Distributed non-parametric Gaussian regression: recent results and open problems

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Part I

Introduction



Problem statement - centralized scenario

inputs: set of noisy measurements of a certain signal:

$$y_m = f(x_m) + \nu_m$$
 $m = 1, \ldots, M$

goal: estimate f(x)



Parametric approach

assumption: known structure *but* unknown parameters example: exponential:



goal: estimate θ starting from the data set $\{(x_m, y_m)\}$ \Rightarrow various approaches depending on the model on f:

- Maximum Likelihood
- Least Squares

. . .

Nonparametric approach

assumption: signal f lives in a certain functions space:

$$f \in \mathcal{H}_{K}$$

goal: search the estimate \hat{f} directly inside this space:

$$\widehat{f} = \arg\min_{\widetilde{f} \in \mathcal{H}_{K}} \left(\text{Loss function}\left(\widetilde{f}, \{y_{m}\}\right) + \gamma \left\|\widetilde{f}\right\|_{\mathcal{H}_{K}}^{2} \right)$$

motivations: functional structure of f could be not easily managed with parametric structures

our approach: use Reproducing Kernel Hilbert Spaces

Part II Centralized Learning



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Introduction to the centralized learning scenario

hypoteses:

- there is only one sensor
- exist a certain and opportune "bidimensional" function

 $\mathcal{K}\left(\cdot,\cdot
ight):$ Input locations imes Input locations o $\mathbb R$

working flow: • $K(\cdot, \cdot)$ defines a function space \mathcal{H}_K • use $K(\cdot, \cdot)$ to construct the estimating function



Reproducing Kernel Hilbert Spaces - hypotheses

question: how $\mathcal{H}_{\mathcal{K}}$ is made?

first assumption: $K(\cdot, \cdot)$ is a Mercer Kernel:

- continuous
- symmetric
- definite positive

second assumption: input locations domain is compact

Reproducing Kernel Hilbert Spaces - implications

implication 1: $K(\cdot, \cdot)$ defines a compact linear positive definite integral operator:

$$(L_{\kappa}f)(x_m) := \int_{\mathcal{X}} K(x_m, x') f(x') dx'$$

implication 2: L_K has at most a numerable set of eigenfunctions:

$$\phi_k(\cdot) = \lambda_k(L_K\phi_k)(\cdot) \qquad k = 1, 2, \dots$$

Reproducing Kernel Hilbert Spaces

Theorem

with the previous hypotheses:

- $\{\lambda_k\}$ are real and non-negative: $\lambda_1 \ge \lambda_2 \ge \ldots \ge 0$
- $\{\phi_k(\cdot)\}$ is an orthonormal basis for the space

$$\mathcal{H}_{K} = \left\{ f \in \mathcal{L}_{2} \quad s.t. \quad f = \sum_{k=1}^{\infty} a_{k} \phi_{k} \\ \text{with } \{a_{k}\} \quad s.t. \quad \sum_{k=1}^{\infty} \frac{a_{k} \cdot a_{k}}{\lambda_{k}} < +\infty \right\}$$

• $f_1 = \sum_{k=1}^{\infty} a_k \phi_k$, $f_2 = \sum_{k=1}^{\infty} b_k \phi_k \Rightarrow$

$$\langle f_1, f_2 \rangle_{\mathcal{H}_K} = \sum_{k=1}^{\infty} \frac{a_k \cdot b_k}{\lambda_k}$$

RKHS based learning

assumption: \mathcal{H}_{K} is defined via the kernel K

 1° question: how we construct the estimate? 2° question: how can we interpret it?



