal{H}} = \sum_{i=1}^{I} \sum_{j=1}^{J} \alpha_i \alpha'_j k(x_i, x'_j).$$

Reproducibility: for $f \in \mathcal{H}$, the function value at x is recovered as

$$f(x) = \langle f, k(x, \cdot) \rangle_{\mathcal{H}}.$$

Example: Matérn prior

Matérn prior: for a *smoothness* parameter $\alpha > 0$, we define

$$k(x, x') = \int_{\mathbb{R}^d} e^{i\lambda^\top (x - x')} \psi(\lambda) \mathrm{d}\lambda,$$

where $\psi : \mathbb{R}^d \to \mathbb{R}$ is the spectral density given by

$$\psi(\lambda) = \frac{1}{(1 + \|\lambda\|^2)^{\alpha + d/2}}.$$

- The support is included in a Hölder space $C^{\alpha'}[0,1]^d$ for any $\alpha' < \alpha$.
- The RKHS $\mathcal{H}$ is included in a Sobolev space $W^{\alpha + d/2}[0,1]^d$ with the regularity $\alpha + d/2$.

For infinite dimensional RKHS $\mathcal{H}$, the support of the prior is typically much larger than $\mathcal{H}$.

Convergence rate of posterior: Matérn prior

Let $\hat{f}$ be the posterior mean.

Theorem (van der Vaart and van Zanten (2011))

Let $f^* \in C^\beta[0,1]^d \cap W^\beta[0,1]^d$ for $\beta > 0$, then for Matérn prior with parameter α, we have

$$\mathrm{E}[\|\hat{f} - f^*\|_n^2] \leq O\left(n^{-\frac{\alpha \wedge \beta}{\alpha + d/2}}\right).$$

- The optimal rate is $O\left(n^{-\frac{\beta}{\beta + d/2}}\right)$.
- The optimal rate is achieved only when $\alpha = \beta$.
- The rate $n^{-\frac{\alpha \wedge \beta}{\alpha + d/2}}$ is tight.
  $\rightarrow$ If $f^* \in \mathcal{H}$ $(\beta = \alpha + d/2)$, then GP does not achieve the optimal rate.

$\rightarrow$ **Scale mixture** is useful (van der Vaart & van Zanten, 2009).

Summary of existing results

- GP is optimal only in quite restrictive situations ($\alpha = \beta$).
  - In particular, if $f^\circ \in \mathcal{H}$, the optimal rate can not be achieved.
- The analysis was given only for restricted classes such as Sobolev and Hölder classes.

Outline

Bayesian-MKL = sparse aggregated estimation + Gaussian process

- **Condition on design:** Does not require any special conditions such as restricted eigenvalue condition.
- **Optimality:** Adaptively achieves the optimal rate for a wide class of true functions. In particular, even if $f^{\circ} \in \mathcal{H}$, it achieves the optimal rate.
- **Generality:** The analysis is given for a general class of spaces utilizing the notion of *interpolation spaces* and *the metric entropy*.

Bayesian MKL

We estimate f^{o} in a Bayesian manner. Let $f = (f_1, \ldots, f_M)$.

Prior of Bayesian MKL:

$$\Pi(\mathrm{d}f) = \sum_{J \subseteq \{1,\ldots,M\}} \pi_J \cdot \prod_{m \in J} \int_{\lambda_m \in \mathbb{R}_+} \mathrm{GP}_m(\mathrm{d}f_m | \lambda_m) \mathcal{G}(\mathrm{d}\lambda_m) \cdot \prod_{m \notin J} \delta_0(\mathrm{d}f_m)$$

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- $\mathrm{GP}_m(\cdot|\lambda_m)$ with a scale parameter λ_m is a *scaled Gaussian process* corresponding to the kernel function $\tilde{k}_{m,\lambda_m}$ where

$$\tilde{k}_{m,\lambda_m} = \frac{k_m}{\lambda_m},$$

for some fixed kernel function k_m.

