Greedy Kernel Techniques with Applications to Machine Learning

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Overview

1. Historical Remarks: From RBF to Kernels
2. Kernel Techniques
3. Simplification by Relaxation
4. Online Learning and Greedy Methods

Development of Kernel Techniques

1. Radial Basis Functions (with a little help from Will)
2. Computer–Aided Design
3. Meshless Methods for PDE Solving in Engineering
4. Learning with Kernels

Reconstruction of Functions

Problem: Find $u\ :\ \Omega \to I\!R$

Given: Data

Discrete scattered data	$(x_j, u(x_j)),\ \ 1 \le j \le N$
PDE data	$\left\{ \begin{array}{ll} (x, \Delta u(x)) & x \in \Omega \\ (y, u(y)) & y \in \partial\Omega \end{array} \right\}$
General functionals	$(\lambda, \lambda(u)),\ \ \lambda \in \Lambda =$ set of functionals

Learning

Problem: Find $u\ :\ \Omega \ni$ Stimulus $\mapsto$ Response

Given: Training data

$$(x_j, u(x_j)),\ \ 1 \le j \le N$$

Why Kernels?

Data $(x_j, u(x_j)) \in \Omega \times I\!R,\ 1 \le j \le N$

General linear reconstruction:

$$\tilde{u}(x) := \sum_{j=1}^{n} \underbrace{L_j(x)}_{=?} u(x_j)$$

Error estimate

$$\begin{aligned}
|u(x) - \tilde{u}(x)|^2 &= \left| u(x) - \sum_{j=1}^{n} L_j(x) u(x_j) \right|^2 \\
&= \left| \left(\delta_x - \sum_{j=1}^{n} L_j(x) \delta_{x_j} \right) (u) \right|^2 \\
&\le \underbrace{\left\| \delta_x - \sum_{j=1}^{n} L_j(x) \delta_{x_j} \right\|_{H^*}^2}_{\text{minimize wrt. } L_j(x)} \|u\|_H^2 \\
\underbrace{(\delta_x, \delta_{x_k})_{H^*}}_{=:K(x,x_k)} &= \sum_{j=1}^{n} L_j^*(x) \underbrace{(\delta_{x_j}, \delta_{x_k})_{H^*}}_{=:K(x_j,x_k)},\ 1 \le k \le N
\end{aligned}$$

Optimal L_j^* is Lagrange interpolant
on span $\{K(x, x_k)\ :\ 1 \le k \le N\}$

Necessary: $u \in$ RKHS H

Generalization: Arbitrary data functionals $\lambda \in H^*$
(meshless collocation methods)

Generalized Data

Data $(\lambda_j, \lambda_j(u)) \in H^* \times I\!R,\ 1 \leq j \leq N$

General linear reconstruction:

$$\tilde{u} := \sum_{j=1}^{n} \underbrace{L_j}_{=?} \lambda_j u$$

Error estimate with test functional $\mu \in H^*$

$$\begin{aligned}
|\mu(u) - \mu(\tilde{u})|^2 &= \left| \mu(u) - \sum_{j=1}^{n} \mu(L_j)\lambda_j(u) \right|^2 \\
&= \left| \left(\mu - \sum_{j=1}^{n} \mu(L_j)\lambda_j \right)(u) \right|^2 \\
&\leq \underbrace{\left\| \mu - \sum_{j=1}^{n} \mu(L_j)\lambda_j \right\|_{H^*}^2}_{\text{minimize wrt. } \mu(L_j)} \|u\|_H^2 \\
\underbrace{(\mu, \lambda_k)_{H^*}}_{=:K(\mu,\lambda_k)} &= \sum_{j=1}^{n} \mu(L_j^*) \underbrace{(\lambda_j, \lambda_k)_{H^*}}_{=:K(\lambda_j,\lambda_k)},\ 1 \leq k \leq N
\end{aligned}$$

Optimal L_j^* is Lagrange interpolant
on span $\{\text{Riesz representer of } \lambda_k\ :\ 1 \leq k \leq N\}$

Necessary: $u \in$ RKHS H, $\lambda_j \in H^*$

Second Optimality Property

Data $(x_j, u(x_j)) \in \Omega \times I\!R,\ 1 \leq j \leq N$

Optimal linear reconstruction:

$$u^*(x) := \sum_{j=1}^{n} L_j^*(x) u(x_j)$$

Minimization of norm under all other interpolants:

$$\|u^*\|_H = \min \left\{ \|v\|_H \ : \ \begin{array}{l} v \in H \\ v(x_j) = u(x_j),\ 1 \leq j \leq N \end{array} \right\}$$

