Kernel approaches to covariate shift

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Transfer learning and covariate shift

- Patterns $\mathcal{X}$, labels $\mathcal{Y}$
- Training: get Z_{tr} are n_{tr} pairs $(x^{\mathrm{tr}}, y^{\mathrm{tr}})$ from $\mathbf{P}_{\mathrm{tr}}$
- Test: get Z_{te} are n_{te} pairs $(x^{\mathrm{te}}, y^{\mathrm{te}})$ from $\mathbf{P}_{\mathrm{te}}$
- Predict on $\mathbf{P}_{\mathrm{te}}$ given data from $\mathbf{P}_{\mathrm{tr}}$
- Examples:
  - Medical diagnosis
  - Brain computer interfaces
  - Gene expression profiles

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Does this make sense?

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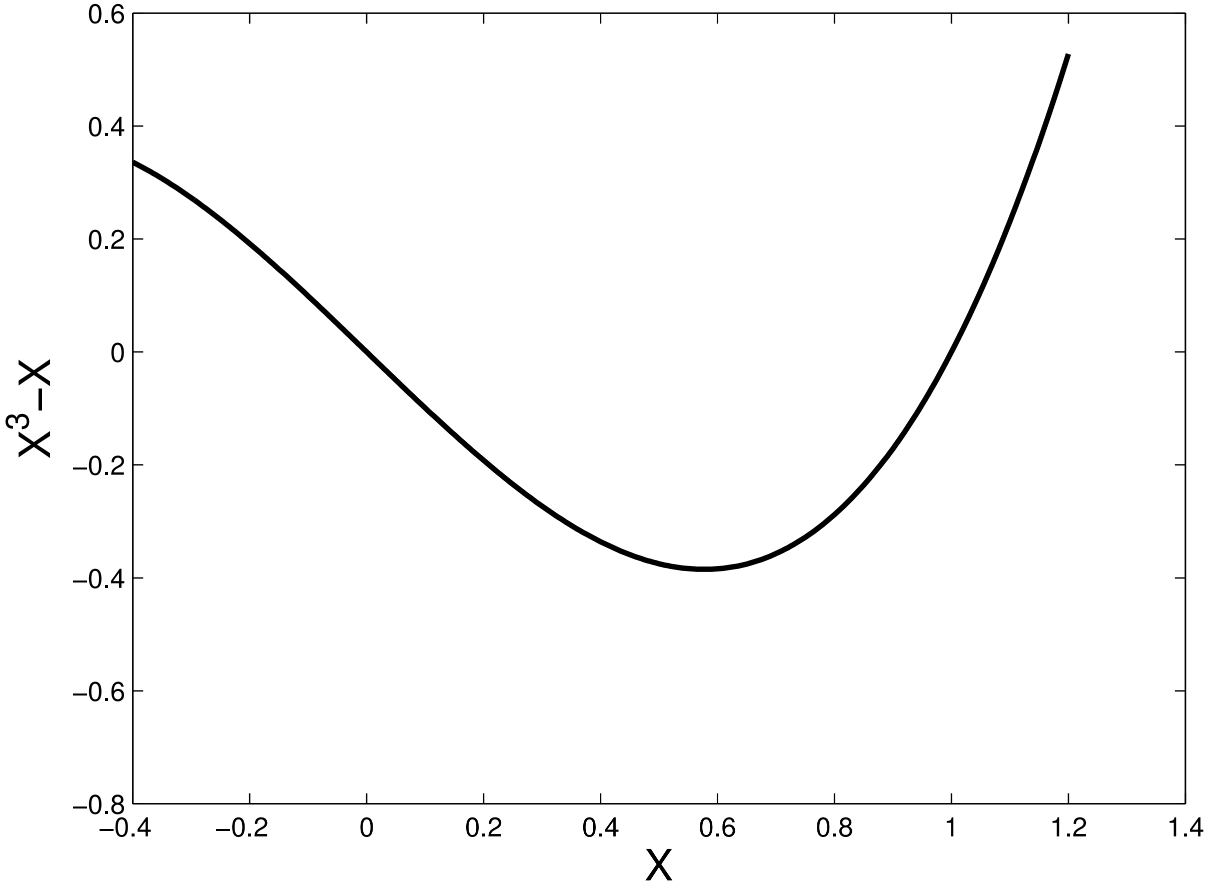
- Examples:
  - Medical diagnosis
  - Brain computer interfaces
  - Gene expression profiles
- Assumption: $\mathbf{P}_{\mathrm{tr}}(x, y) = \mathbf{P}(y|x)\mathbf{P}_{\mathrm{tr}}(x)$ and $\mathbf{P}_{\mathrm{te}}(x, y) = \mathbf{P}(y|x)\mathbf{P}_{\mathrm{te}}(x)$

Conditional probs unchanged: covariate shift

A toy example

- Toy data [Shimodaira, 2000]
  - $\mathbf{P}_{\mathrm{tr}}(x) \sim \mathcal{N}(0.5, 0.5^2)$,
  - $\mathbf{P}_{\mathrm{te}}(x) \sim \mathcal{N}(0, 0.3^2)$

- $y = -x + x^3 + \epsilon$, where $\epsilon \sim \mathcal{N}(0, 0.3^2)$
- Linear regression



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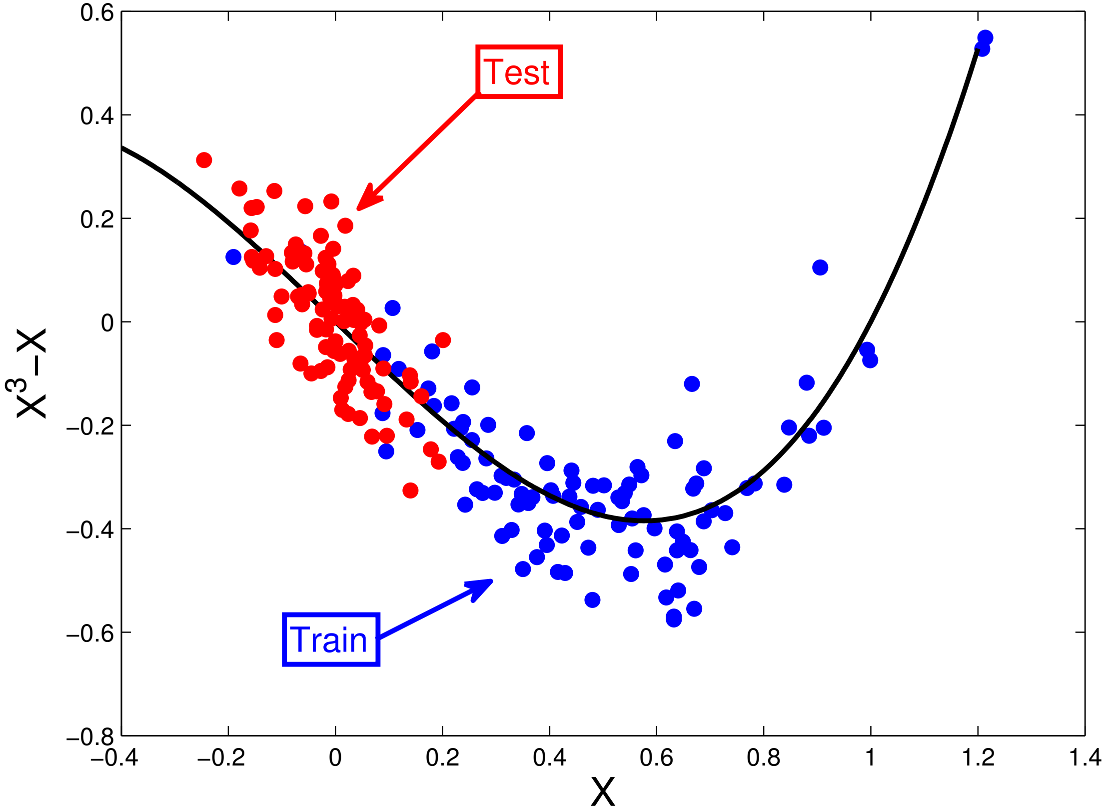

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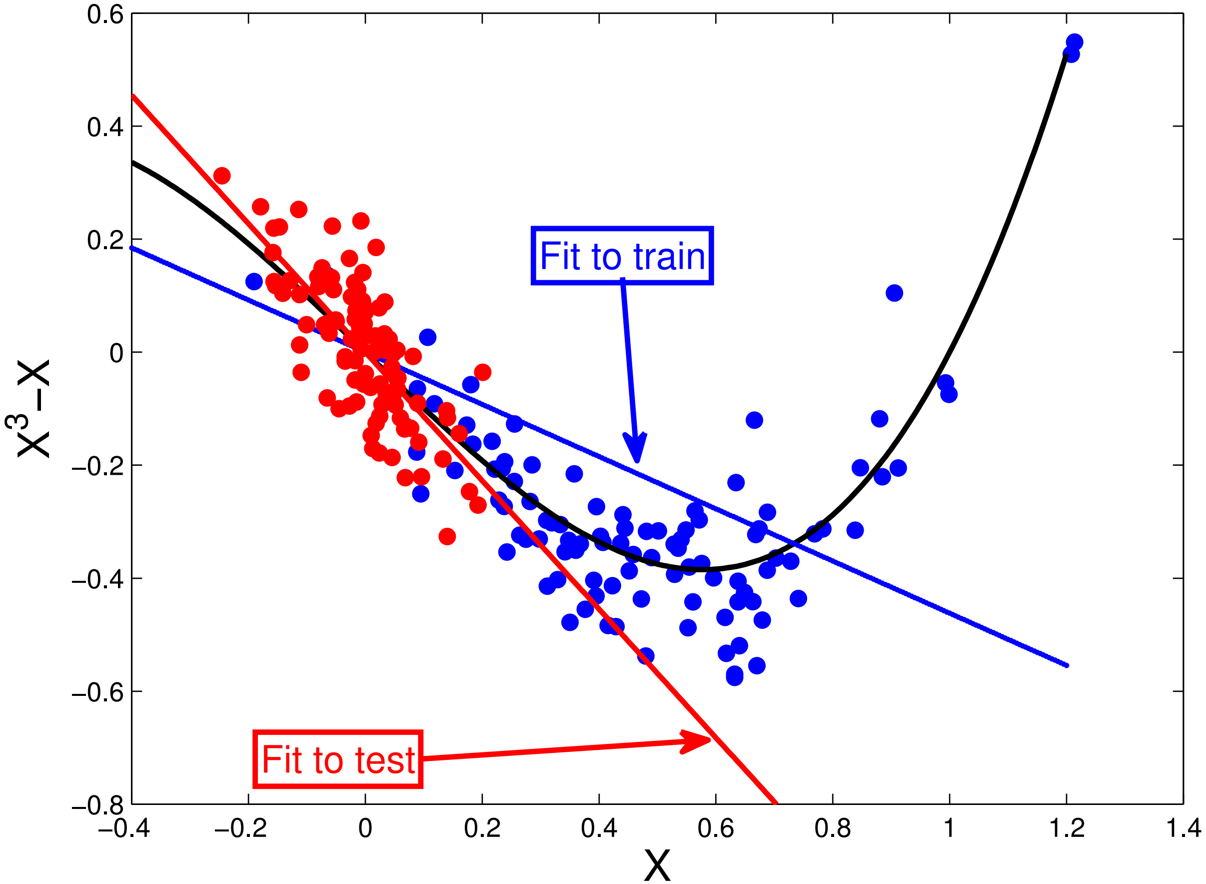

The solution procedure

- Classical setting: (regularized) expected risk

$$R[\mathbf{P}, l(x, y, \theta)] = \mathbf{E}\left[l(x, y, \theta)\right] + \lambda\Omega[\theta]$$

  - Loss $l(x, y, \theta)$, eg $-\log \mathbf{P}(y|x, \theta)$
  - Minimize over θ

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- Covariate shift setting:

$$\begin{aligned} R[\mathbf{P}_{\mathrm{te}}, l(x,y,\theta)] &= \mathbf{E}_{\mathbf{P}_{\mathrm{te}}}\left[l(x,y,\theta)\right] + \lambda\Omega[\theta] \\ &= \mathbf{E}_{\mathbf{P}_{\mathrm{tr}}}\left[\beta(x,y) l(x,y,\theta)\right] + \lambda\Omega[\theta] \end{aligned}$$

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- Importance weighting:

$$\mathbf{E}_{\mathbf{P}_{\mathrm{te}}}\left[l(x,y,\theta)\right] = \mathbf{E}_{\mathbf{P}_{\mathrm{tr}}}\Bigg[\underbrace{\frac{\mathbf{P}_{\mathrm{te}}(x,y)}{\mathbf{P}_{\mathrm{tr}}(x,y)}}_{:=\beta_{\mathrm{imp}}(x,y)} l(x,y,\theta)\Bigg] \quad \text{provided} \quad \mathbf{P}_{\mathrm{te}} \ll \mathbf{P}_{\mathrm{tr}}$$

