Optimal kernel methods for large scale learning

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Learning problem

The problem $\mathcal{P}$

Find

$$f_{\mathcal{H}} = \operatorname*{argmin}_{f \in \mathcal{H}} \mathcal{E}(f), \qquad \mathcal{E}(f) = \int d\rho(x,y)(y - f(x))^2$$

with ρ **unknown** but given $(x_i, y_i)_{i=1}^n$ i.i.d. samples.

Remarks:

- stochastic optimization problem
- $\mathcal{H}$ is a space of candidate solutions.

Outline

Learning with kernels

Random projections

FALKON: Random projections and preconditioning

Kernel ridge regression

Let K p.d. kernel (e.g. $K(x, x') = e^{-\gamma\|x-x'\|^2}$) and

$$\mathcal{H} = \overline{\mathsf{span}\{K(x, \cdot) | x \in X\}},$$

Problem $\widehat{\mathcal{P}}_n$

$$\widehat{f}_\lambda = \underset{f \in \mathcal{H}}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^{n} (y_i - f(x_i))^2 + \lambda \|f\|_{\mathcal{H}}^2$$

KRR: Statistic (worst case)

Noise

$$\mathbb{E}[|Y|^p \mid X = x] \leq \frac{1}{2} p! \sigma^2 b^{p-2}, \quad \forall p \geq 2$$

Kernel boundness $\sup_x K(x, x) < \infty$.

Best model There exists $f_{\mathcal{H}}$ solving

$$\min_{f \in \mathcal{H}} \mathcal{E}(f).$$

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Best model There exists $f_{\mathcal{H}}$ solving

$$\min_{f \in \mathcal{H}} \mathcal{E}(f).$$

Theorem[(Caponnetto, De Vito '05)] Under the assumptions above

$$\mathbb{E}\mathcal{E}(\widehat{f}_\lambda) - \mathcal{E}(f_{\mathcal{H}}) \lesssim \frac{1}{\lambda n} + \lambda.$$

By selecting $\lambda_n = \frac{1}{\sqrt{n}}$

$$\mathbb{E}\mathcal{E}(\widehat{f}_{\lambda_n}) - \mathcal{E}(f_{\mathcal{H}}) \lesssim \frac{1}{\sqrt{n}}$$

KRR: Statistics (refined case)

Let $Lf(x') = \mathbb{E}K(x', x)f(x)$ and $\mathcal{N}(\lambda) = \mathrm{Trace}((L + \lambda I)^{-1}L)$
Capacity condition:

$$\mathcal{N}(\lambda) = O(\lambda^{-\gamma}), \qquad \gamma \in [0, 1]$$

Source condition:

$$f_{\mathcal{H}} \in \mathrm{Range}(L^r), \qquad r \geq 1/2$$

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Theorem[(Caponnetto, De Vito '05)] Under (basic) and (refined)

$$\mathbb{E}\mathcal{E}(\widehat{f}_\lambda) - \mathcal{E}(f_{\mathcal{H}}) \lesssim \frac{\mathcal{N}(\lambda)}{n} + \lambda^{2r}.$$

By selecting $\lambda_n = n^{-\frac{1}{2r+\gamma}}$

$$\mathbb{E}\mathcal{E}(\widehat{f}_{\lambda_n}) - \mathcal{E}(f_{\mathcal{H}}) \lesssim n^{-\frac{2r}{2r+\gamma}}$$

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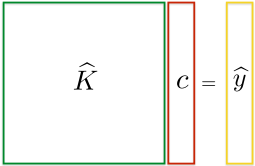
KRR: Optimization

$$\widehat{f}_\lambda(x) = \sum_{i=1}^{n} K(x, x_i) c_i$$

$$(\widehat{K} + \lambda n I)c = \widehat{y}$$

Linear System



Computations

Space $O(n^2)$ **Kernel eval.** $O(n^2)$ **Time** $O(n^3)$

Large scale ML:

Running out of time and space ... can we fix it?