Learning with Kernels

Training data $(x_j, u(x_j)) \in \Omega \times I\!R,\ 1 \le j \le N$

Kernel Trick:

$$\begin{array}{rcl} \Phi & & \Omega \to H = \textbf{feature space} \\ \Phi(x) & := & K(x,\cdot) \in H \\ K(x,y) & = & (K(x,\cdot), K(y,\cdot))_H \\ & = & (\Phi(x), \Phi(y))_H \\ u^*(x) & = & \sum_{j=1}^{N} L_j^* u(x_j) \\ & = & \sum_{j=1}^{N} \alpha_j^* K(x, x_j) \end{array}$$

Optimal L_j^* is Lagrange interpolant
on span $\{K(x, x_k)\ :\ 1 \le k \le N\}$

Minimization of norm
under all other interpolants:

$$\|u^*\|_H = \min \left\{ \|v\|_H\ :\ \begin{array}{l} v \in H \\ v(x_j) = u(x_j),\ 1 \le j \le N \end{array} \right\}$$

For Classification:

Minimization of $\|v\|_H$ is maximization
of separation margin

Simplification by Relaxation

Unrelaxed:

$$\begin{aligned} \|u^*\|_H &= \min \left\{ \|v\|_H \;:\; \begin{array}{l} v \in H \\ v(x_j) = u(x_j),\ 1 \le j \le N \end{array} \right\} \\ u^*(x) &= \sum_{j=1}^{N} L_j^* u(x_j) \\ &= \sum_{j=1}^{N} \alpha_j^* K(x, x_j) \qquad \textbf{full}\text{ sum!} \end{aligned}$$

Relaxed: Given $\epsilon \ge 0$

$$\begin{aligned} \|u^*\|_H &= \min \left\{ \|v\|_H \;:\; \begin{array}{l} v \in H \\ |v(x_j) - u(x_j)| \le \epsilon,\ 1 \le j \le N \end{array} \right\} \\ u^*(x) &= \sum_{\substack{j=1 \\ |v(x_j)-u(x_j)|=\epsilon}}^{N} \alpha_j^* K(x, x_j) \qquad \textbf{reduced}\text{ sum!} \end{aligned}$$

Reason: Kuhn–Tucker conditions for linear constraints

Support Vectors: $x_j^{\pm}$ with $v(x_j^{\pm}) - u(x_j^{\pm}) = \pm\epsilon$

Quadratic problem: Minimize $\|v\|_H^2 = \sum_{j,k=1}^{N} \alpha_j \alpha_k K(x_k, x_j)$

Open problem: Bound on # of support vectors

Online Learning

Given $\epsilon \geq 0$. Current "knowledge":

$$u^*(x) = \sum_{\substack{j=1 \\ |v(x_j)-u(x_j)|=\epsilon}}^{\mathbf{n}} \alpha_j^* K(x, x_j) \text{ **reduced** sum!}$$

Iteration of Online Learning:

1. Wait for new training sample $(x, u(x))$
2. If $|u(x) - u^*(x)| \leq \epsilon$ do nothing.
3. If $|u(x) - u^*(x)| > \epsilon$ set $x_{n+1} := x$ and update u^* to u^{**} with (**Learning by new blunders**)

$$|u(x_j) - u^{**}(x_j)| \leq \epsilon, \quad 1 \leq j \leq n+1.$$

Theorem $\|u^*\|_H < \|u^{**}\|_H$ (knowledge gain)

The increase can be quantified and bounded below.

Theorem If Ω is compact, and if the presented samples satisfy

$$h_k := \sup_{y \in \Omega} \min_{1 \leq j \leq k} \|y - x_j\|_2 \to 0 \text{ for } k \to \infty$$

the algorithm performs only a finite number of steps.

Snape Teaching

Theorem If Ω is compact, and if the teacher always poses the hardest possible problem, i.e.

$$|u(x_{n+1}) - u^*(x_{n+1})| = \|u - u^*\|_{\infty,\Omega}$$

then the algorithm performs only a finite number of steps.