Importance weighting

- Variance of importance weighted risk [Robert and Casella, 2004]

$$\mathrm{var}\left(l(x,y,\theta)\frac{\mathbf{P}_{\mathrm{te}}(x,y)}{\mathbf{P}_{\mathrm{tr}}(x,y)} \right)$$
$$= \mathbf{E}_{\mathbf{P}_{\mathrm{tr}}}\left[l^2(x,y,\theta)\frac{{\mathbf{P}_{\mathrm{te}}}^2(x,y)}{{\mathbf{P}_{\mathrm{tr}}}^2(x,y)} \right] - \left(\mathbf{E}_{\mathbf{P}_{\mathrm{te}}}\left[l(x,y,\theta)\right]\right)^2$$

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$$\begin{aligned}
&\mathrm{var}\left(l(x,y,\theta)\frac{\mathsf{P}_{\mathrm{te}}(x,y)}{\mathsf{P}_{\mathrm{tr}}(x,y)}\right)\\
&= \mathbf{E}_{\mathsf{P}_{\mathrm{tr}}}\left[l^2(x,y,\theta)\frac{{\mathsf{P}_{\mathrm{te}}}^2(x,y)}{{\mathsf{P}_{\mathrm{tr}}}^2(x,y)}\right] - R^2[\mathsf{P}_{\mathrm{te}},\theta,l(x,y,\theta)]\\
&= \mathbf{E}_{\mathsf{P}_{\mathrm{te}}}\left[l^2(x,y,\theta)\frac{\mathsf{P}_{\mathrm{te}}(x,y)}{\mathsf{P}_{\mathrm{tr}}(x,y)}\right] - R^2[\mathsf{P}_{\mathrm{te}},\theta,l(x,y,\theta)]
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&= \mathbf{E}_{\mathbf{P}_{\mathrm{te}}}\left[l^2(x,y,\theta)\underbrace{\frac{\mathbf{P}_{\mathrm{te}}(x,y)}{\mathbf{P}_{\mathrm{tr}}(x,y)}}_{\leq B}\right] - R^2[\mathbf{P}_{\mathrm{te}},\theta,l(x,y,\theta)]
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\end{aligned}$$

- $\mathbf{P}_{\mathrm{tr}}$ should have heavier tails than $\mathbf{P}_{\mathrm{te}}$

Importance weighting

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- Loss $l(x, y, \theta) = (y - \langle \Phi(x), \theta \rangle)^2$

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$$\underset{\theta}{\text{minimize}} \sum_{i=1}^{n_{\text{tr}}} \beta_i (y_i^{\text{tr}} - \left\langle \Phi(x_i^{\text{tr}}), \theta \right\rangle)^2 + \lambda \left\| \theta \right\|^2. \tag{2}$$

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- Equivalently:

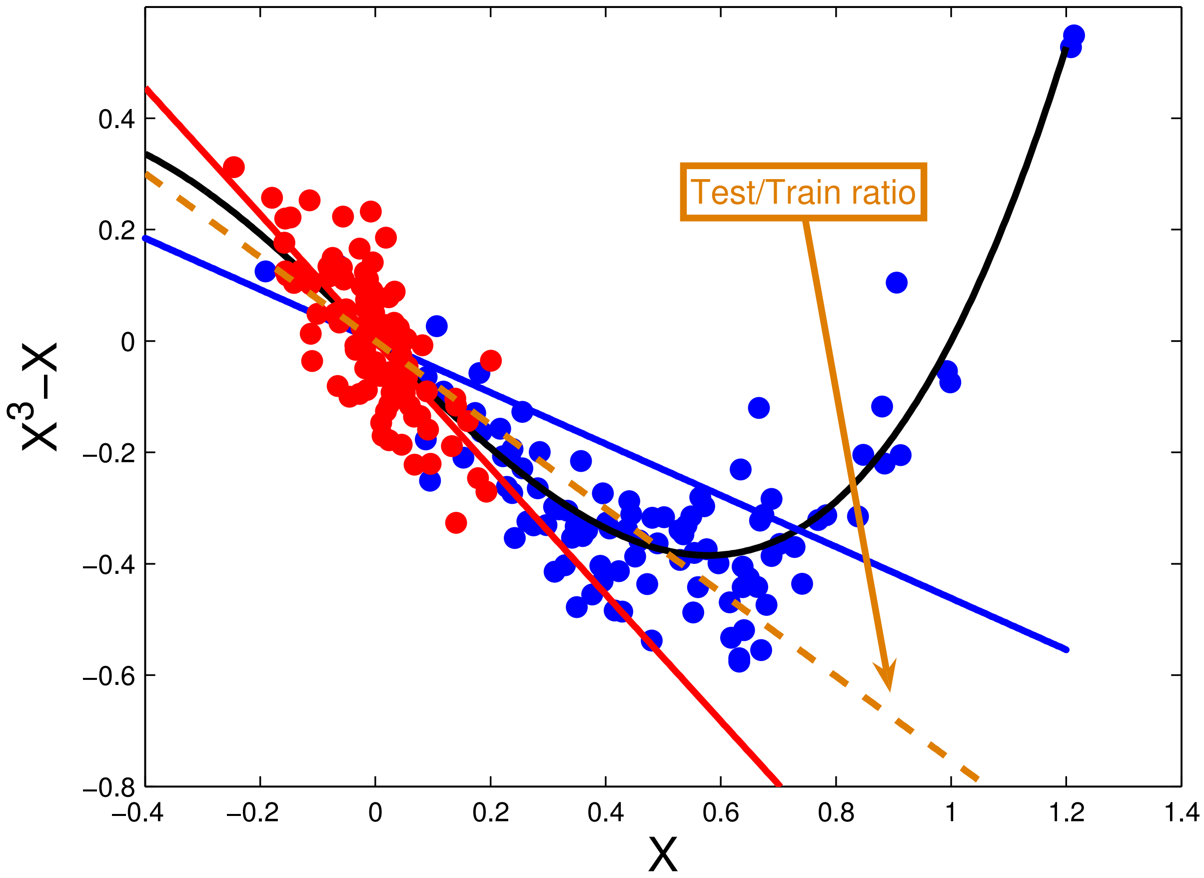
$$\underset{\alpha}{\text{minimize}} \quad (y - K\alpha)^\top \bar{\beta} (y - K\alpha) + \lambda \alpha^\top K \alpha$$

  - $\bar{\beta} = \text{diag}(\beta_1, \ldots, \beta_{n_{\text{tr}}})$
  - $K_{ij} = k(x_i^{\text{tr}}, x_j^{\text{tr}}) = \left\langle \Phi(x_i^{\text{tr}}), \Phi(x_j^{\text{tr}}) \right\rangle$
- Solution

$$\alpha = (\lambda \bar{\beta}^{-1} + K)^{-1} y$$

Importance weighting

- Ridge regression, linear kernel
- Importance weighting improves performance



Alternatives to density estimation

- Difficulties with direct density estimation
  - Empirical $\mathbf{P}_{\mathrm{tr}}$ and $\mathbf{P}_{\mathrm{te}}$ difficult for structured/high dimensional data
  - Variance can be large if empirical $\mathbf{P}_{\mathrm{te}}/\mathbf{P}_{\mathrm{tr}}$ large

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- Some other reweighting approaches:
  - Minimize classification error of $\mathbf{P}_{\text{tr}}$ vs $\mathbf{P}_{\text{te}}$ [Qin, 1998, Cheng and Chu, 2004, Bickel et al., 2009]
  - Minimize KL divergence between $\mathbf{P}_{\text{tr}}$ and $\mathbf{P}_{\text{te}}$ (KLIEP) [Sugiyama et al., 2008]
  - Ratio $\mathbf{P}_{\text{te}}/\mathbf{P}_{\text{tr}}$ via least-squares function fitting [Kanamori et al., 2009]
  - Minimize Maximum Mean Discrepancy (MMD) between $\mathbf{P}_{\text{tr}}$ and $\mathbf{P}_{\text{te}}$ [Huang et al., 2007, Gretton et al., 2008]

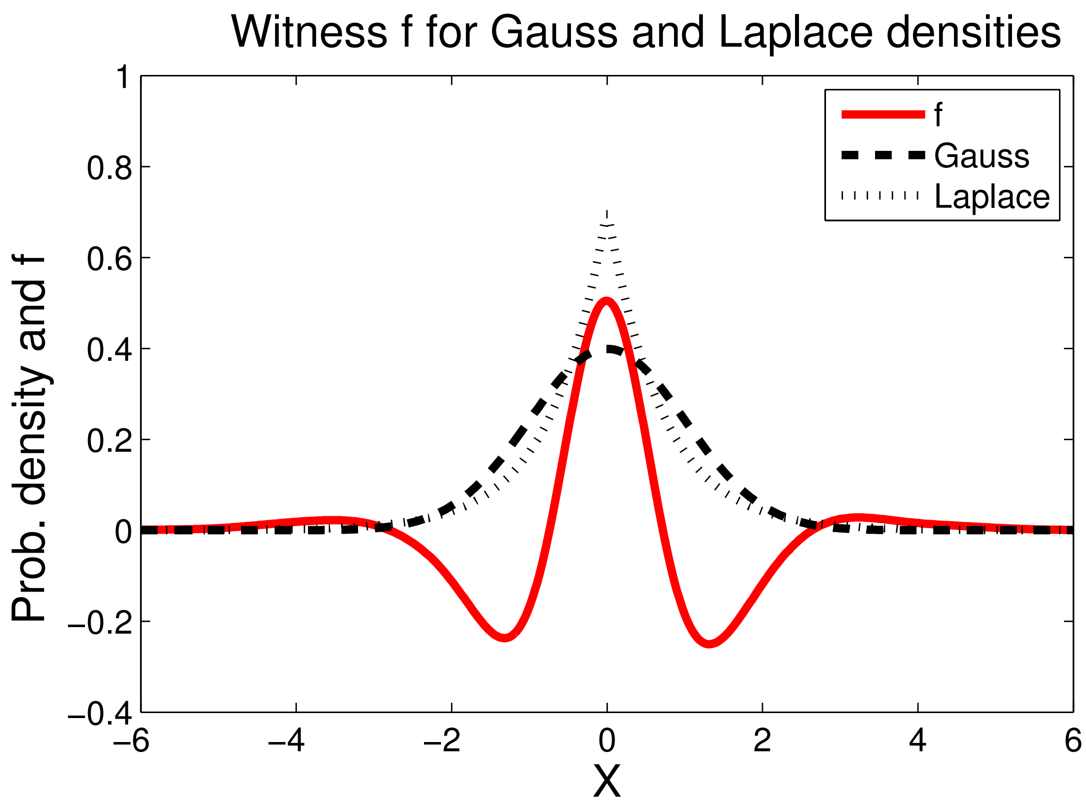
Maximum mean discrepancy

Function Showing Difference in Distributions

- Idea: avoid density estimation when comparing distributions **P** and **Q**

$$\mathrm{MMD}(\mathbf{P}, \mathbf{Q}; F) := \sup_{f \in F} \left[\mathbf{E}_{\mathbf{P}} f(x) - \mathbf{E}_{\mathbf{Q}} f(y) \right].$$

- Example: Gauss **P** vs Laplace **Q**



Function Showing Difference in Distributions

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  [Fortet and Mourier, 1953]

$$\mathrm{MMD}(\mathbf{P},\mathbf{Q};F) := \sup_{f\in F}\left[\mathbf{E}_{\mathbf{P}} f(\mathsf{x}) - \mathbf{E}_{\mathbf{Q}} f(\mathsf{y})\right].$$

- Classical results: $\mathrm{MMD}(\mathbf{P},\mathbf{Q};F) = 0$ iff $\mathbf{P} = \mathbf{Q}$, when
  - $F =$bounded continuous [Dudley, 2002]
  - $F =$ bounded variation 1 (Kolmogorov metric) [Müller, 1997]
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- $\mathrm{MMD}(\mathbf{P}, \mathbf{Q}; F) = 0$ iff $\mathbf{P} = \mathbf{Q}$ when $F =$the unit ball in a characteristic RKHS $\mathcal{F}$ [Fukumizu et al., 2008, Sriperumbudur et al., 2008]

Function Showing Difference in Distributions (2)

- $\mathcal{F}$ RKHS from $\mathcal{X}$ to $\mathbb{R}$ with positive definite kernel $k(x_i, x_j)$
- $\mathcal{F} = \overline{\text{span}\{k(x, \cdot) | x \in \mathcal{X}\}}$
  - Example: $f(\cdot) = \sum_{i=1}^{m} \alpha_i k(x_i, \cdot)$ for arbitrary $m \in \mathbb{N}$, $\alpha_i \in \mathbb{R}$, $x_i \in \mathcal{X}$.