Computations for optimal statistical accuracy

Model:	$O(n)$
Space:	$O(n^2)$
Kernel eval.:	$O(n^2)$
Time:	$O(n^3)$

Outline

Learning with kernels

Random projections

FALKON: Random projections and preconditioning

Random projections

Solve $\widehat{\mathcal{P}}_n$ on $\mathcal{H}_M = \mathrm{span}\{K(\tilde{x}_1, \cdot), \dots, K(\tilde{x}_M, \cdot)\}$

$$\widehat{f}_{\lambda, M} = \underset{f \in \mathcal{H}_M}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^{n} (y_i - f(x_i))^2 + \lambda \|f\|_{\mathcal{H}}^2$$

Random projections

Solve $\widehat{\mathcal{P}}_n$ on $\mathcal{H}_M = \operatorname{span}\{K(\tilde{x}_1,\cdot),\dots,K(\tilde{x}_M,\cdot)\}$

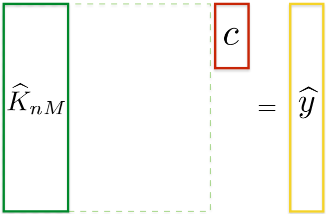
$$\widehat{f}_{\lambda,M} = \operatorname*{argmin}_{f\in\mathcal{H}_M} \frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2 + \lambda\|f\|_{\mathcal{H}}^2$$

- ... that is, pick M columns at random

$$\widehat{f}_{\lambda,M}(x) = \sum_{i=1}^{M} K(x,\tilde{x}_i)c_i$$

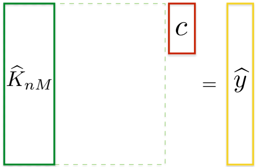
$$(\widehat{K}_{nM}^\top \widehat{K}_{nM} + \lambda n \widehat{K}_{MM})c = \widehat{K}_{nM}^\top \widehat{y}$$

Linear System



- **Nyström methods** (Smola, Scholköpf '00)
- Gaussian processes: inducing inputs (Quionero-Candela et al '05)

Nyström KRR: Computations



$$(\widehat{K}_{nM}^{\top}\widehat{K}_{nM} + \lambda n \widehat{K}_{MM})c = \widehat{K}_{nM}^{\top}\widehat{y}$$

Computations (train)

- **Space** $\cancel{O(n^2)} \to O(M_n^2)$
- **Kernel eval.** $\cancel{O(n^2)} \to O(nM_n)$
- **Time** $\cancel{O(n^3)} \to O(nM_n^2)$

Computations (test) $\cancel{O(n)} \to O(M_n)$

Nyström KRR: Statistics (worst case)

Theorem[Rudi, Camoriano, Rosasco '15] Under the basic assumptions

$$\mathbb{E}\mathcal{E}(\widehat{f}_{\lambda,M}) - \mathcal{E}(f_{\mathcal{H}}) \lesssim \frac{1}{\lambda n} + \lambda + \frac{1}{M}.$$

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By selecting $\lambda_n = \frac{1}{\sqrt{n}}$, $M_n = \frac{1}{\lambda_n}$

$$\mathbb{E}\mathcal{E}(\widehat{f}_{\lambda_n,M_n}) - \mathcal{E}(f_{\mathcal{H}}) \lesssim \frac{1}{\sqrt{n}}$$

Remarks

$$\boxed{M = O(\sqrt{n}) \text{ suffices for optimal generalization}}$$

- Previous works: only for fixed design
  (Bach '13, Alaoui, Mahoney, '15, Yang et al. '15, Musco, Musco '16)
- Matches statistical minimax lower bounds [Caponnetto, De Vito '05].
- Special case: Sobolev spaces with $s = d/2$, e.g. exponential kernel and Fourier features.
- Same statistical bound of (kernel) ridge regression [Caponnetto, De Vito '05].

Nyström KRR: Statistics (refined)

Theorem[Rudi, Camoriano, Rosasco '15] Under (basic) and (refined)

$$\mathbb{E}\mathcal{E}(\widehat{f}_{\lambda,M}) - \mathcal{E}(f_{\mathcal{H}}) \lesssim \frac{\mathcal{N}(\lambda)}{n} + \lambda^{2r} + \frac{1}{M}.$$

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By selecting $\lambda_n = n^{-\frac{1}{2r+\gamma}}$, $M_n = \frac{1}{\lambda_n}$

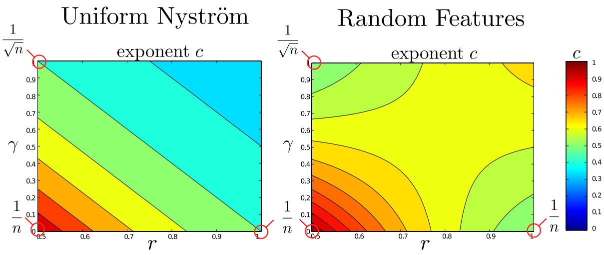
$$\mathbb{E}\mathcal{E}(\widehat{f}_{\lambda_n,M_n}) - \mathcal{E}(f_{\mathcal{H}}) \lesssim n^{-\frac{2r}{2r+\gamma}}$$

Remarks

- The obtained rate is minmax optimal [Caponnetto, De Vito '05].
- Reduces to worst case for $\gamma = 1, r = 1/2$.