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- $\mathcal{G}(\lambda_m) = \exp(-\lambda_m)$ (Gamma distribution: conjugate prior)
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- $\mathcal{G}(\lambda_m) = \exp(-\lambda_m)$ (Gamma distribution: conjugate prior) $\rightarrow$ **scale mixture**.
- Set all components f_m for $m \notin J$ as 0.
- Put a prior π_J on each sub-model J.

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We estimate f^{o} in a Bayesian manner. Let $f = (f_1, \ldots, f_M)$.

Prior of Bayesian MKL:

$$\Pi(\mathrm{d}f) = \sum_{J \subseteq \{1,\ldots,M\}} \pi_J \cdot \prod_{m \in J} \int_{\lambda_m \in \mathbb{R}_+} \mathrm{GP}_m(\mathrm{d}f_m | \lambda_m) \mathcal{G}(\mathrm{d}\lambda_m) \cdot \prod_{m \notin J} \delta_0(\mathrm{d}f_m)$$

- π_J is given as

$$\pi_J = \frac{\zeta^{|J|}}{\sum_{j=1}^{M} \zeta^j} \binom{M}{|J|}^{-1},$$

with some $\zeta \in (0, 1)$.

The estimator

The posterior: For some constant $\beta > 0$, the posterior probability measure is given as

$$\Pi(\mathrm{d}f|D_n) := \frac{\exp\left(-\frac{\sum_{i=1}^n (y_i - \sum_{m=1}^M f_m(x_i))^2}{\beta}\right)}{\int \exp\left(-\frac{\sum_{i=1}^n (y_i - \sum_{m=1}^M \tilde{f}_m(x_i))^2}{\beta}\right) \Pi(\mathrm{d}\tilde{f})} \Pi(\mathrm{d}f),$$

for $f = (f_1, \ldots, f_M)$.

The estimator: The Bayesian estimator $\hat{f}$ (Bayesian-MKL estimator) is given as the expectation of the posterior:

$$\hat{f} = \int \sum_{m=1}^M f_m \Pi(\mathrm{d}f|y_1, \ldots, y_n).$$

Point

- Model averaging
- Scale mixture of Gaussian process prior

Outline

Mean Squared Error

We want to bound the mean squared error:

$$\|f^{\mathrm{o}} - \hat{f}\|_n^2 := \frac{1}{n}\sum_{i=1}^{n}(f^{\mathrm{o}}(x_i) - \hat{f}(x_i))^2,$$

where $\hat{f}$ is the Bayesian estimator. We utilize a *PAC-Bayesian bound*.

PAC-Bayesian Bound

Under some conditions for the noise (explained in the next slide), we have the following theorem.

Theorem (Dalalyan and Tsybakov (2008))

For all probability measure ρ, we have

$$\mathrm{E}_{Y_{1:n}|x_{1:n}}\left[\|\hat{f}-f^{\mathrm{o}}\|_n^2\right] \leq \int \|f-f^{\mathrm{o}}\|_n^2 \mathrm{d}\rho(f) + \frac{\beta \mathcal{K}(\rho,\Pi)}{n},$$

where $\mathcal{K}(\rho,\Pi)$ is the KL-divergence between ρ and Π:

$$\mathcal{K}(\rho,\Pi) := \int \log\left(\frac{\mathrm{d}\rho}{\mathrm{d}\Pi}\right)\mathrm{d}\rho.$$

Noise Condition

Let

$$m_\xi(z) := -\mathrm{E}[\xi_1 \mathbf{1}\{\xi_1 \leq z\}],$$

where $\mathbf{1}\{\cdot\}$ is the indicator function. Then we impose the following assumption on m_ξ.