RKHS based learning - cost-function interpretation

recall: estimation \hat{f} has to:

- fit \rightarrow loss functions
- $\bullet\,$ not to overfit $\rightarrow\,$ Tikhonov regularizator

our approach: loss functions = quadratic functions



RKHS based learning - Bayesian interpretation

goal: construct the Bayesian estimator of f:

$$\widehat{f} = \operatorname{cov}(f, \mathbf{y}) \operatorname{var}(\mathbf{y})^{-1} \mathbf{y} \qquad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_M \end{bmatrix}$$

Proposition

lf:

• *f* is a Gaussian process with covariance *K*:

$$\operatorname{cov}\left(f\left(x_{m}\right) f\left(x_{n}\right)^{T}\right) = K\left(x_{m}, x_{n}\right)$$

• loss functions = quadratic functions

then cost-function regularization is equivalent to Bayes estimation

RKHS based learning - numerical results

$$\widehat{f}(\cdot) = \sum_{m=1}^{M} c_m K(x_m, \cdot) \quad \text{with} \quad \begin{bmatrix} c_1 \\ \vdots \\ c_M \end{bmatrix} = (K_{\mathbf{x}} + \gamma I_M)^{-1} \begin{bmatrix} y_1 \\ \vdots \\ y_M \end{bmatrix}$$

Example:

RKHS based learning - drawbacks

$$\widehat{f}\left(\cdot\right) = \sum_{m=1}^{M} c_{m} \mathcal{K}\left(x_{m},\cdot\right)$$

1° feature: must invert $(K_{\mathbf{x}} + \gamma I_M)^{-1}$ 2° feature: must store $[c_1, \ldots, c_M]$

caveat: $M \text{ big} \Rightarrow$

- computationally hard to invert $M \times M$ matrices
- function representations pretty big

our requirements:

compact representations (necessary for distributed algorithms)

 \Box light computations (preferable)



Approximated RKHS learning

want compact representations & light computations? \Rightarrow must approximate

model:
$$f = \sum_{k=1}^{+\infty} a_k \phi_k \implies y_m = \sum_{k=1}^{+\infty} a_k \phi_k (x_m) + \nu_m$$

new goal: estimate only the first *E* coefficients with $E \ll M$

definition: Reduced Hilbert Space:

$$\mathcal{H}_{K}^{E} := \left\{ \widetilde{f} \in \mathcal{L}_{2} \text{ s.t. } \widetilde{f} = \sum_{k=1}^{E} a_{k} \phi_{k} \\ \mathbf{a} := \left[a_{1} \dots a_{E} \right]^{T} \in \mathbb{R}^{E} \right\}$$

Approximated learning - example

Kernel for BIBO stable linear time-invariant systems:

$$\mathcal{K}(x, x'; \beta) = \begin{cases} \frac{\exp\left(-2\beta x\right)}{2} \left(\exp\left(-\beta x'\right) - \frac{\exp\left(-\beta x\right)}{3}\right) & \text{if } x \le x' \\ \frac{\exp\left(-2\beta x'\right)}{2} \left(\exp\left(-\beta x\right) - \frac{\exp\left(-\beta x'\right)}{3}\right) & \text{if } x \ge x' \end{cases}$$



Approximated learning - kind of approaches

cost-function based:

- $\bullet~$ data fitting $\rightarrow~$ loss functions
- $\bullet \ \ not \ overfit \rightarrow Tikhonov \ regularizer$



Bayesian approach:

- consider a prior
- find the best linear estimator

$$\widehat{\mathbf{a}} = \operatorname{cov}\left(\mathbf{a}, \ \mathbf{y}
ight) \operatorname{var}\left(\mathbf{y}
ight)^{-1} \mathbf{y}$$

Approximated learning - compact notation

notation:
$$y_m = \sum_{k=1}^{+\infty} a_k \phi_k(x_m) + \nu_m \quad \rightarrow \quad \mathbf{y} = C\mathbf{a} + \mathbf{e} + \nu$$

definitions:

$$\mathbf{y} := \begin{bmatrix} y_1 \\ \vdots \\ y_M \end{bmatrix} \quad C := \begin{bmatrix} \phi_1(x_1) & \dots & \phi_E(x_1) \\ \vdots & & \vdots \\ \phi_1(x_M) & \dots & \phi_E(x_M) \end{bmatrix}$$

$$\mathbf{a} := \begin{bmatrix} a_1 \\ \vdots \\ a_E \end{bmatrix} \qquad \mathbf{e} := \begin{bmatrix} \sum_{k=E+1}^{+\infty} a_k \phi_k(x_1) \\ \vdots \\ \sum_{k=E+1}^{+\infty} a_k \phi_k(x_M) \end{bmatrix} \qquad \nu := \begin{bmatrix} \nu_1 \\ \vdots \\ \nu_E \end{bmatrix}$$