Drawback: Number of memorized samples grows

Goal: Forgetting well–learned samples

Forgetful Students

Given $\epsilon > \delta \geq 0$. Current “knowledge”:

$$u^*(x) = \sum_{\substack{j=1 \\ |v(x_j)-u(x_j)|=\delta}}^{\mathbf{n}} \alpha_j^* K(x, x_j) \text{ \textbf{reduced} sum!}$$

Iteration of Forgetful Online Learning:

1. Wait for new training sample $(x, u(x))$
2. If $|u(x) - u^*(x)| \leq \epsilon$ do nothing.
3. If $|u(x) - u^*(x)| > \epsilon$ set $x_{n+1} := x$ and update u^* to u^{**} with (**Learning by new blunders**)

$$|u(x_j) - u^{**}(x_j)| \leq \delta, \quad 1 \leq j \leq n+1.$$

4. Discard old samples with $< \delta$ above.
   (**Forget well–managed samples**)

Theorem Similar results as in the “memorizing” case.

Implementation

Given $\epsilon \geq 0$, training data $(x_j, u(x_j)),\ 1 \leq j \leq n$.

Quadratic Optimization Problem

$$\text{Minimize} \quad \sum_{j,k=1}^{n} \alpha_j \alpha_k K(x_j, x_k)$$

$$-\epsilon \leq \sum_{j=1}^{n} \alpha_j K(x_j, x_k) - u(x_k) \leq \epsilon, \quad 1 \leq k \leq n$$

Required:
Fast update method based on active sets

Problem:
Quadratic objective function

Current workaround:
Linear systems for interpolation,
Greedy Techniques

Example: Previous algorithm with $\delta = 0$.