Assumption

$\mathrm{E}[\xi_1^2] < \infty$ *and the measure* $m_\xi(z)\mathrm{d}z$ *is absolutely continuous with respect to the density function* $p_\xi(z)$ *with a bounded Radon-Nikodym derivative, i.e., there exists a bounded function* $g_\xi : \mathbb{R} \to \mathbb{R}_+$ *such that*

$$\int_a^b m_\xi(z)\mathrm{d}z = \int_a^b g_\xi(z)p_\xi(z)\mathrm{d}z, \quad \forall a, b \in \mathbb{R}.$$

- The Gaussian noise $\mathcal{N}(0, \sigma^2)$ satisfies the assumption with $g_\xi(z) = \sigma^2$,
- The uniform distribution on $[-a, a]$ satisfies the assumption with $g_\xi(z) = \max(a^2 - z^2, 0)/2$.

Concentration Function

We define the **concentration function** as

$$\phi_{f_m^*}^{(m)}(\epsilon, \lambda_m) := \underbrace{\inf_{h \in \mathcal{H}_m : \|h - f_m^*\|_n \leq \epsilon} \|h\|_{\mathcal{H}_{m,\lambda_m}}^2}_{\text{bias}} \underbrace{- \log \mathrm{GP}_m(\{f : \|f\|_n \leq \epsilon\} | \lambda_m)}_{\text{variance}}.$$

It is known that $\phi_{f_m^*}^{(m)}(\epsilon, \lambda_m) \sim -\log \mathrm{GP}_m(\{f : \|f_m^* - f\|_n \leq \epsilon\} | \lambda_m)$ (van der Vaart & van Zanten, 2011; van der Vaart & van Zanten, 2008b).

General Result

Let $I_0 := \{m \mid f_m^* \neq 0\}$, $\check{I}_0 := \{m \in I_0 \mid f_m^* \notin \mathcal{H}_m\}$, and $\kappa := \zeta(1-\zeta)$.

Theorem (Convergence rate of Bayesian-MKL)

The convergence rate of Bayesian-MKL is bounded as

$$\mathrm{E}_{Y_{1:n}|x_{1:n}}\left[\|\hat{f} - f^{\mathrm{o}}\|_n^2\right] \leq 2\|f^{\mathrm{o}} - f^*\|_n^2$$
$$+ C_1 \inf_{\epsilon_m, \lambda_m > 0} \left\{ \sum_{m \in I_0} \left(\epsilon_m^2 + \frac{1}{n}\phi_{f_m^*}^{(m)}(\epsilon_m, \lambda_m) + \frac{\lambda_m}{n} - \frac{\log(\lambda_m)}{n} \right) \right.$$
$$\left. + \sum_{\substack{m, m' \in \check{I}_0: \\ m \neq m'}} \epsilon_m \epsilon_{m'} + \frac{|I_0|}{n} \log\left(\frac{Me}{\kappa |I_0|}\right) \right\}.$$

Interpretation of the theorem

Let $\hat{\epsilon}_m^2 = \inf_{\epsilon_m, \lambda_m > 0} \left(\epsilon_m^2 + \frac{1}{n} \phi_{f_m^*}^{(m)}(\epsilon_m, \lambda_m) + \frac{\lambda_m}{n} - \frac{\log(\lambda_m)}{n} \right)$ and suppose $f^{\mathrm{o}} = f^*$. Typically $\hat{\epsilon}_m^2$ achieves the optimal learning rate for the *single kernel* learning.

- (Correctly specified) If $f_m^* \in \mathcal{H}_m$ for all m, then we have

$$\mathrm{E}_{Y_{1:n}|x_{1:n}} \left[\|\hat{f} - f^{\mathrm{o}}\|_n^2 \right] = O\left[\sum_{m \in I_0} \hat{\epsilon}_m^2 + \frac{|I_0|}{n} \log\left(\frac{Me}{\kappa |I_0|} \right) \right].$$

  ⇒ Optimal learning rate for MKL.
  Note that we imposed no condition on the design such as restricted eigenvalue condition.