Approximated learning - numerical solutions

$$(\Sigma_{\mathbf{a}} := \mathsf{diag} \left(\lambda_1, \dots, \lambda_E \right) \quad \Sigma_{\mathbf{e}} := \ \mathsf{var} \left(\Sigma_{\mathbf{e}} \right))$$

cost-function approach:

$$\widehat{\mathbf{a}} = \left(\sigma^2 \Sigma_{\mathbf{a}} C^T C + \gamma I_E
ight)^{-1} \Sigma_{\mathbf{a}} C^T \mathbf{y}$$

(computations load: $O(E^3 + E^2M + EM^2)$ operations) Bayesian approach:

$$\widehat{\mathbf{a}} = \boldsymbol{\Sigma}_{\mathbf{a}} \boldsymbol{C}^{\mathsf{T}} \left(\boldsymbol{C} \boldsymbol{\Sigma}_{\mathbf{a}} \boldsymbol{C}^{\mathsf{T}} + \boldsymbol{\Sigma}_{\mathbf{e}} + \sigma^{2} \boldsymbol{I}_{\mathcal{M}} \right)^{-1} \mathbf{y}$$

(computations load: $O(M^3)$ operations)

never equivalent!

∜

Part III

Distributed Approximated Learning



Distributed approximated learning - introduction



Distributed approx. learning - starting hypotheses

Simplifications:

- each sensor knows exactly S (n° of sensors)
- Ino time-delay between measured signals
- common input-locations grid among sensors



Bayesian strategy: when distributed = centralized?

$$(\mathbf{y}_i := \text{set of measurements of sensor } i$$

$$\widehat{\mathbf{a}}_{cent} = \operatorname{cov}\left(\mathbf{a}, \begin{bmatrix} \mathbf{y}_{1} \\ \vdots \\ \mathbf{y}_{S} \end{bmatrix}\right) \operatorname{var}\left(\begin{bmatrix} \mathbf{y}_{1} \\ \vdots \\ \mathbf{y}_{S} \end{bmatrix}\right)^{-1} \begin{bmatrix} \mathbf{y}_{1} \\ \vdots \\ \mathbf{y}_{S} \end{bmatrix}$$
$$= (\dots \text{ some massages} \dots)$$
$$= \frac{1}{S} \sum_{i=1}^{S} \left(\sum_{\mathbf{a}} C^{T} \left(C \sum_{\mathbf{a}} C^{T} + \sum_{\mathbf{e}} + \frac{\sigma^{2}}{S} I_{M} \right)^{-1} \mathbf{y}_{i} \right)$$
$$\Rightarrow \text{ equivalent to an average consensus on locally computable quantities!}$$



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Bayesian strategies: distributed vs local

local Bayesian strategy:

$$\widehat{\mathbf{a}}_{\mathsf{loc},s} = \operatorname{cov}\left(\mathbf{a},\mathbf{y}_{i}\right) \operatorname{var}\left(\mathbf{y}_{i}\right)^{-1} \mathbf{y}_{i} = \Sigma_{\mathbf{a}} C^{T} \left(C \Sigma_{\mathbf{a}} C^{T} + \Sigma_{\mathbf{e}} + \sigma^{2} I_{\mathcal{M}} \right)^{-1} \mathbf{y}_{s}$$

distributed strategy: (equivalent to centralized)

• initial local estimation:

$$\widehat{\mathbf{a}}_{s}(0) = \Sigma_{\mathbf{a}} C^{T} \left(C \Sigma_{\mathbf{a}} C^{T} + \Sigma_{\mathbf{e}} + \frac{\sigma^{2}}{S} I_{M} \right)^{-1} \mathbf{y}_{s}$$

2 average consensus on the varios $\widehat{a}_s(0)$

difference = how to weight the measurement noise!