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- Kernel is inner product between two feature maps:

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- Evaluating functions at x

$$f(x) = \langle f, \Phi(x) \rangle_{\mathcal{F}}$$

  - $\Phi(x)$ feature map

Function Showing Difference in Distributions

- The (kernel) MMD: [Gretton et al., 2007]

$$\mathrm{MMD}^2(\mathsf{P}, \mathsf{Q}; F)$$

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using

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$$=: \langle \mu_x, f \rangle_{\mathcal{F}}$$

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$$= \|\mu_x - \mu_y\|_{\mathcal{F}}^2$$

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$$= \mathbf{E}_{\mathbf{P},\mathbf{P}} k(\mathsf{x}, \mathsf{x}') + \mathbf{E}_{\mathbf{Q},\mathbf{Q}} k(\mathsf{y}, \mathsf{y}') - 2\mathbf{E}_{\mathbf{P},\mathbf{Q}} k(\mathsf{x}, \mathsf{y})$$

- x' is a R.V. independent of x with distribution $\mathbf{P}$
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- Mean map:

$$\mu_x := \mathbf{E}_{\mathbf{P}} \Phi(\mathsf{x}) = \int k(\cdot, x)\, d\mathbf{P}(x)$$

Transfer learning using maximum mean discrepancy

Transfer learning by KMM

Kernel mean matching (KMM)

Transfer learning by KMM

Kernel mean matching (KMM)

- Reweight training points so feature means match

$$\underset{\beta}{\text{minimize}} \quad \left\| \mu(\mathsf{P}_{\text{te}}) - \mathbf{E}_{\mathsf{P}_{\text{tr}}}\left[\beta(x)\Phi(x)\right] \right\|$$
$$\text{subject to } \beta(x) \geq 0 \text{ and } \mathbf{E}_{\mathsf{P}_{\text{tr}}}\left[\beta(x)\right] = 1.$$

- If $\mathsf{P}_{\text{te}} \ll \mathsf{P}_{\text{tr}}$, characteristic kernel, solution is $\mathsf{P}_{\text{te}}(x) = \beta_{\text{imp}}(x)\mathsf{P}_{\text{tr}}(x)$

Transfer learning by KMM

Kernel mean matching (KMM)

- Reweight training points so feature means match

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- What about non-characteristic?

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- Empirical:

$$\min_{\beta} \left\| \frac{1}{n_{\text{tr}}} \sum_{i=1}^{n_{\text{tr}}} \beta_i \Phi(x_i^{\text{tr}}) - \frac{1}{n_{\text{te}}} \sum_{i=1}^{n_{\text{te}}} \Phi(x_i^{\text{te}}) \right\|^2 = \frac{1}{{n_{\text{tr}}}^2} \beta^\top K \beta - \frac{2}{{n_{\text{tr}}}^2} \kappa^\top \beta + \text{const.}$$

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$$\text{subject to } \beta_i \in [0, B] \quad \text{and} \quad \left| \sum_{i=1}^{n_{\text{tr}}} \beta_i - n_{\text{tr}} \right| \leq \sqrt{n_{\text{tr}}}\epsilon.$$

Transfer learning by KMM

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Transfer learning by KMM

- What if given β_{imp}: finite sample effects?
- Assume $k(x, x) \leq R^2$ for all $x \in \mathcal{X}$.

Transfer learning by KMM

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- Assume $k(x,x) \leq R^2$ for all $x \in \mathcal{X}$.
- With probability at least $1-\delta$,

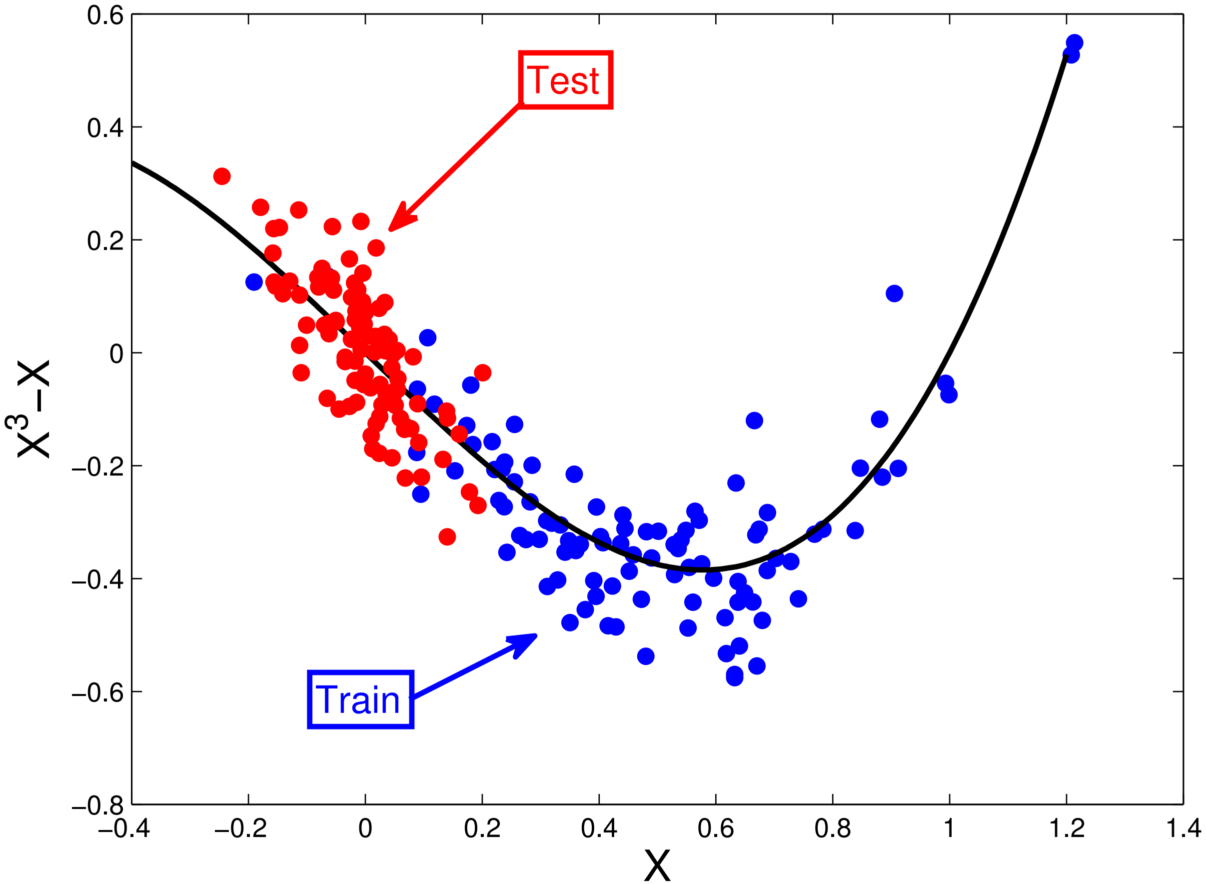
$$\left\| \frac{1}{n_{\mathrm{tr}}} \sum_{i=1}^{n_{\mathrm{tr}}} \beta_{\mathrm{imp}}(x_i^{\mathrm{tr}}) \Phi(x_i^{\mathrm{tr}}) - \frac{1}{n_{\mathrm{te}}} \sum_{i=1}^{n_{\mathrm{te}}} \Phi(x_i^{\mathrm{te}}) \right\| \leq \left(1 + \sqrt{2 \log 2/\delta}\right) R \sqrt{B^2/n_{\mathrm{tr}} + 1/n_{\mathrm{te}}}.$$

- Still (potentially) high variance for large B.

- Convergence of KMM procedure: [Cortes et al., 2008]

Transfer learning by KMM

- Compare KMM and importance sampling



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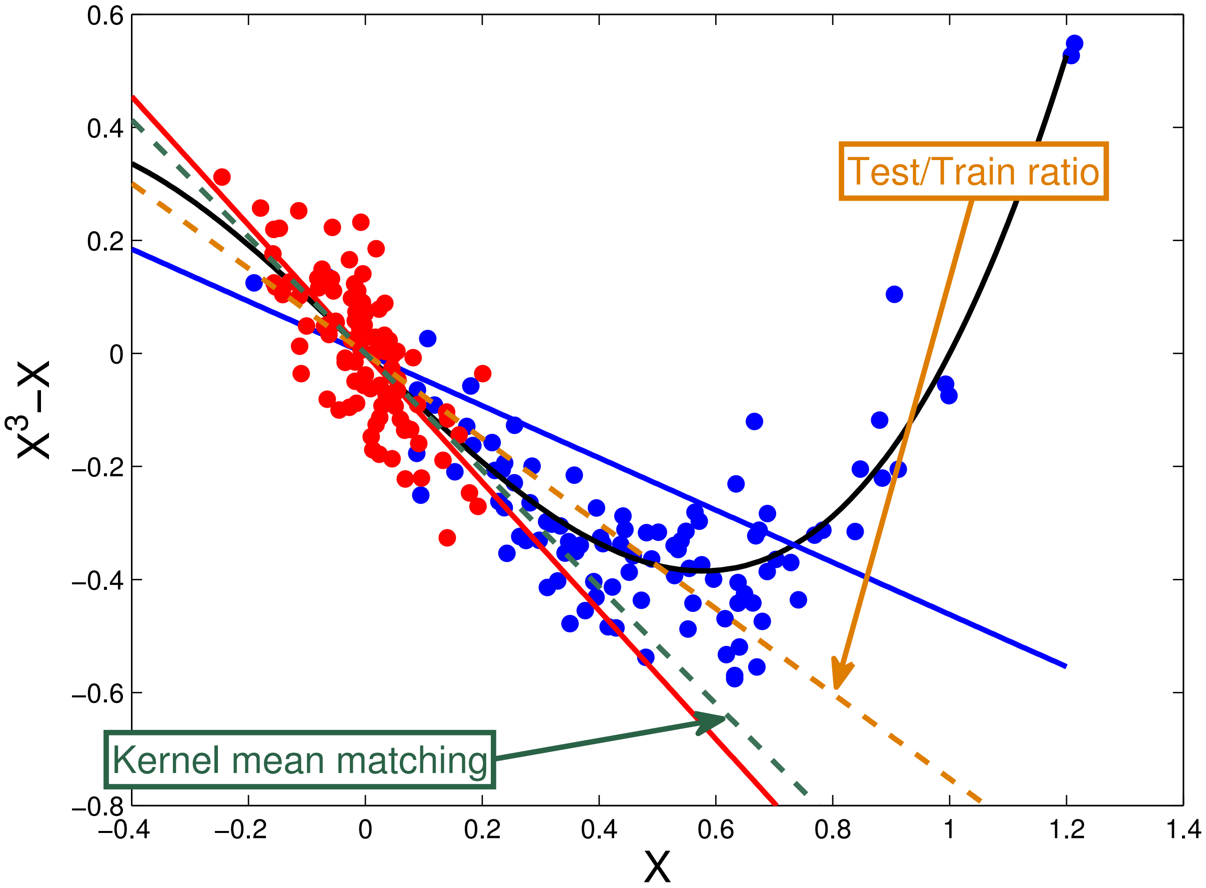

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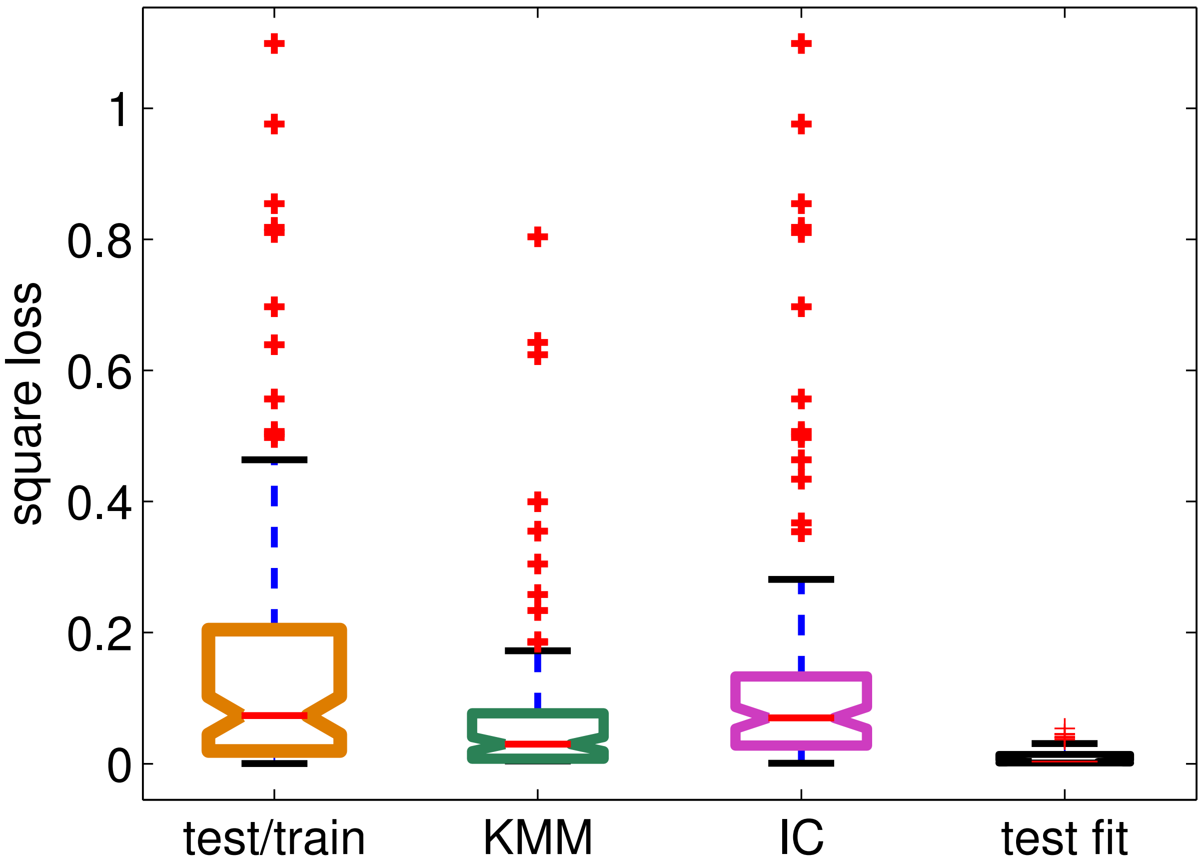