Comparison with Random Features: [Rudi, Rosasco '17]

$$M = n^c$$



Computations required for $1/\sqrt{n}$ rate

$$\begin{aligned} \text{Model:} &\quad O(\sqrt{n}) \\ \text{Space:} &\quad O(n) \\ \text{Kernel eval.:} &\quad O(n\sqrt{n}) \\ \text{Time:} &\quad O(n^2) \end{aligned}$$

Possible improvements:

- adaptive sampling
- **optimization**

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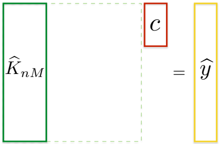
Beyond $O(n^2)$ time?

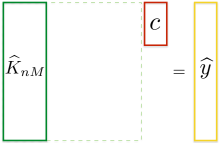
$$(\widehat{K}_{nM}^\top \widehat{K}_{nM} + \lambda n \widehat{K}_{MM})\ c \ = \ \widehat{K}_{nM}^\top \widehat{y}.$$



Bottleneck: compute $\widehat{K}_{nM}^\top \widehat{K}_{nM}$ requires $O(nM^2)$ time.

Optimization to rescue

$$\underbrace{\widehat{K}_{nM}^\top \widehat{K}_{nM} + \lambda n \widehat{K}_{MM}}_{H}\, c = \underbrace{\widehat{K}_{nM}^\top \widehat{y}}_{b}.$$



Idea: First order methods

$$c_t = c_{t-1} - \frac{\tau}{n}\left[\widehat{K}_{nM}^\top(\widehat{K}_{nM} c_{t-1} - y_n) \;+\; \lambda n \widehat{K}_{MM} c_{t-1}\right]$$

Pros: requires $O(nMt)$

Cons: $t \propto \kappa(H)$ arbitrarily large- $\kappa(H) = \sigma_{\max}(H)/\sigma_{\min}(H)$ condition number.

Preconditioning

Idea: solve an equivalent linear system with better condition number

Preconditioning

$$Hc = b \quad \mapsto \quad P^\top H P \beta = P^\top b, \quad c = P\beta.$$

Ideally $PP^\top = H^{-1}$, so that

$$t = O(\kappa(H)) \quad \mapsto \quad t = O(1)!$$

Computing a good preconditioning can be hard!

Remarks

- Preconditioning KRR (Fasshauer et al '12, Avron et al '16, Cutajat '16, Ma, Belkin '17)

$$H = K + \lambda n I$$

Can we precondition Nystrom-KRR?

Preconditioning Nystom-KRR

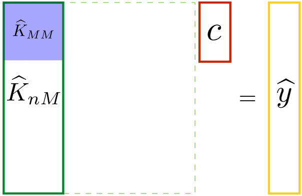
Consider $$H := \widehat{K}_{nM}^\top \widehat{K}_{nM} + \lambda n \widehat{K}_{MM}$$

Proposed Preconditioning

$$PP^\top = \left(\frac{n}{M} \widehat{K}_{MM}^2 + \lambda n \widehat{K}_{MM} \right)^{-1}$$

Compare to naive preconditioning

$$PP^\top = \left(\widehat{K}_{nM}^\top \widehat{K}_{nM} + \lambda n \widehat{K}_{MM} \right)^{-1}.$$



Baby FALKON

Proposed Preconditioning

$$PP^\top = \left(\frac{n}{M}\widehat{K}_{MM}^2 + \lambda n \widehat{K}_{MM}\right)^{-1},$$

Gradient descent

$$\widehat{f}_{\lambda,M,t}(x) = \sum_{i=1}^{M} K(x,\widetilde{x}_i)c_{t,i}, \qquad c_t = P\beta_t$$

$$\beta_t = \beta_{t-1} - \frac{\tau}{n}P^\top\left[\widehat{K}_{nM}^\top(\widehat{K}_{nM}P\beta_{t-1} - y_n) \;+\; \lambda n \widehat{K}_{MM}P\beta_{t-1}\right]$$

FALKON

- Gradient descent $\mapsto$ conjugate gradient
- Computing P

$$P = \frac{1}{\sqrt{n}} T^{-1} A^{-1}, \quad T = \mathrm{chol}(K_{MM}), \quad A = \mathrm{chol}\left(\frac{1}{M}\, TT^\top + \lambda I\right),$$

where $\mathrm{chol}(\cdot)$ is the Cholesky decomposition.