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Guessed distributed strategy

hypothesis removal: sensors do not know S (n° of sensors)

all sensors make the same guess: S_g ("g" = guess)

how distributed estimator changes?

distributed strategy:

Comparison: centralized vs guessed distributed

centralized (or distributed) strategy:

$$\widehat{\mathbf{a}}_{cent} = \Sigma_{\mathbf{a}} C^{T} \left(C \Sigma_{\mathbf{a}} C^{T} + \Sigma_{\mathbf{e}} + \frac{\sigma^{2}}{S} I_{M} \right)^{-1} \overline{\mathbf{y}}$$

guessed distributed strategy:

$$\widehat{\mathbf{a}}_{\text{dist}}\left(\mathbf{S}_{\mathbf{g}}\right) = \Sigma_{\mathbf{a}} C^{T} \left(C \Sigma_{\mathbf{a}} C^{T} + \Sigma_{\mathbf{e}} + \frac{\sigma^{2}}{\mathbf{S}_{\mathbf{g}}} I_{M} \right)^{-1} \overline{\mathbf{y}}$$

centralized strategy use the correct measurements variance!



Comparisons between estimators performances

performance "=" estimation error variance

centralized vs local: centralized is always better than local

centralized vs guessed distributed: centralized is always better than guessed distributed (equal iff $S = S_g$, (guess is correct))

guessed distributed vs local: depends!!



Comparison: guessed distributed vs local (1)

Proposition

If $S_g \in [1, 2(S - 1)]$ then guessed distributed strategy is better than local independently of the kernel, noise power, number of measurements, etc.



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Comparison: guessed distributed vs local (2)

Proposition

If we consider kernel then the previous bound can be enlarged



Comparison: guessed distributed vs local (3)

Proposition

lf

$$\min\left(\operatorname{eig}\left(\mathcal{K}_{\mathsf{x}}\right)\right) \geq \frac{\sigma^2}{S-1}$$

then the guessed distributed strategy is always better than the local one, for all guesses ${\bf S_g}\in[1,+\infty)$



implication: in this case communications always improve estimation

Loss of performances: TODO

TODO: characterize the loss of performance when making wrong guesses (i.e. $S_g \neq S$)

desired propositions: small error in guessing (say Δ) $\stackrel{?}{\Rightarrow}$ loss of performance is small (say ε)? When? How much is ε ? Does it depend on K_x ? ...



Distributed estimation without initial guessings (1)

Initial guessing ${\bf S_g}$ could be undesirable \Rightarrow look for estimators without required initializations

requested features:

- must not require guessings
- must be a linear tranformation of the measurements \mathbf{y}_i
- must lead to the smallest possible estimation error variance
- \bullet dimension of exchanged vectors must be at most E

Distributed estimation without initial guessings (2)

Proposed algorithm:

- **(**) whiten the noise $\mathbf{e} + \nu$
- 2 compress information using an SVD decomposition
- run an average consensus algorithm

$$\rightarrow$$
 $\widehat{\mathbf{a}} = A(\mathbf{y}_1, \dots, \mathbf{y}_S)$

"Corollary algorithm": maximum likelihood estimator for the number of sensors *S*:

$$\widehat{S}_{\mathsf{ML}} := \arg \max_{S} P\left(A\left(\mathbf{y}_{1}, \ldots, \mathbf{y}_{S}\right) \mid S\right)$$

TODO: comparisons between this and "guessed distributed":

- estimation error variance
- computational requirements



Adding temporal shifts to the measured function

hypothesis removal: there are unknown time-delays between measured signals



implication: unknown delays \Rightarrow no common sampling grid

\Rightarrow much more difficult scenario!