IC method due to [Shimodaira, 2000]

Reweighting by classification

- Use train/test classification error to reweight [Qin, 1998, Cheng and Chu, 2004, Bickel et al., 2009]
- $\mathbf{P}\left(S|x^{\mathrm{tr}}, x^{\mathrm{te}}, \theta_{\mathrm{shift}}\right)$ classifies training $(s = 1)$ vs test $(s = 0)$

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- Learn two classifiers: train vs test and covariate to label

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- Learn two classifiers: train vs test and covariate to label
- Single joint optimization? [Bickel et al., 2009]

$$\max_{\theta_{\text{shift}}, \theta_{\text{learn}}} \mathbf{P}\left(y^{\text{tr}}|S, x^{\text{tr}}, \theta_{\text{shift}}, \theta_{\text{learn}}\right) \mathbf{P}\left(S|x^{\text{tr}}, x^{\text{te}}, \theta_{\text{shift}}\right) \mathbf{P}(\theta_{\text{shift}})\mathbf{P}(\theta_{\text{learn}})$$

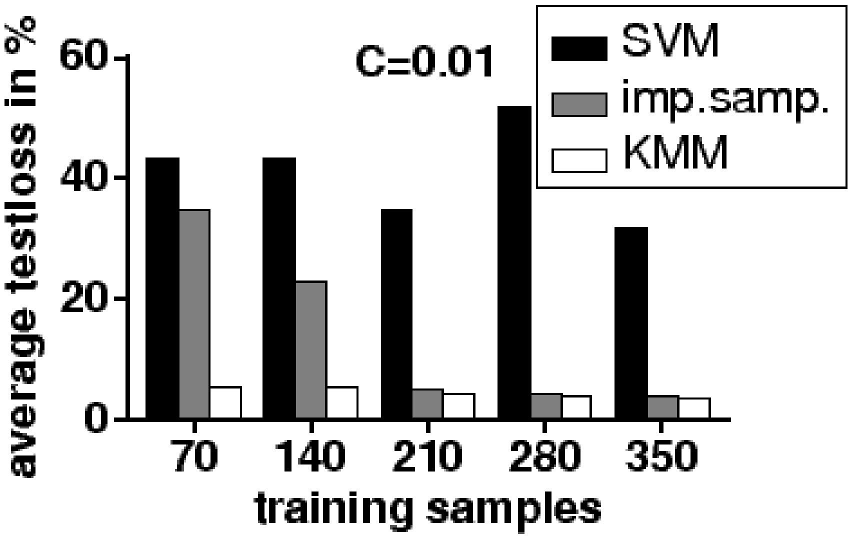
Experiments

Breast Cancer data

- Gaussian kernel $\exp(-|x_i - x_j|^2/(2\sigma))$ for KMM and SVN, $\sigma = 5$
- Performance vs C
  - Small C $\rightarrow$ prioritize smoothness
- Selection procedure:
  - Random training/test split
  - Training set from 10% - 50% of test
  - $P(s_i = 1|x_i) \propto \exp(-0.05\|x_i - \overline{x}\|^2)$

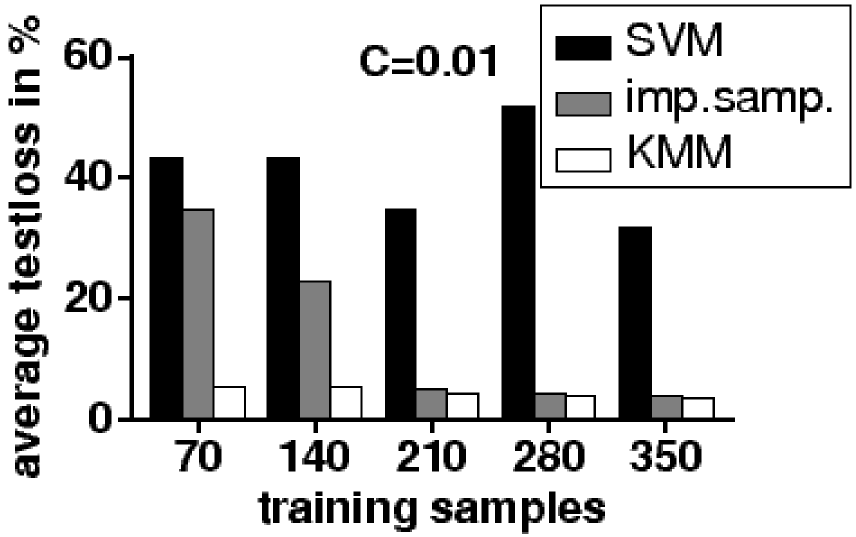
Breast Cancer data

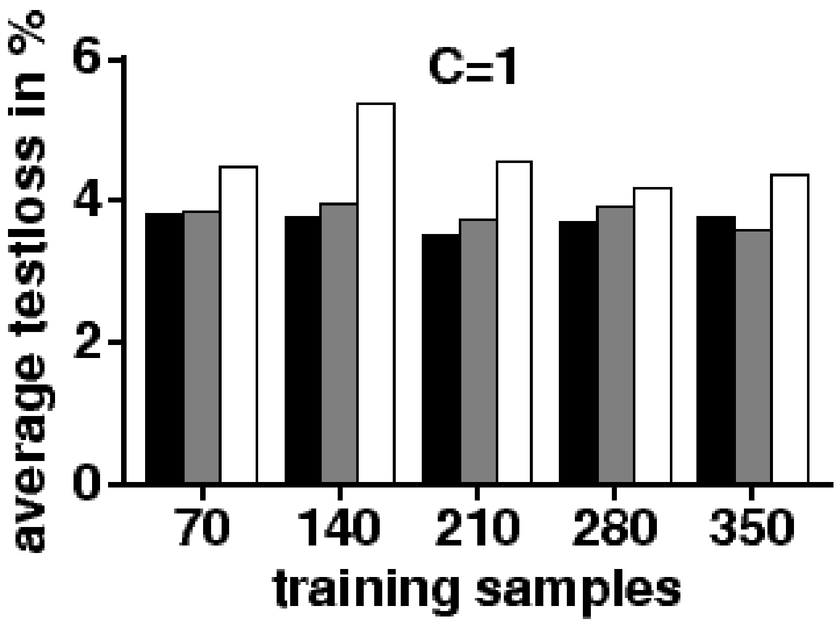
- Reweighting greatly improves performance
- KMM outperforms IS at small sample sizes



Breast Cancer data

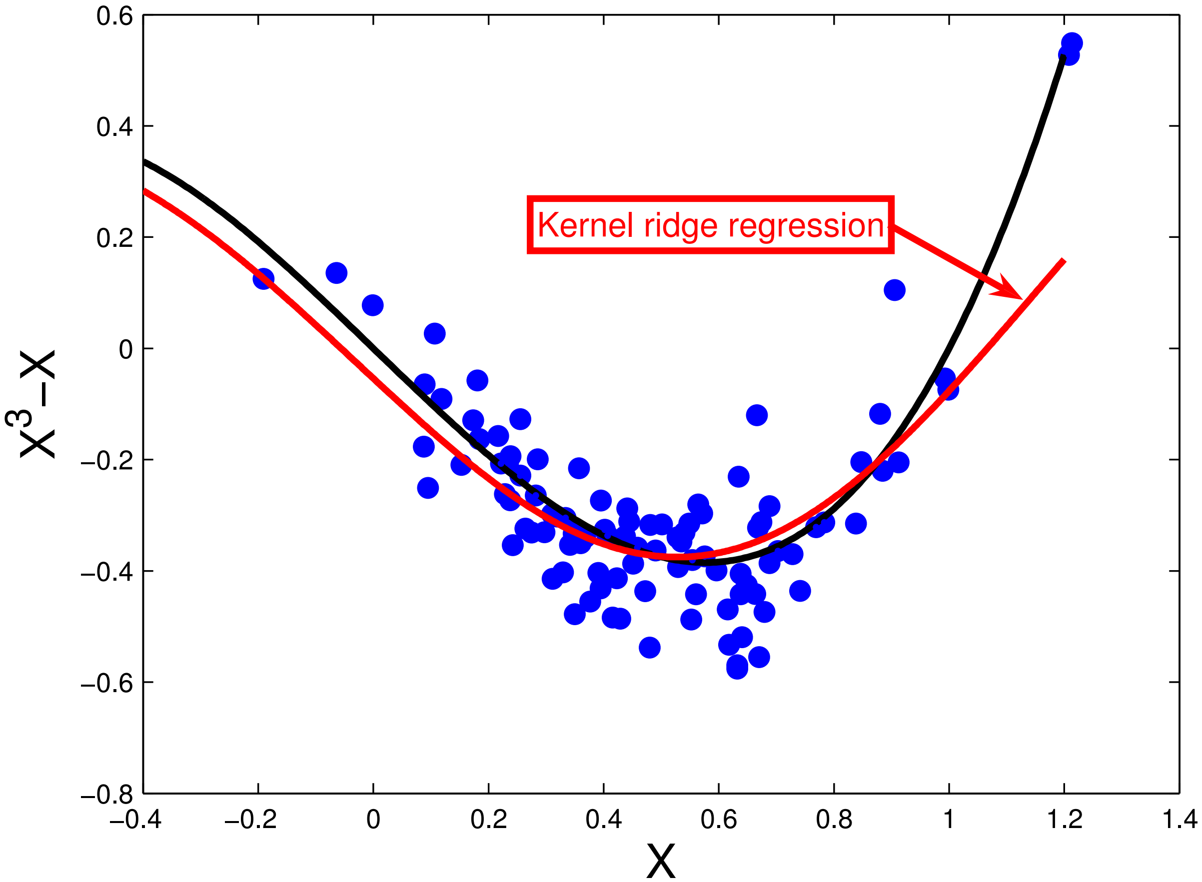
- KMM slightly decreases performance
- IS does not help





Toy example revisited

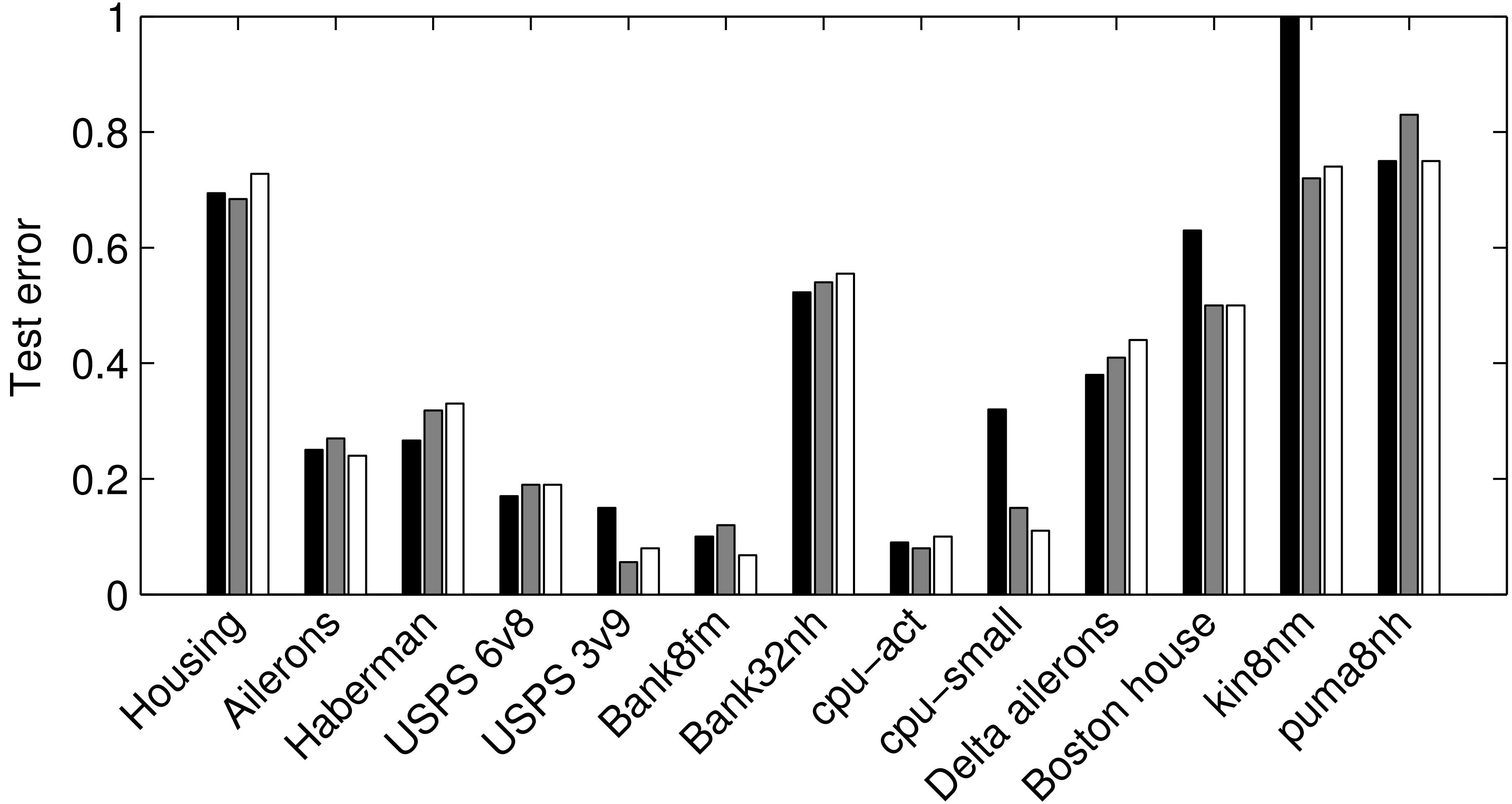
- Kernel ridge regression result



Large scale experiments

- Regression and classification
- Sampling scheme: training data missing at random
  - Sampling by Gaussian distribution on first principal component
- Cross validate on unweighted training set for C and σ
- Same σ for classifier/regressor and KMM