Falkon statistics (worst case)

Theorem

Under (basic), when $M > \frac{\log n}{\lambda}$*,*

$$\mathbb{E}\mathcal{E}(\widehat{f}_{\lambda_n, M_n, t_n}) - \mathcal{E}(f_{\mathcal{H}}) \lesssim \frac{1}{\lambda n} + \lambda + \frac{1}{M} + \exp\left[-t\ \left(1 - \frac{\log n}{\lambda M}\right)^{1/2}\right]$$

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By selecting

$$\lambda_n = 1/\sqrt{n}, \qquad M_n = \frac{2\log n}{\lambda}, \qquad t_n = \log n,$$

then

$$\mathbb{E}\mathcal{E}(\widehat{f}_{\lambda_n, M_n, t_n}) - \mathcal{E}(f_{\mathcal{H}}) \lesssim \frac{1}{\sqrt{n}}$$

Falkon statistics (refined results)

Theorem

Under (basic) and (refined), when $M > \frac{\log n}{\lambda}$*,*

$$\mathbb{E}\mathcal{E}(\widehat{f}_{\lambda_n, M_n, t_n}) - \mathcal{E}(f_{\mathcal{H}}) \lesssim \frac{\mathcal{N}(\lambda)}{n} + \lambda^{2r} + \frac{1}{M} + \exp\left[-t \, \left(1 - \frac{\log n}{\lambda M}\right)^{1/2}\right]$$

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By selecting

$$\lambda_n = n^{-\frac{1}{2r+\gamma}}, \qquad M_n = \frac{2\log n}{\lambda}, \qquad t_n = \log n,$$

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$$\mathbb{E}\mathcal{E}(\widehat{f}_{\lambda_n, M_n, t_n}) - \mathcal{E}(f_{\mathcal{H}}) \lesssim n^{-\frac{2r}{2r+\gamma}}$$

Remarks

Relevant works

- SGD
- RF-KRR (Rahimi, Recht '07; Bach '15; Rudi, Rosasco '17)
- Divide and conquer (Zhang et al. '13)
- NYTRO (Angles et al '16)
- Nyström SGD (Lin, Rosasco '16)

- Same statistical properties/memory requirements
- Much smaller time complexity

Proof: bridging statistics and optimization

Lemma

Let $\delta > 0$, $\kappa_P := \kappa(P^\top HP)$, $c_\delta = c_0 \log \frac{1}{\delta}$. *When* $\lambda \geq \frac{1}{n}$

$$\mathcal{E}(\widehat{f}_{\lambda,M,t}) - \mathcal{E}(f_{\mathcal{H}}) \quad \leq \quad \mathcal{E}(\widehat{f}_{\lambda,M}) - \mathcal{E}(f_{\mathcal{H}}) \quad + \quad c_\delta \exp(-t/\sqrt{\kappa_P}).$$

with probability $1 - \delta$.

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with probability $1 - \delta$.

Lemma

Let $\delta \in (0, 1], \lambda > 0$. *When*

$$M = \frac{2 \log \frac{1}{\delta}}{\lambda},$$

then

$$\kappa(P^\top H P) \leq \left(1 - \frac{\log \frac{1}{\delta}}{\lambda M}\right)^{-1} < 4$$

with probability $1 - \delta$.

Computational implications

Cost for optimal generalization with FALKON

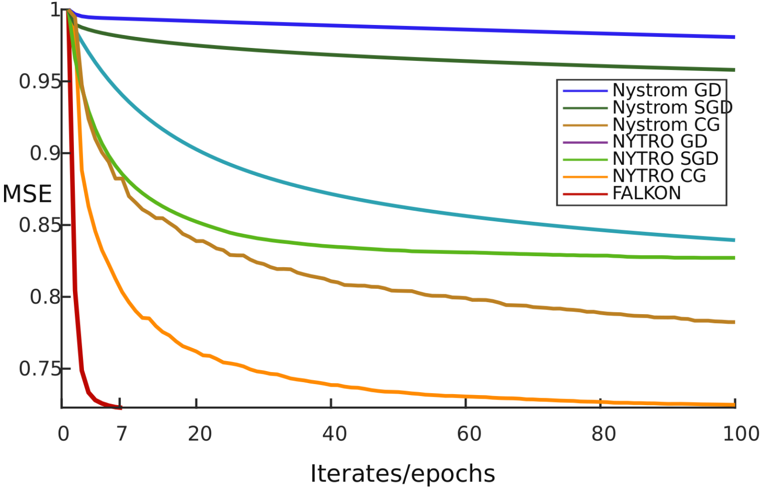
$$M_n = O(\sqrt{n}), \quad t_n = \log n$$