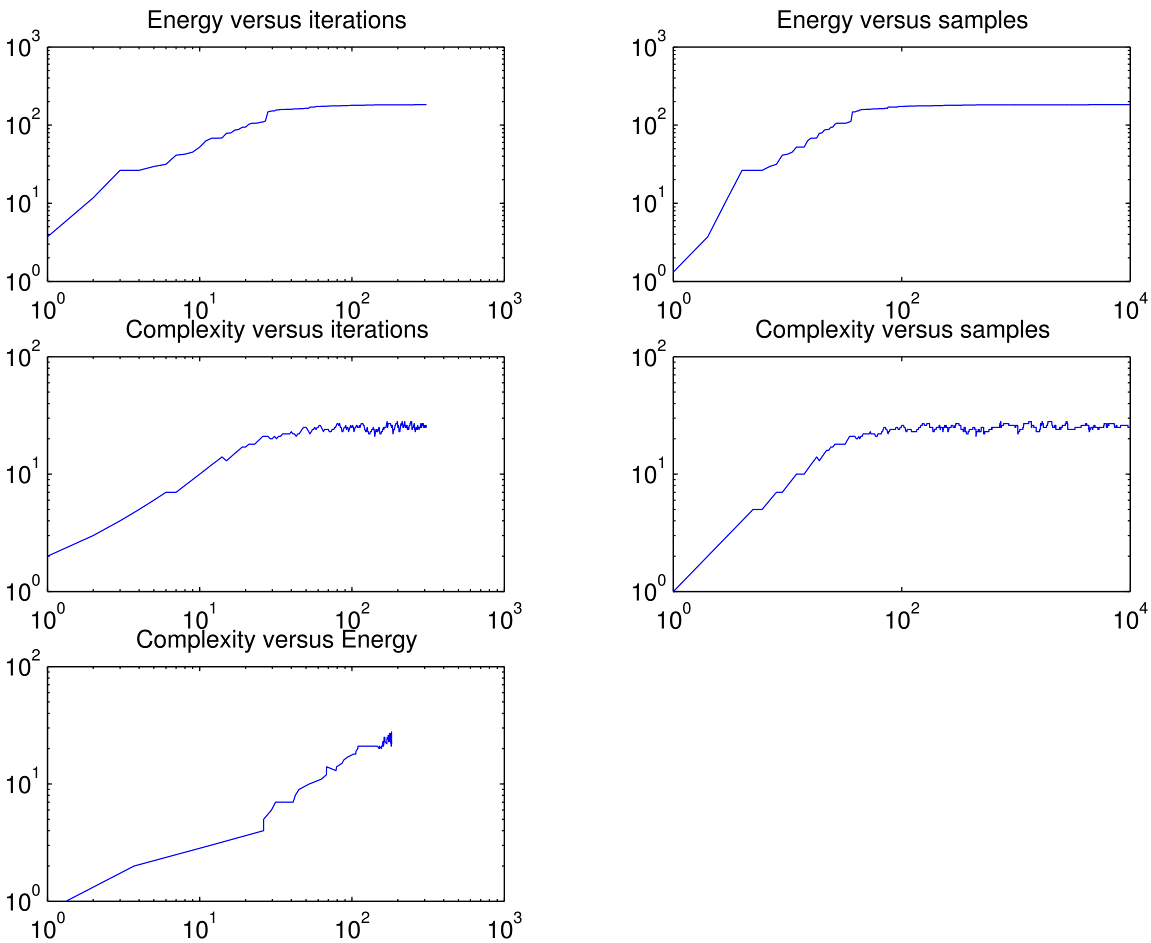
Learning the "peaks" Function

Online learning, random samples, $\epsilon = 0.01$

After some 100 samples: starts to discard

After some 400 learning steps: nothing to learn

Final complexity: about 35 support vectors



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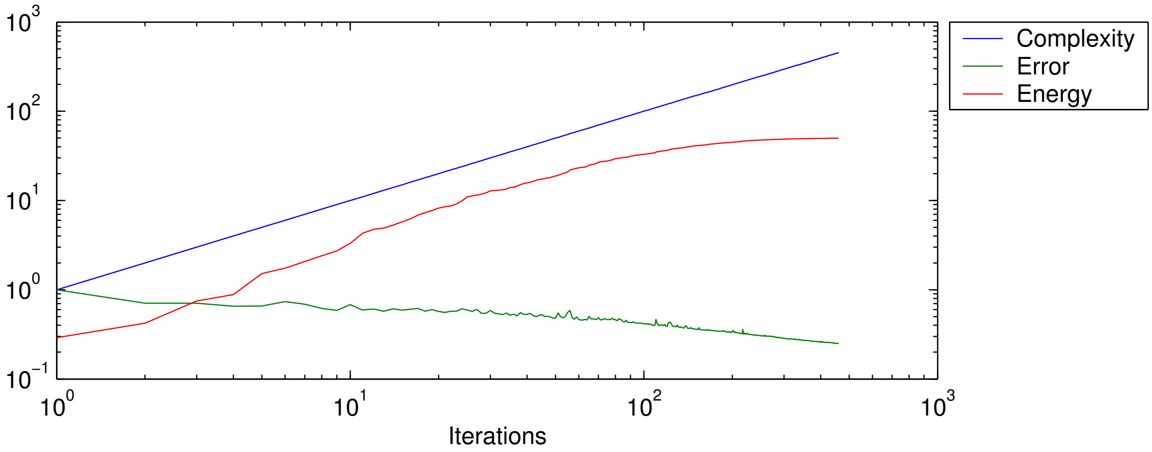
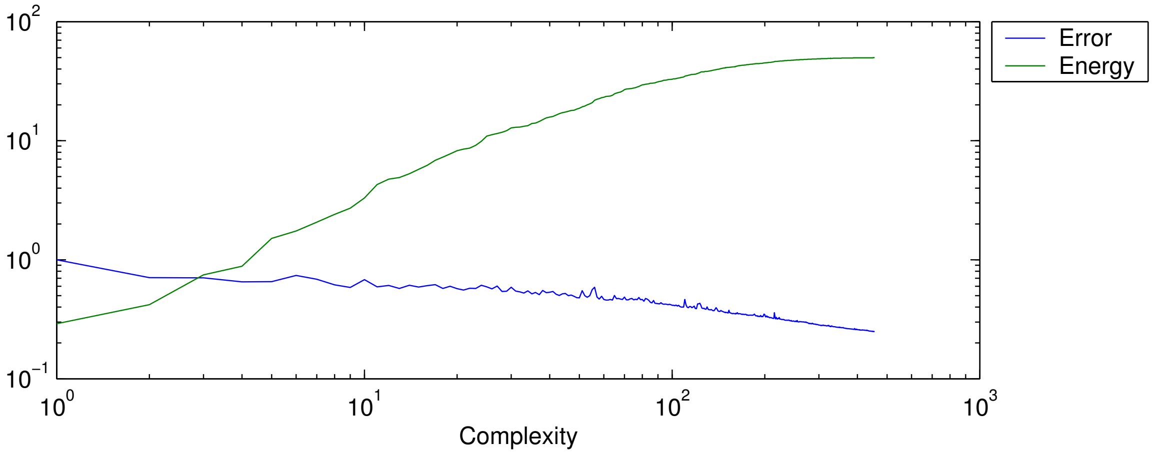
Boston Census Data

22784 training samples with 16 variables describing input data for estimating the price of houses from the 1990 US census. Method: Greedy with Snape teaching





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Open Problems

Find non–quadratic forgetful method

Find fast quadratic update method

Prove upper bounds for number of support vectors

Understand bias–variance tradeoff

Use learning techniques for solving PDEs