Large scale experiments



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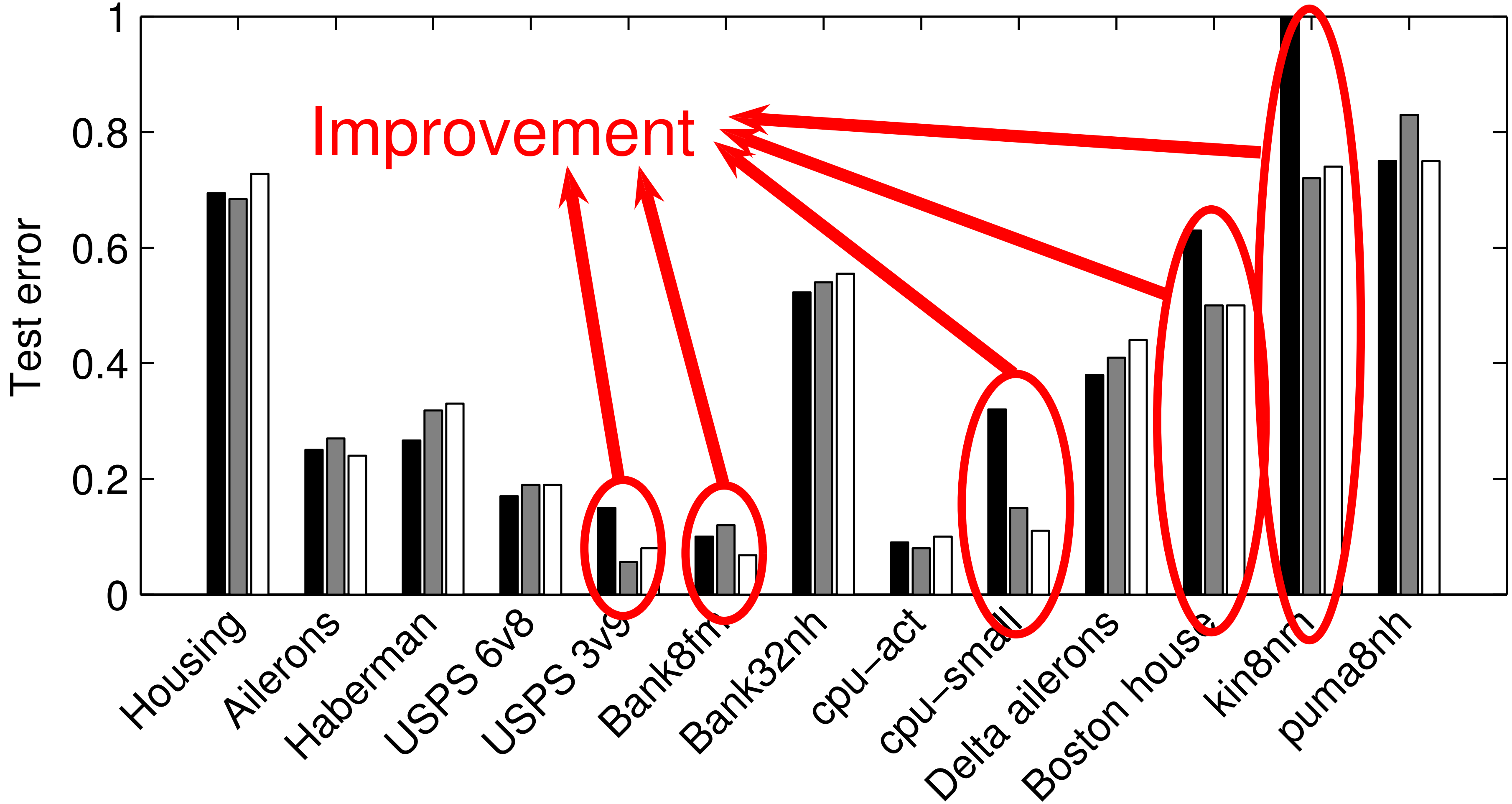

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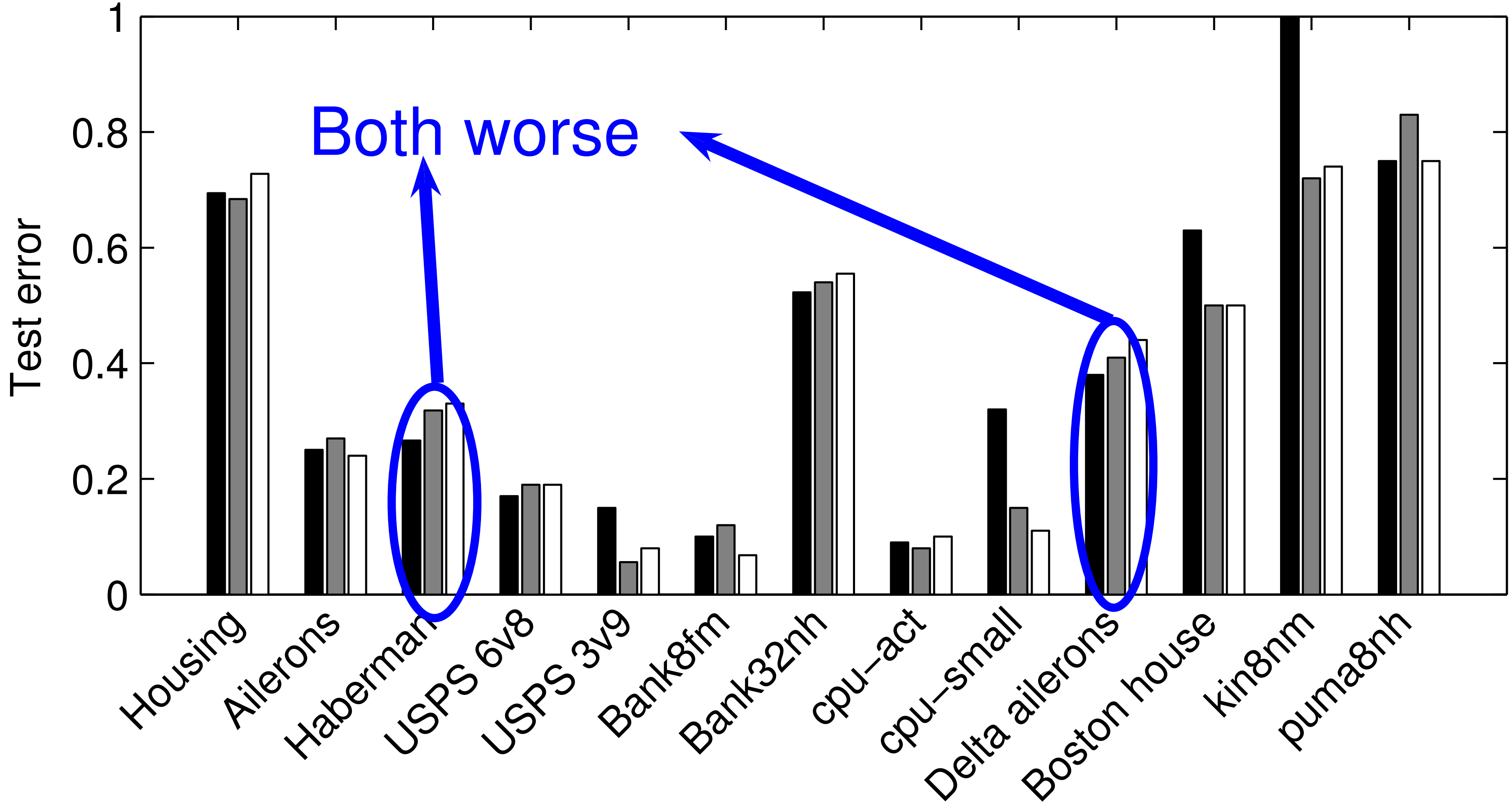

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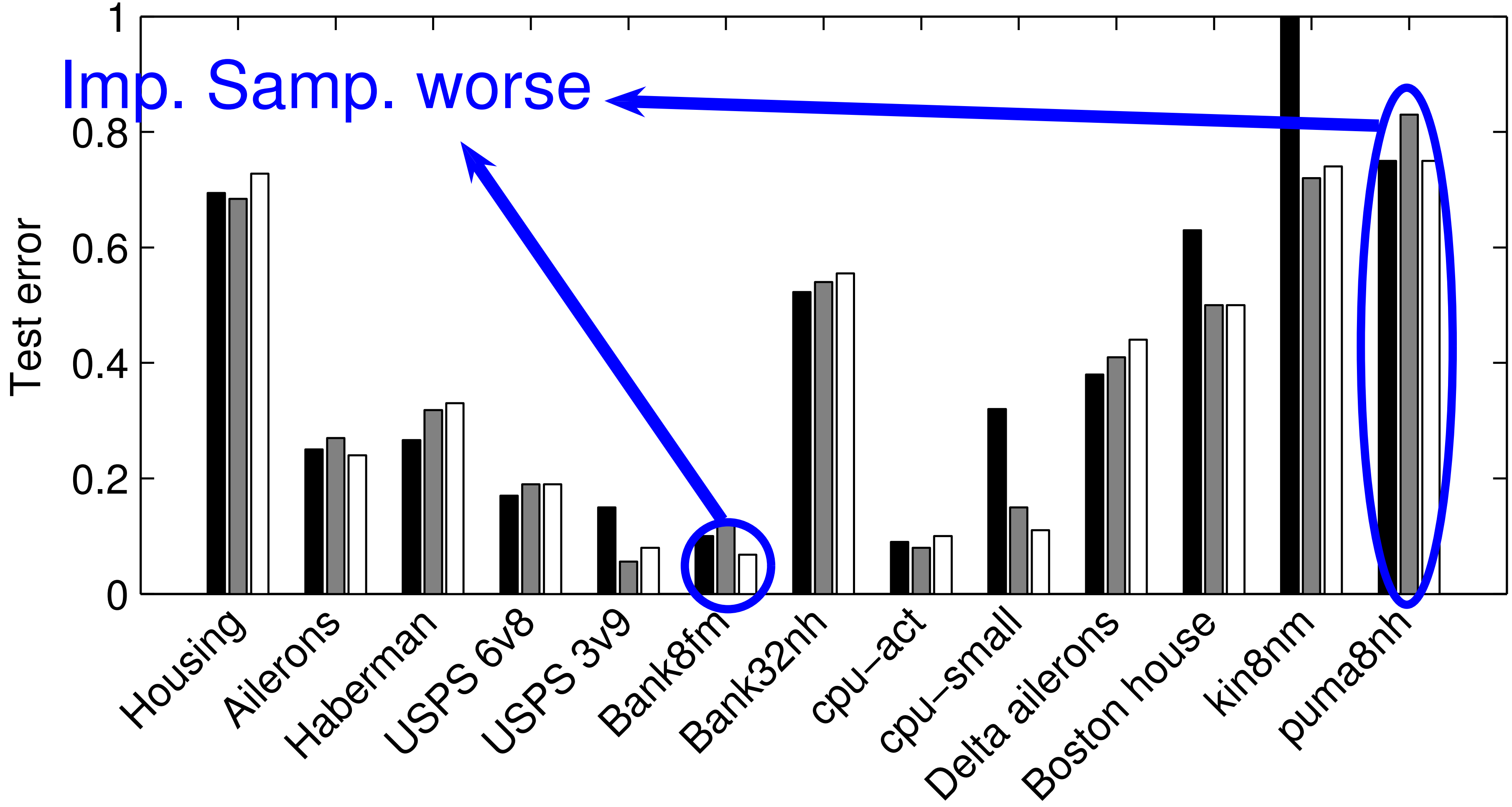