$$\Downarrow$$

$$\begin{aligned}
\text{Model:} \quad & O(\sqrt{n}) \\
\text{Space:} \quad & O(n) \\
\text{Kernel eval.:} \quad & O(n\sqrt{n}) \\
\text{Time:} \quad & \cancel{O(n^2)} \to O(n\sqrt{n})
\end{aligned}$$

In practice

Higgs dataset: $n = 10,000,000, \quad M = 50,000$



Some experiments

	MillionSongs ($n \sim 10^6$)			YELP ($n \sim 10^6$)		TIMIT ($n \sim 10^6$)	
	MSE	Relative error	Time(s)	RMSE	Time(m)	c-err	Time(h)
FALKON	**80.30**	$\mathbf{4.51 \times 10^{-3}}$	**55**	**0.833**	**20**	32.3%	**1.5**
Prec. KRR	-	4.58×10^{-3}	$289^{\dagger}$	-	-	-	-
Hierarchical	-	4.56×10^{-3}	$293^{\star}$	-	-	-	-
D&C	80.35	-	737^{*}	-	-	-	-
Rand. Feat.	80.93	-	772^{*}	-	-	-	-
Nyström	80.38	-	876^{*}	-	-	-	-
ADMM R. F.	-	5.01×10^{-3}	$958^{\dagger}$	-	-	-	-
BCD R. F.	-	-	-	0.949	$42^{\ddagger}$	34.0%	$1.7^{\ddagger}$
BCD Nyström	-	-	-	0.861	$60^{\ddagger}$	33.7%	$1.7^{\ddagger}$
KRR	-	4.55×10^{-3}	-	0.854	$500^{\ddagger}$	33.5%	$8.3^{\ddagger}$
EigenPro	-	-	-	-	-	32.6%	$3.9^{\wr}$
Deep NN	-	-	-	-	-	32.4%	-
Sparse Kernels	-	-	-	-	-	**30.9%**	-
Ensemble	-	-	-	-	-	33.5%	-

Table: MillionSongs, YELP and TIMIT Datasets. Times obtained on: $\ddagger$ = cluster of 128 EC2 r3.2xlarge machines, $\dagger$ = cluster of 8 EC2 r3.8xlarge machines, $\wr$ = single machine with two Intel Xeon E5-2620, one Nvidia GTX Titan X GPU and 128GB of RAM, $\star$ = cluster with 512 GB of RAM and IBM POWER8 12-core processor, $*$ = unknown platform.

Some more experiments

	SUSY ($n \sim 10^6$)			HIGGS ($n \sim 10^7$)		IMAGENET ($n \sim 10^6$)	
	c-err	AUC	Time(m)	AUC	Time(h)	c-err	Time(h)
FALKON	**19.6%**	0.877	**4**	0.833	**3**	20.7%	**4**
EigenPro	19.8%	-	$6^{\wr}$	-	-	-	-
Hierarchical	20.1%	-	$40^{\dagger}$	-	-	-	-
Boosted Decision Tree	-	0.863	-	0.810	-	-	-
Neural Network	-	0.875	-	0.816	-	-	-
Deep Neural Network	-	**0.879**	$4680^{\ddagger}$	**0.885**	$78^{\ddagger}$	-	-
Inception-V4	-	-	-	-	-	**20.0%**	-

Table: Architectures: $\dagger$ cluster with IBM POWER8 12-core cpu, 512 GB RAM, $\wr$ single machine with two Intel Xeon E5-2620, one Nvidia GTX Titan X GPU, 128GB RAM, $\ddagger$ single machine.

Contributions

- Best computations so far for optimal statistics

$$\boxed{\textbf{Space } O(n) \qquad \textbf{Time } O(n\sqrt{n})}$$

- Random projections+iterative solvers+preconditioning
- ... fast rates
- ... adaptive sampling

Next?