- (Misspecified) If $f_m^* \notin \mathcal{H}_m$ for all $m \in I_0$, then we have

$$\mathrm{E}_{Y_{1:n}|x_{1:n}} \left[\|\hat{f} - f^{\mathrm{o}}\|_n^2 \right] = O\left[\left(\sum_{m \in I_0} \hat{\epsilon}_m \right)^2 + \frac{|I_0|}{n} \log\left(\frac{Me}{\kappa |I_0|} \right) \right].$$

Outline of the Proof

Fix $\epsilon_m, \lambda_m > 0$ arbitrary. Next we define a "representer" element $\tilde{h}_m \in \mathcal{H}_m$ that is close to f_m^*. If $f_m^* \in \mathcal{H}_m$, then set $\tilde{h}_m = f_m^*$. Otherwise, we take $\tilde{h}_m \in \mathcal{H}_{m,\lambda_m}$ such that $\|\tilde{h}_m\|^2_{\mathcal{H}_m,\lambda_m} \leq 2 \inf_{h \in \mathcal{H}_m : \|h - f_m^*\|_n \leq \epsilon_m} \|h\|^2_{\mathcal{H}_{m,\lambda_m}}$. We substitute the following "dummy" posterior into ρ:

$$\rho(\mathrm{d}f) = \prod_{m \in I_0} \frac{\int_{\frac{\lambda_m}{2} \leq \tilde{\lambda}_m \leq \lambda_m} \frac{\mathrm{GP}_m(\mathrm{d}f_m - \tilde{h}_m | \tilde{\lambda}_m) \mathbf{1}\{\|f_m - \tilde{h}_m\|_n \leq \epsilon_m\}}{\mathrm{GP}_m(\{\Delta f_m : \|\Delta f_m\|_n \leq \epsilon_m\} | \tilde{\lambda}_m)} \mathcal{G}(\mathrm{d}\tilde{\lambda}_m)}{\mathcal{G}(\{\tilde{\lambda}_m : \frac{\lambda_m}{2} \leq \tilde{\lambda}_m \leq \lambda_m\})} \cdot \prod_{m \notin I_0} \delta_0(\mathrm{d}f_m).$$

One can show that the KL-divergence betweenρ and the prior Π is bounded as

$$\frac{1}{n}\mathcal{K}(\rho, \Pi) \leq C_1' \sum_{m \in I_0} \left(\frac{1}{n} \phi_{f_m^*}^{(m)}(\epsilon_m, \lambda_m) + \frac{1}{n}\lambda_m - \frac{1}{n} \log(\lambda_m) \right) + \frac{|I_0|}{n} \log\left(\frac{Me}{|I_0|\kappa} \right),$$

where C_1' is a universal constant. A key to prove this is an infinite dimensional extension of the Brascamp and Lieb inequality (Brascamp & Lieb, 1976; Hargé, 2004). Since $\{\epsilon_m, \lambda_m\}_{m=1}^M$ are arbitrary, this gives the assertion.

Example 1: Metric Entropy Characterization (Correctly specified)

Define the ϵ-*covering number* $N(\mathcal{B}_{\mathcal{H}_m}, \epsilon, \|\cdot\|_n)$ as the number of $\|\cdot\|_n$-norm balls covering the unit ball $\mathcal{B}_{\mathcal{H}_m}$ in $\mathcal{H}_m$.
The metric entropy is its logarithm:

$$\log N(\mathcal{B}_{\mathcal{H}_m}, \epsilon, \|\cdot\|_n).$$

Example 1: Metric Entropy Characterization

We assume that there exits a real value $0 < s_m < 1$ such that

$$\log N(\mathcal{B}_{\mathcal{H}_m}, \epsilon, \|\cdot\|_n) = O(\epsilon^{-2s_m}),$$

where $\mathcal{B}_{\mathcal{H}_m}$ is the unit ball of the RKHS $\mathcal{H}_m$.