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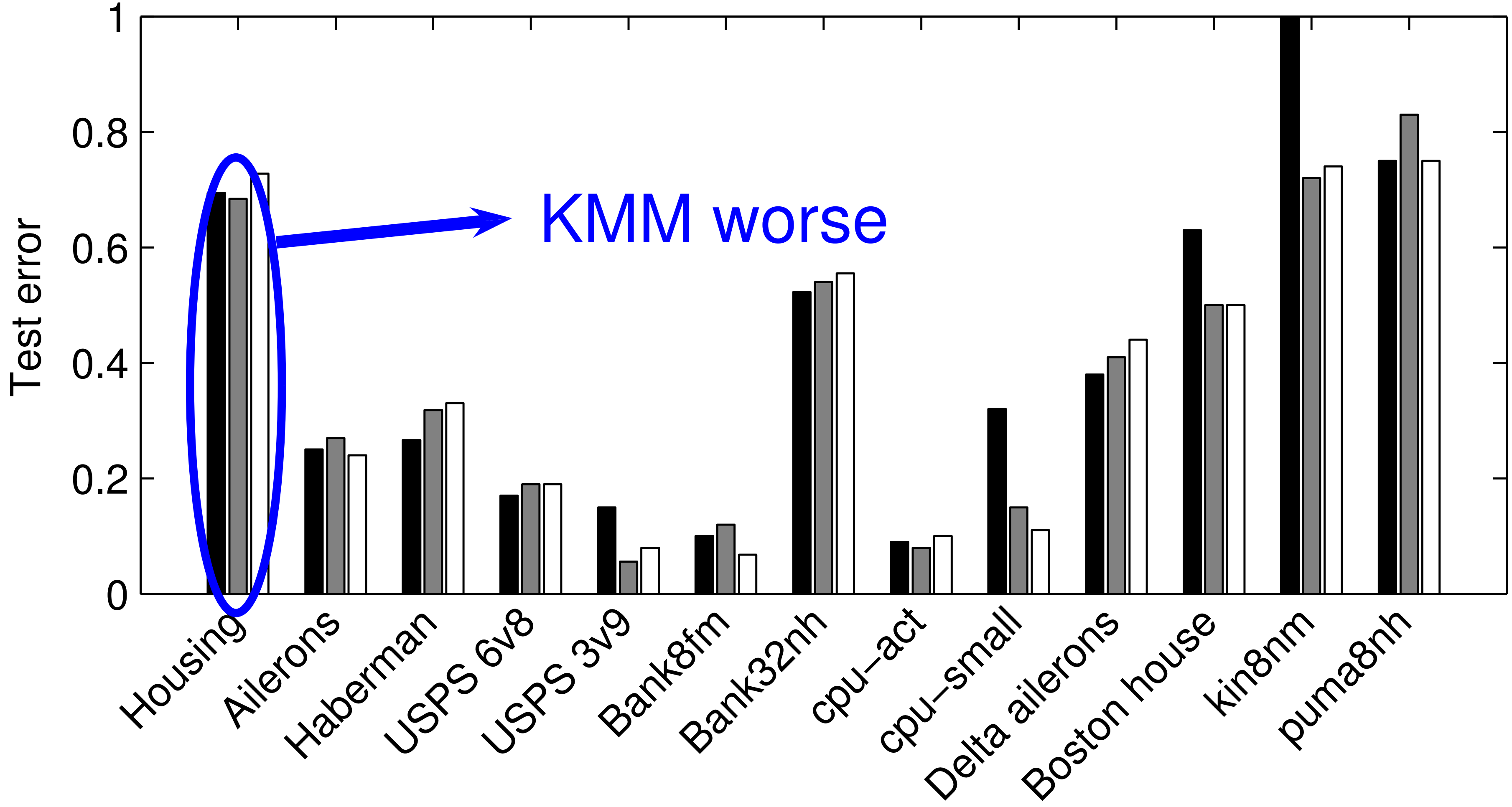

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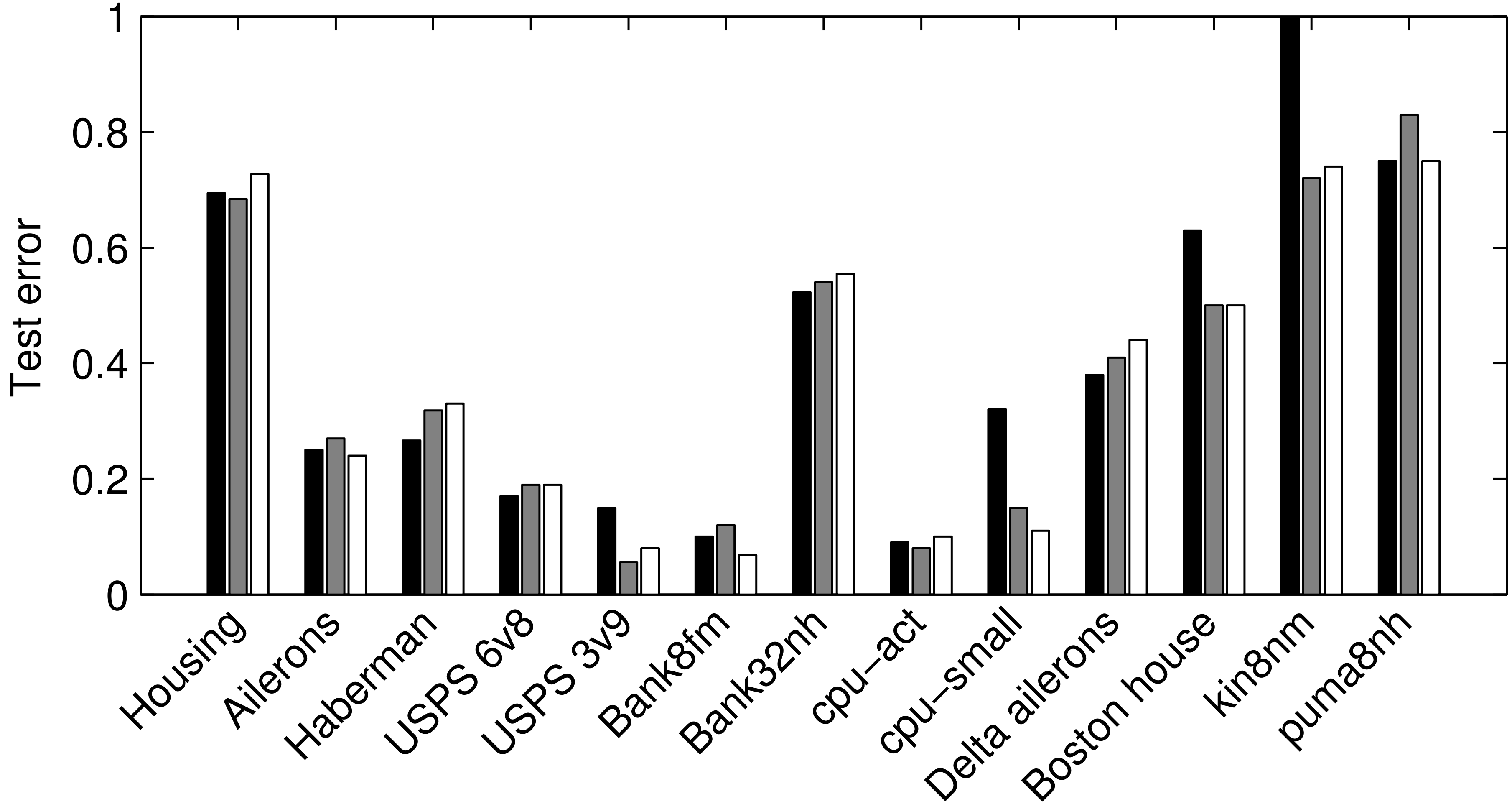
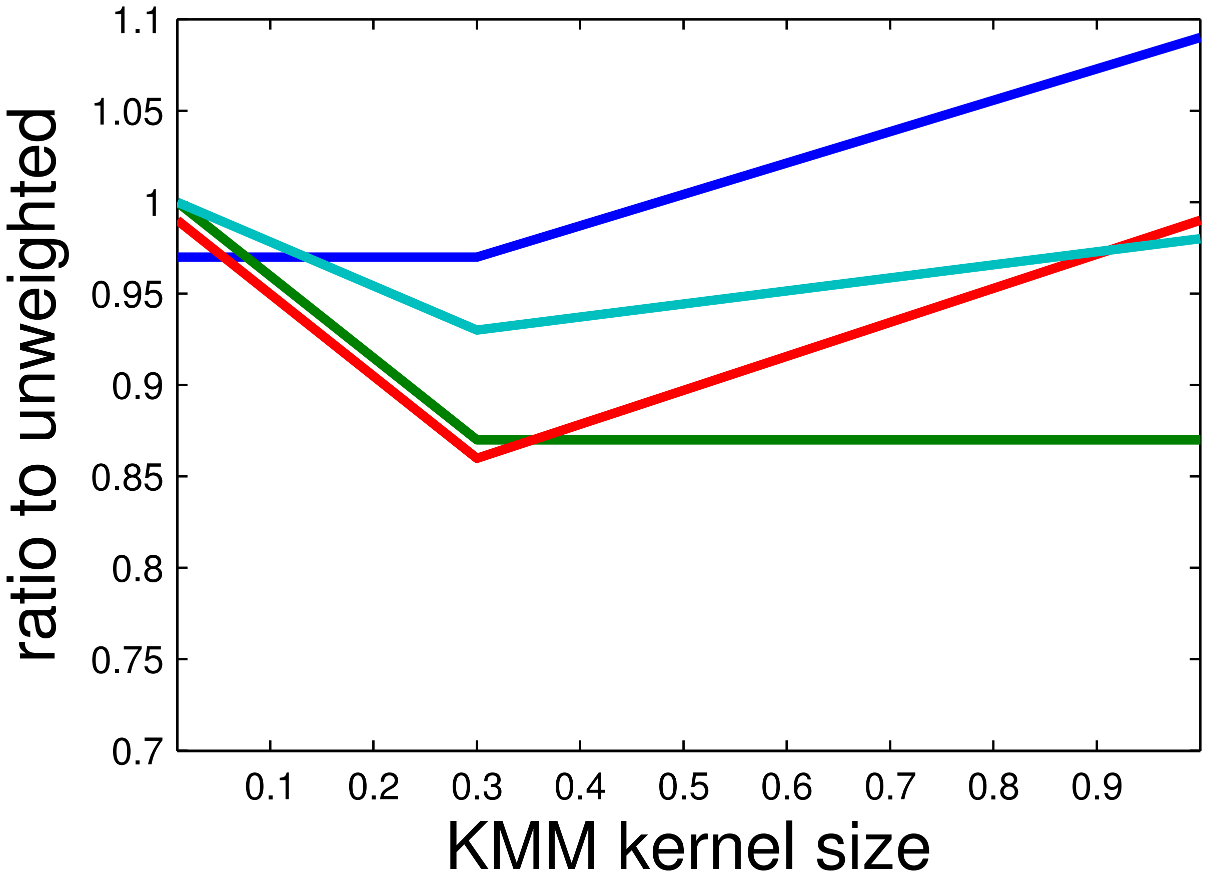


Further work: model selection

- Model selection for covariate shift
- Results from [Sugiyama et al., 2008]
- Data have 18-21 dimensions



Further work: model selection

- Model selection for covariate shift

- Some strategies [Bickel et al., 2009]
  - Systematic drift: can be learned [Bickel et al., 2009]
  - Cross validation to obtain error for current β estimate [Sugiyama et al., 2008, Kanamori et al., 2009]
  - Classifier of training vs test: again, cross-validate [Bickel et al., 2009]
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- Does knowing something about the learning problem help?

- Model selection for weighted learning: bias for unweighted? [Kanamori et al., 2009]

Summary

- Kernel mean matching: perform covariate shift. . .
  - . . .without density estimation
  - . . .using only particular covariate features
  - . . .on structured domains
- Large performance advantage for “simple” learning algorithms
- Mixed results for powerful learning algorithms
- Model selection remains an issue

Acknowledgements

- Co-authors on KMM papers:
  - Karsten Borgwardt
  - Jiayuan Huang
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  - Bernhard Schölkopf
  - Alex Smola
- Discussions
  - Paul von Bünau
  - Corinna Cortes
  - Klaus-Robert Müller
  - Masashi Sugiyama

Questions?