Classic Time Delay Estimation

notation: f_1, f_2 = noisy delayed versions of the same f classic TDE: maximization of \mathcal{L}_2 's inner product:

$$\tau_{\mathsf{optimal}} = \arg \max_{\tau} \langle f_1(x), f_2(x - \tau) \rangle_{\mathcal{L}_2}$$





Time Delay Estimation in RKHS framework

RKHS based TDE: maximization of $\mathcal{H}_{\mathcal{K}}$'s inner product:

$$\tau_{\mathsf{optimal}} = \arg \max_{\tau} \langle f_1(x), f_2(x - \tau) \rangle_{\mathcal{H}_{\mathcal{K}}} = \arg \max_{\tau} \sum_{k=1}^{\infty} \frac{a_k \cdot b_k(\tau)}{\lambda_k}$$

Note: requires $f_1(x)$ and $f_2(x - \tau)$ in the same reference system



Joint "function and TD" Estimation - centralized scenario

proposed solution: Maximum likelihood strategy:

$$\mathcal{L}\left(\widetilde{f}\right) := -J\left(\widetilde{f}\right) = -\sum_{s=1}^{S}\sum_{m=1}^{M_{s}} \frac{\left(\widetilde{f}\left(x_{s,m} - \tau_{s}\right) - y_{s,m}\right)^{2}}{\sigma^{2}} - \gamma \left\|\widetilde{f}\right\|_{\mathcal{H}_{K}}^{2}$$

implies:

$$\widehat{f}_{\mathsf{ML}} := \arg \max_{\widetilde{f} \in \mathcal{H}_{K}^{\mathcal{E}}} \mathcal{L}\left(\widetilde{f}\right)$$

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 \Rightarrow maximization via descent algorithms Caveat: initialization strongly affects results!

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Joint "function and TDE" - distributed scenario

proposed solution: distributed minimization of the centralized likelihood:

• find the minimal *bridged sensor network* topology:



- introduce some constraints in the centralized likelihood (one for each bridge)
- S construct a Lagrangian from the constrained likelihood
- solve the Lagrangian via a distributed minimization algorithm
- Caveat: initialization strongly affects results!

Part IV

Other Open Problems



Grid based distributed estimation (1)

hypotheses:

- no time delays between measured functions
- sensors share a common sampling grid
- sensors have also some own sampling locations



Grid based distributed estimation (2)

proposed algorithm:

- run distributed estimation on the grid (guessed / without guessing) $\rightarrow \widehat{a}_{dist}(\theta)$
- fuse distributed estimation & data not previously used: $\widehat{\mathbb{E}}[f \mid \widehat{\mathbf{a}}_{dist}(\theta) \mathbf{y}_s]$

TODOs:

- characterize the combined estimation error variance (always better than pure local? no? when? why?)
- find suboptimal combination strategies of local estimates + distributed estimates (no recomputing everything)

Recursively updated approximated estimators

problematic issue: all current implementations of approximated estimators work "offline":

single new measurement arrive \rightarrow recompute everything

desired strategy: find recursive equations:

$$\widehat{\mathbf{a}}(t+1) = \Theta\left(\widehat{\mathbf{a}}(t), (x_{t+1}, y_{t+1})\right)$$

TODO: everything (first step: find at least some suboptimal equations)



No-common-grid suboptimal strategy

previously proposed strategy: distributed lagrangian minimization \rightarrow slow convergence + local minima

suboptimal alternative idea:

cycle the following

- estimate the delays between the functions
- construct an artificial grid
- Oreate some measurements on this grid
- In this grid strategy on this grid
- o update the local estimations using the distributed one

TODO: everything (numerical equations, convergence, stability, error **e** bounds, . . .)

Time Delay Estimation using RKHS techniques

TDE via RKHS-based approximated representations: in our knowledge never been proposed

Distributed Fault Detection (1)

hypotheses:

- sensors measure the same (or quite the same) function
- sensors can be faulty

Distributed Fault Detection (2)

proposed solution: each sensor:

- do distributed estimation
- do local estimation
- compare local and distributed estimations



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Bibliography





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