Theorem (Correctly specified)

If $f_m^* \in \mathcal{H}_m$ for all $m \in I_0$, then we have

$$\mathrm{E}_{Y_{1:n}|X_{1:n}}\left[\|\hat{f} - f^{\mathrm{o}}\|_n^2\right] \leq C\left\{\sum_{m\in I_0} n^{-\frac{1}{1+s_m}} + \frac{|I_0|}{n}\log\left(\frac{Me}{|I_0|\kappa}\right)\right\} + 2\|f^{\mathrm{o}} - f^*\|_n^2$$

It is known that, if there is no scale mixture prior, the optimal rate $n^{-\frac{1}{1+s_m}}$ can not be achieved (Castillo, 2008).

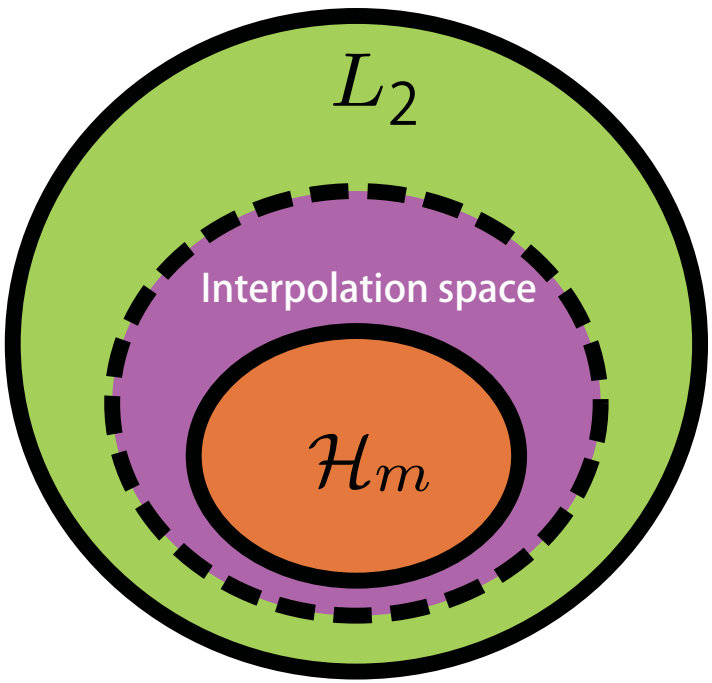
Example 1: Metric Entropy Characterization (Misspecified)

Let $[L_2(P_n), \mathcal{H}_m]_{\theta,\infty}$ be the *interpolation space* equipped with the norm,

$$\|f\|_{\theta,\infty}^{(m)} := \sup_{t>0} t^{-\theta} \inf_{g_m \in \mathcal{H}_m} \{\|f - g_m\|_n + t\|g_m\|_{\mathcal{H}_m}\}.$$

One has

$$\mathcal{H}_m \hookrightarrow [L_2(P_n), \mathcal{H}_m]_{\theta,\infty} \hookrightarrow L_2(P_n).$$



Example 1: Metric Entropy Characterization (Misspecifi d)

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One has

$$\mathcal{H}_m \hookrightarrow [L_2(P_n), \mathcal{H}_m]_{\theta,\infty} \hookrightarrow L_2(P_n).$$

Theorem (Misspecified)

If $f_m^* \in [L_2(P_n), \mathcal{H}_m]_{\theta,\infty}$ with $0 < \theta \leq 1$, then we have

$$\mathrm{E}_{Y_{1:n}|X_{1:n}}\left[\|\hat{f} - f^{\mathrm{o}}\|_n^2\right] \leq C\left\{\left(\sum_{m \in I_0} n^{-\frac{1}{2(1+s_m/\theta)}}\right)^2 + \frac{|I_0|}{n}\log\left(\frac{Me}{|I_0|\kappa}\right)\right\} + 2\|f^{\mathrm{o}} - f^*\|_n^2$$

Thanks to the scale mixture prior, the estimator adaptively achieves the optimal rate for $\theta \in (s_m, 1]$.