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Characteristic kernels

Characteristic Kernels (1)

- Characteristic: MMD a metric (MMD = 0 iff $\mathbf{P} = \mathbf{Q}$) [NIPS07b, COLT08]

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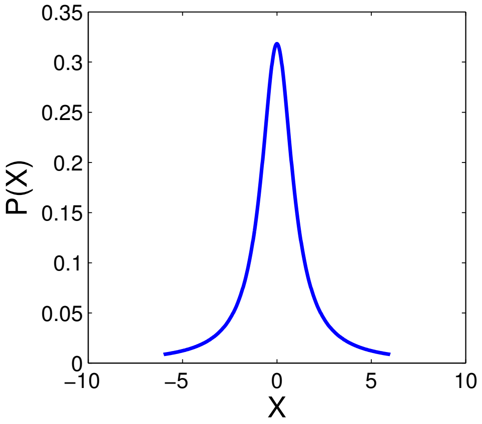
- Fourier representation of MMD:

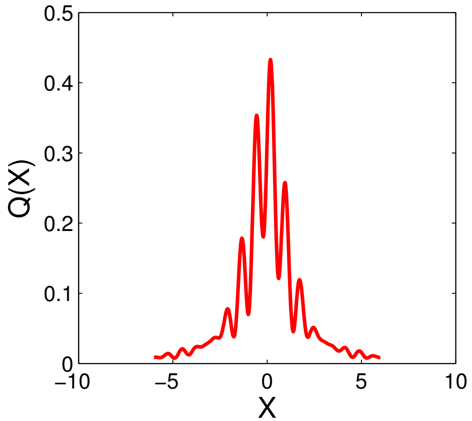
$$\text{MMD}(\mathbf{P}, \mathbf{Q}; F) := \left\| \left[\left(\bar{\phi}_{\mathbf{P}} - \bar{\phi}_{\mathbf{Q}} \right) \Lambda \right]^{\vee} \right\|_{\mathcal{F}}$$

  - $\phi_{\mathbf{P}}$ characteristic function of $\mathbf{P}$
  - $f^{\wedge}$ is Fourier transform, $f^{\vee}$ is inverse Fourier transform
  - $\mu_x := \int k(\cdot, x)\, d\mathbf{P}(x)$

Characteristic Kernels (2)

- Example: **P** differs from **Q** at (roughly) one frequency





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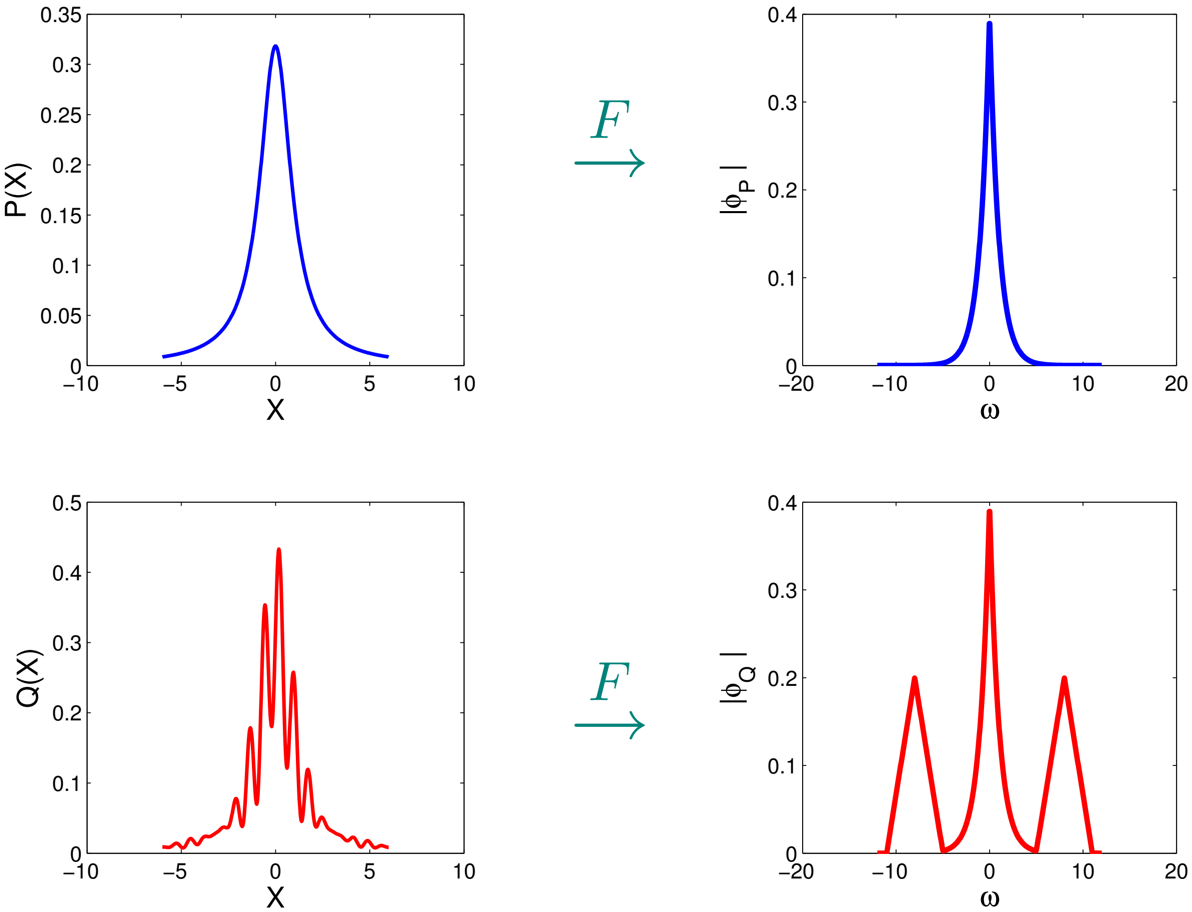

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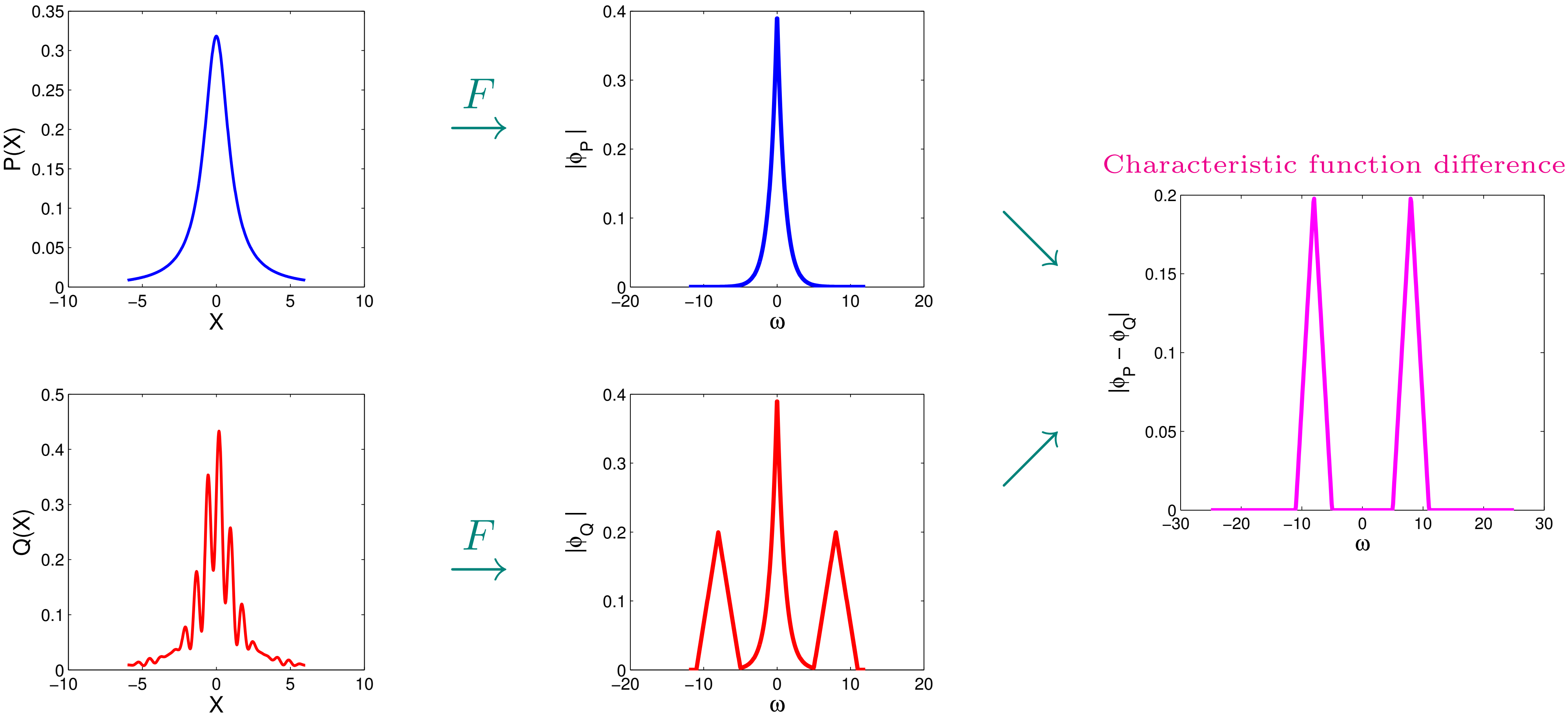
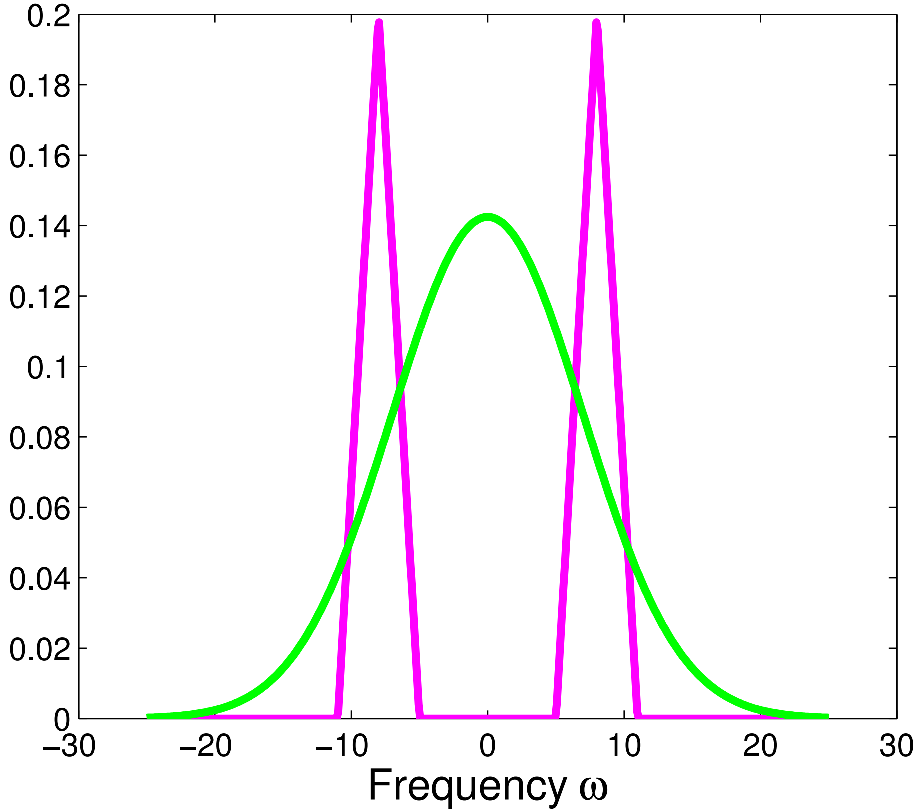


Characteristic Kernels (3)

- Example: **P** differs from **Q** at (roughly) one frequency

Gaussian kernel

Difference $|\phi_P - \phi_Q|$



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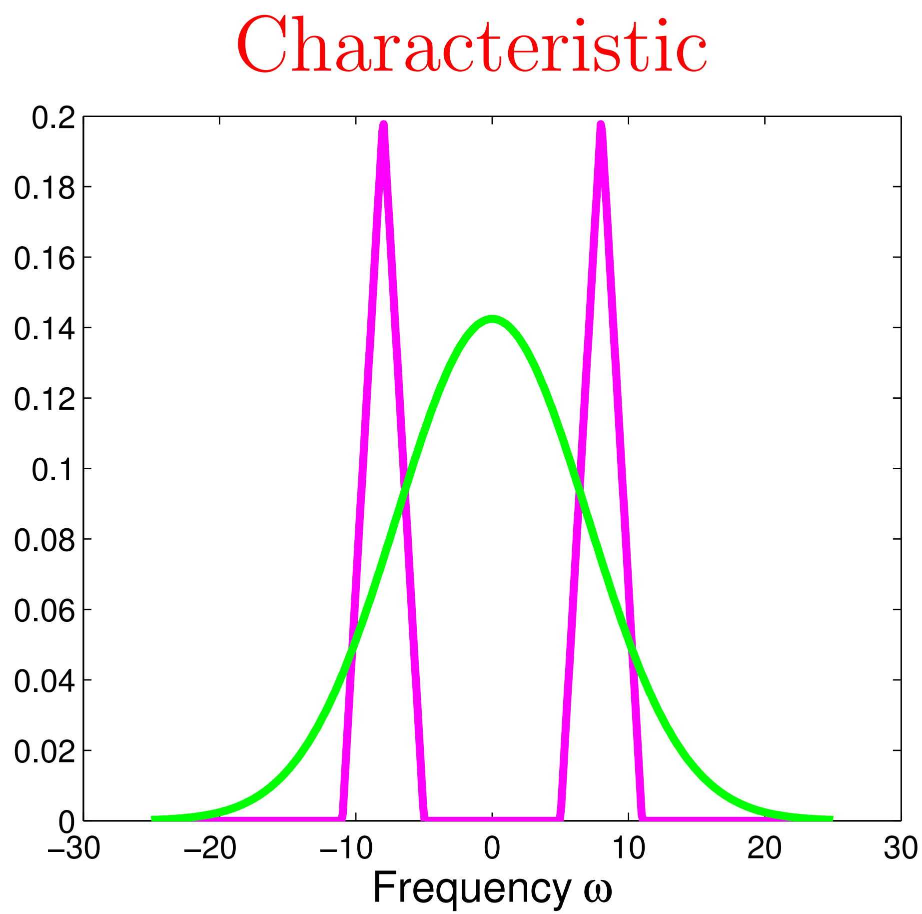