- Distributed architectures...
- Open the **kernel blackbox**!

Proving $\kappa(P^\top HP) \approx 1$

Let $K_x = K(x,\cdot) \in \mathcal{H}$,

$$C = \int K_x \otimes K_x d\rho_X(x), \quad \widehat{C}_n = \frac{1}{n}\sum_{i=1}^{n} K_{x_i} \otimes K_{x_i}, \quad \widehat{C}_M = \frac{1}{M}\sum_{j=1}^{M} K_{\tilde{x}_j} \otimes K_{\tilde{x}_j}.$$

Recall that $P = \frac{1}{\sqrt{n}} T^{-1}A^{-1}, T = \mathrm{chol}(K_{MM}), A = \mathrm{chol}\left(\frac{1}{M}\ TT^\top + \lambda I\right)$.

Steps

$$1. \quad P^\top HP = A^{-\top}V^*(\widehat{C}_n + \lambda I)VA^{-1}$$

Proving $\kappa(P^\top HP) \approx 1$

Let $K_x = K(x, \cdot) \in \mathcal{H}$,

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Steps

$$2. \quad P^\top HP \;=\; A^{-\top}V^*(\widehat{C}_M + \lambda I)VA^{-1} \;+\; A^{-\top}V^*(\widehat{C}_n - \widehat{C}_M)VA^{-1}$$

Proving $\kappa(P^\top HP) \approx 1$

Let $K_x = K(x, \cdot) \in \mathcal{H}$,

$$C = \int K_x \otimes K_x d\rho_X(x), \quad \widehat{C}_n = \frac{1}{n}\sum_{i=1}^{n} K_{x_i} \otimes K_{x_i}, \quad \widehat{C}_M = \frac{1}{M}\sum_{j=1}^{M} K_{\tilde{x}_j} \otimes K_{\tilde{x}_j}.$$

Recall that $P = \frac{1}{\sqrt{n}} T^{-1} A^{-1}, T = \mathrm{chol}(K_{MM}), A = \mathrm{chol}\left(\frac{1}{M}\ TT^\top + \lambda I\right)$.

Steps

$$3. \quad P^\top HP \;=\; I \;+\; A^{-\top} V^* (\widehat{C}_n - \widehat{C}_M) V A^{-1}$$

Proving $\kappa(P^\top H P) \approx 1$

Let $K_x = K(x, \cdot) \in \mathcal{H}$,

$$C = \int K_x \otimes K_x d\rho_X(x), \quad \widehat{C}_n = \frac{1}{n}\sum_{i=1}^{n} K_{x_i} \otimes K_{x_i}, \quad \widehat{C}_M = \frac{1}{M}\sum_{j=1}^{M} K_{\tilde{x}_j} \otimes K_{\tilde{x}_j}.$$

Recall that $P = \frac{1}{\sqrt{n}} T^{-1} A^{-1}, T = \mathrm{chol}(K_{MM}), A = \mathrm{chol}\left(\frac{1}{M}\ TT^\top + \lambda I\right).$

Steps

$$3. \quad P^\top H P \;=\; I \;+\; E \quad \text{with } E = A^{-\top} V^* (\widehat{C}_n - \widehat{C}_M) V A^{-1}$$

Proving $\kappa(P^\top H P) \approx 1$

Let $K_x = K(x, \cdot) \in \mathcal{H}$,

$$C = \int K_x \otimes K_x d\rho_X(x), \quad \widehat{C}_n = \frac{1}{n}\sum_{i=1}^{n} K_{x_i} \otimes K_{x_i}, \quad \widehat{C}_M = \frac{1}{M}\sum_{j=1}^{M} K_{\tilde{x}_j} \otimes K_{\tilde{x}_j}.$$

Recall that $P = \frac{1}{\sqrt{n}} T^{-1} A^{-1}, T = \mathrm{chol}(K_{MM}), A = \mathrm{chol}\left(\frac{1}{M}\ TT^\top + \lambda I\right)$.

Steps

$$4. \quad \kappa(P^\top H P) = \kappa(I + E) \le \frac{1 + \|E\|}{1 - \|E\|}, \quad \text{when } \|E\| < 1,$$

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Steps

$$5. E = A^{-\top} V^* (\widehat{C}_n - \widehat{C}_M) V A^{-1} \leq 1/2 \text{ w.h.p. when } M \geq \frac{c_0 \log \frac{1}{\delta}}{\lambda}$$