Example 2: Matérn prior

Suppose that $\mathcal{X}_m = [0,1]^{d_m}$. The Matérn priors on $\mathcal{X}_m$ correspond to the kernel function defined as

$$k_m(z, z') = \int_{\mathbb{R}^{d_m}} e^{\mathrm{i} s^\top (z - z')} \psi_m(s) \mathrm{d}s,$$

where $\psi_m(s)$ is the spectral density given by $\psi_m(s) = (1 + \|s\|^2)^{-(\alpha_m + d_m/2)}$, for a smoothness parameter $\alpha_m > 0$.

Theorem (Matérn prior, correctly specified)

If $f_m^* \in \mathcal{H}_m$, then we have that

$$\mathrm{E}_{Y_{1:n}|x_{1:n}} \left[\|\hat{f} - f^{\mathrm{o}}\|_n^2 \right] \leq C \left\{ \sum_{m \in I_0} n^{-\frac{1}{1 + \frac{d_m}{2\alpha_m + d_m}}} + \frac{|I_0|}{n} \log \left(\frac{Me}{|I_0|\kappa} \right) \right\} + 2\|f^{\mathrm{o}} - f^*\|_n^2$$

Example 2: Matérn prior

Theorem (Matérn prior, Misspecified)

If $f_m^* \in C^{\beta_m}[0,1]^{d_m} \cap W^{\beta_m}[0,1]^{d_m}$ *and* $\beta_m < \alpha_m + d_m/2$, *then we have that*

$$\mathrm{E}_{Y_{1:n}|X_{1:n}}\left[\|\hat{f} - f^{\mathrm{o}}\|_n^2\right] \leq C\left\{\left(\sum_{m\in I_0} n^{-\frac{\beta_m}{2\beta_m+d_m}}\right)^2 + \frac{|I_0|}{n}\log\left(\frac{Me}{|I_0|\kappa}\right)\right\} + 2\|f^{\mathrm{o}} - f^*\|_n^2$$

Although $f_m^* \notin \mathcal{H}_m$, the convergence rate achieves the optimal rate adaptively.

Example 3: Group Lasso

$\mathcal{X}_m$ is a finite dimensional Euclidean space: $\mathcal{X}_m = \mathbb{R}^{d_m}$. The kernel function corresponding to the Gaussian process prior is $k_m(x, x') = x^\top x'$:

$$f_m(x) = \mu^\top x, \ \mu \sim \mathcal{N}(0, I_{d_m}).$$

Theorem (Group Lasso)

If $f_m^* = \mu_m^\top x$, then we have that

$$\mathrm{E}_{Y_{1:n}|X_{1:n}}\left[\|\hat{f} - f^{\mathrm{o}}\|_n^2\right] = C\left\{\frac{\sum_{m\in I_0} d_m \log(n)}{n} + \frac{|I_0|}{n}\log\left(\frac{Me}{|I_0|\kappa}\right)\right\} + 2\|f^{\mathrm{o}} - f^*\|_n^2$$

This is rate optimal up to $\log(n)$-order.

Gaussian correlation conjecture

We use an infinite dimensional version of the following inequality (Brascamp-Lieb inequality (Brascamp & Lieb, 1976; Hargé, 2004)):

$$\mathrm{E}[\langle X, \phi \rangle^2 | X \in A] \leq \mathrm{E}[\langle X, \phi \rangle^2],$$

where $X \sim \mathcal{N}(0, \Sigma)$ and A is a symmetric convex set centered on the origin.

Gaussian correlation conjecture:

$$\mu(A \cap B) \geq \mu(A)\mu(B),$$

where μ is any centered Gaussian measure and A and B are any two symmetric convex sets.

Brascamp-Lieb inequality can be seen as an application of a particular case of the Gaussian correlation conjecture. See the survey by Li and Shao (2001) for more details.

Conclusion

- We developed a PAC-Bayesian bound for Gaussian process model and generalized it to sparse additive model.
- The optimal rate is achieved *without* any conditions on the design.
- We have observed that Gaussian processes with scale mixture adaptively achieve the minimax optimal rate on both correctly-specified and misspecified situations.

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