Characteristic Kernels (4)

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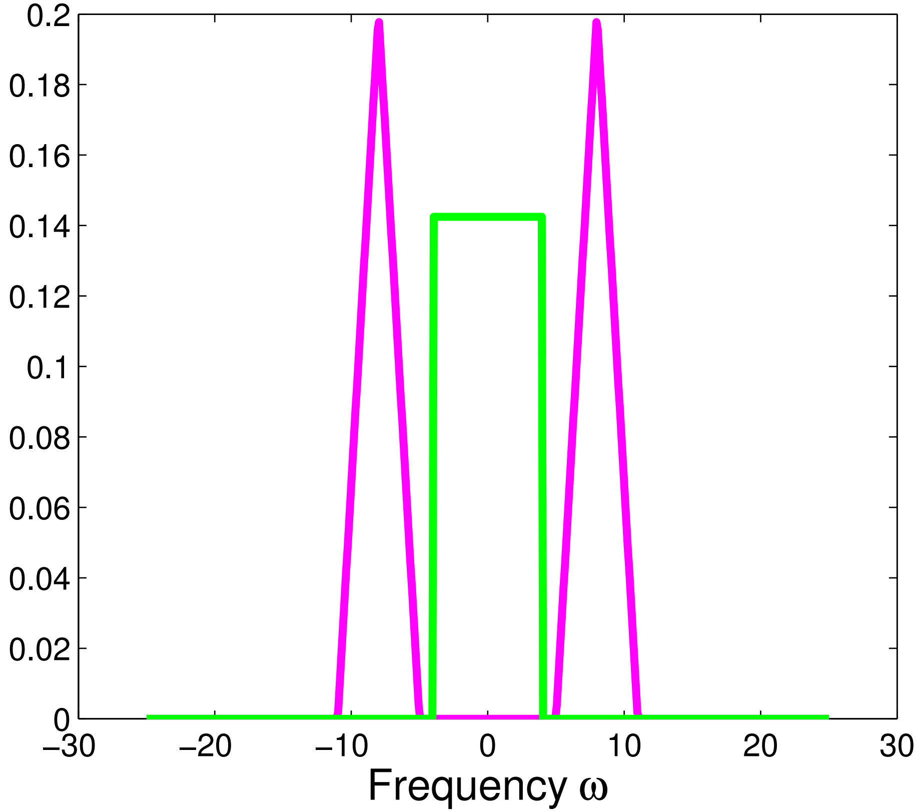
Sinc kernel

Difference $|\phi_P - \phi_Q|$



Characteristic Kernels (4)

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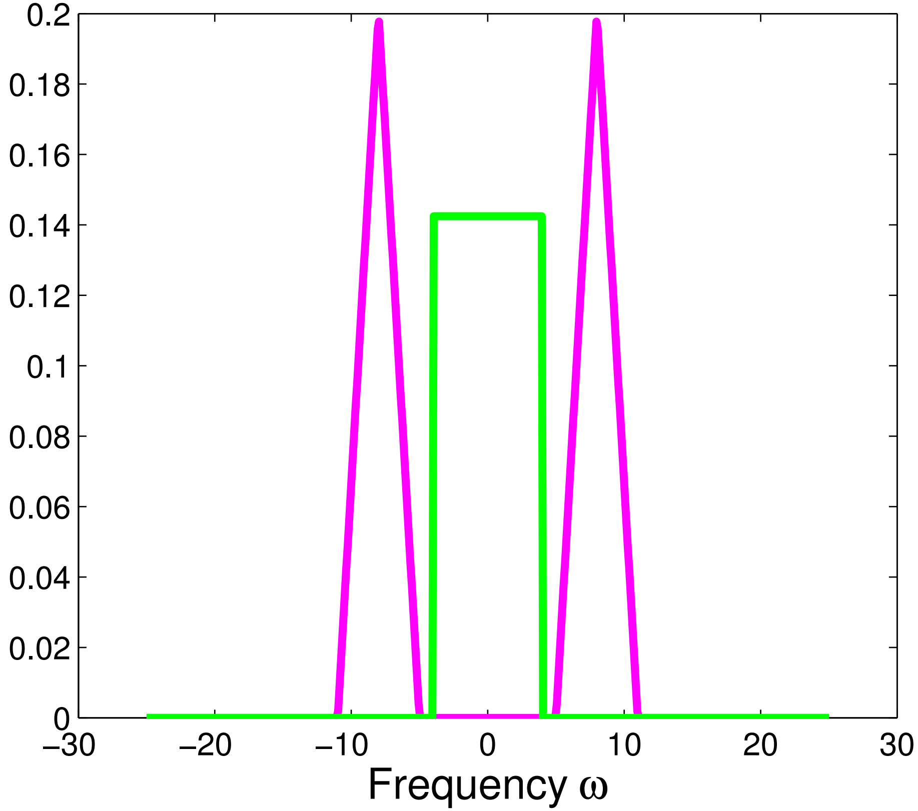
NOT characteristic



Characteristic Kernels (5)

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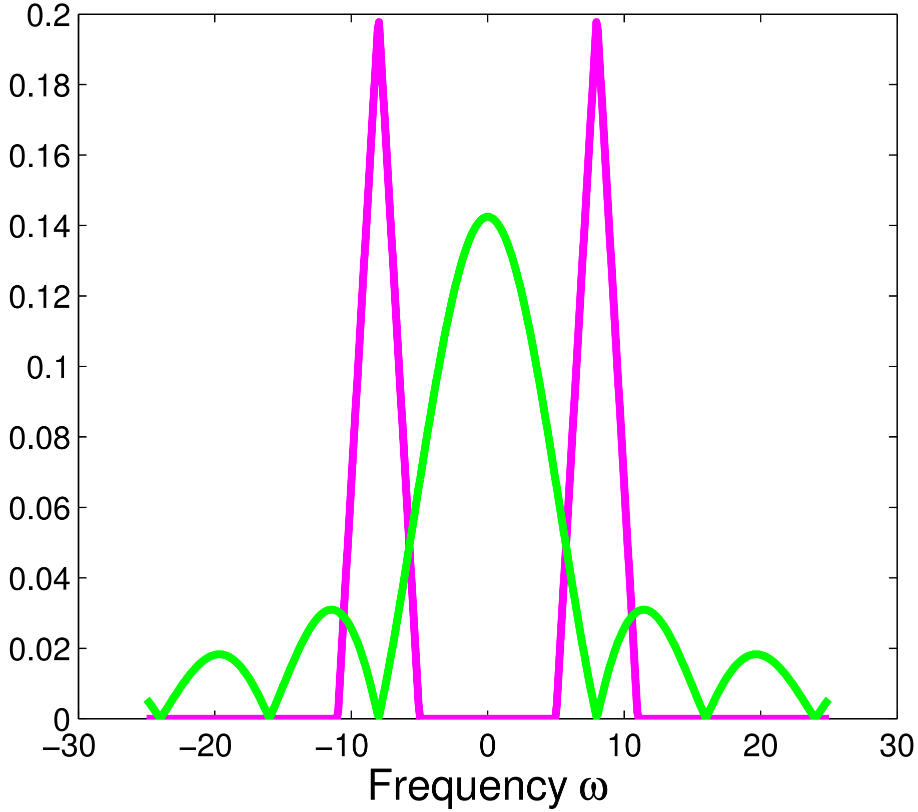
B-Spline kernel

Difference $|\phi_P - \phi_Q|$



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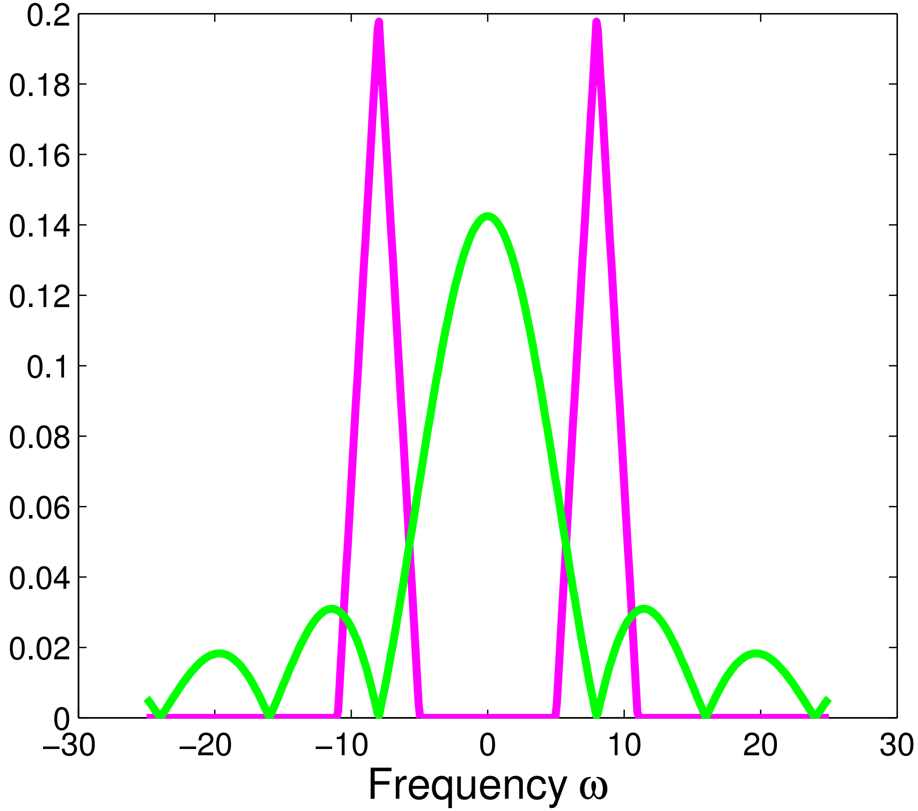
???



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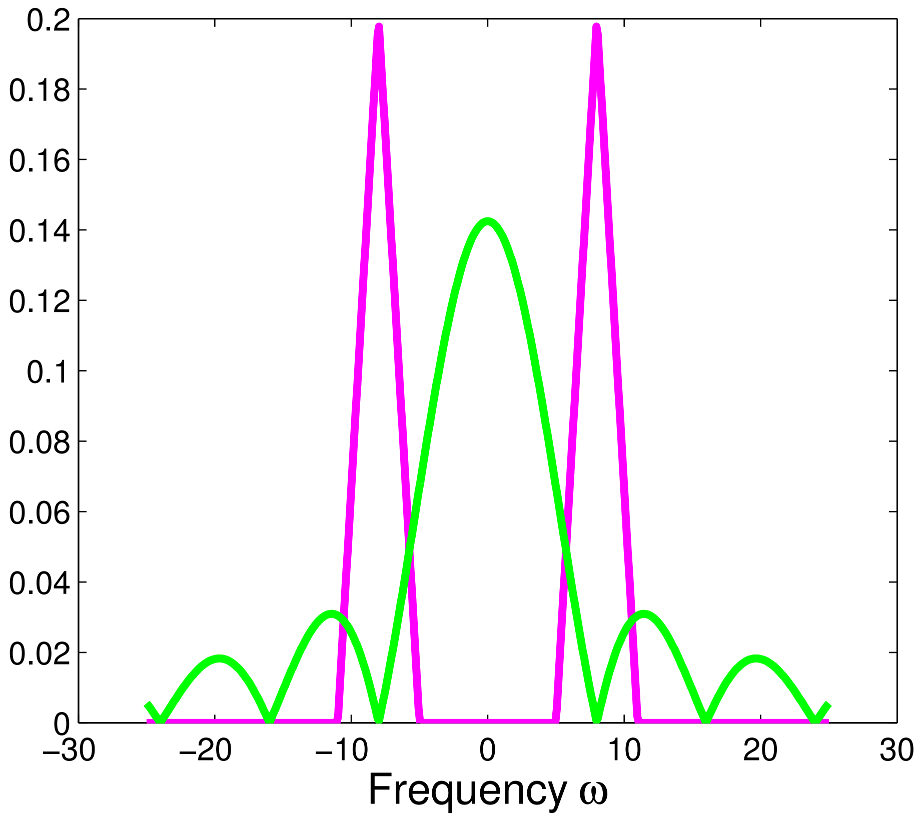
Characteristic



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- Similar reasoning wherever extensions of Bochner's theorem exist: [NIPS08a]
  - Locally compact Abelian groups (periodic domains)
  - Compact, non-Abelian groups (orthogonal matrices)
  - The semigroup $\mathbb{R}_n^+$ (histograms)