Preliminary Analysis of MKL

Flat Maxima, Diversity and Fisher Information

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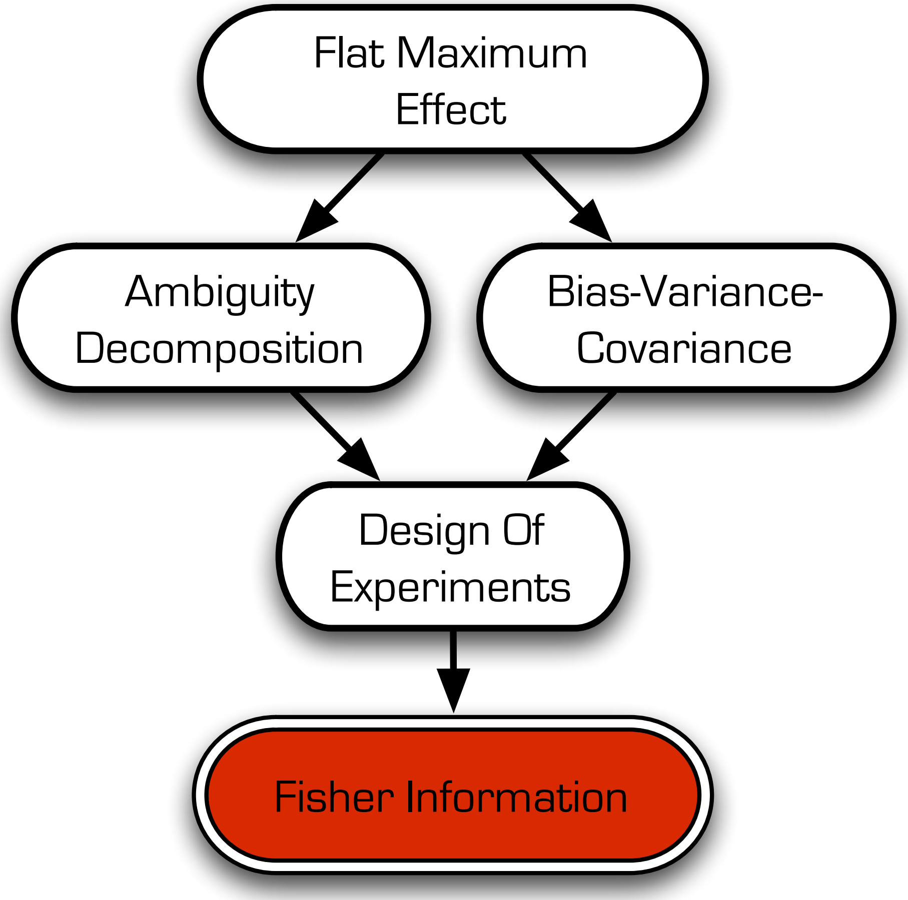


Flat Maximum Effect

- D. J. Hand (Statistical Science, 21(1) p. 1-15, 2006) - Linear regression

$$w = \sum_{i=1}^{d} w_i x_i \qquad u = \sum_{i=1}^{d} u_i x_i \qquad w_i, u_i \geq 0 \quad \sum_{i=1}^{d} w_i = \sum_{i=1}^{d} u_i = 1$$

$$\rho(u, w) \geq \sum_{i,j=1}^{d} u_i w_j \rho(x_i, x_j)$$

"Often quite large deviations from the optimal set of weights will yield predictive performance not substantially worse than the optimal weights"

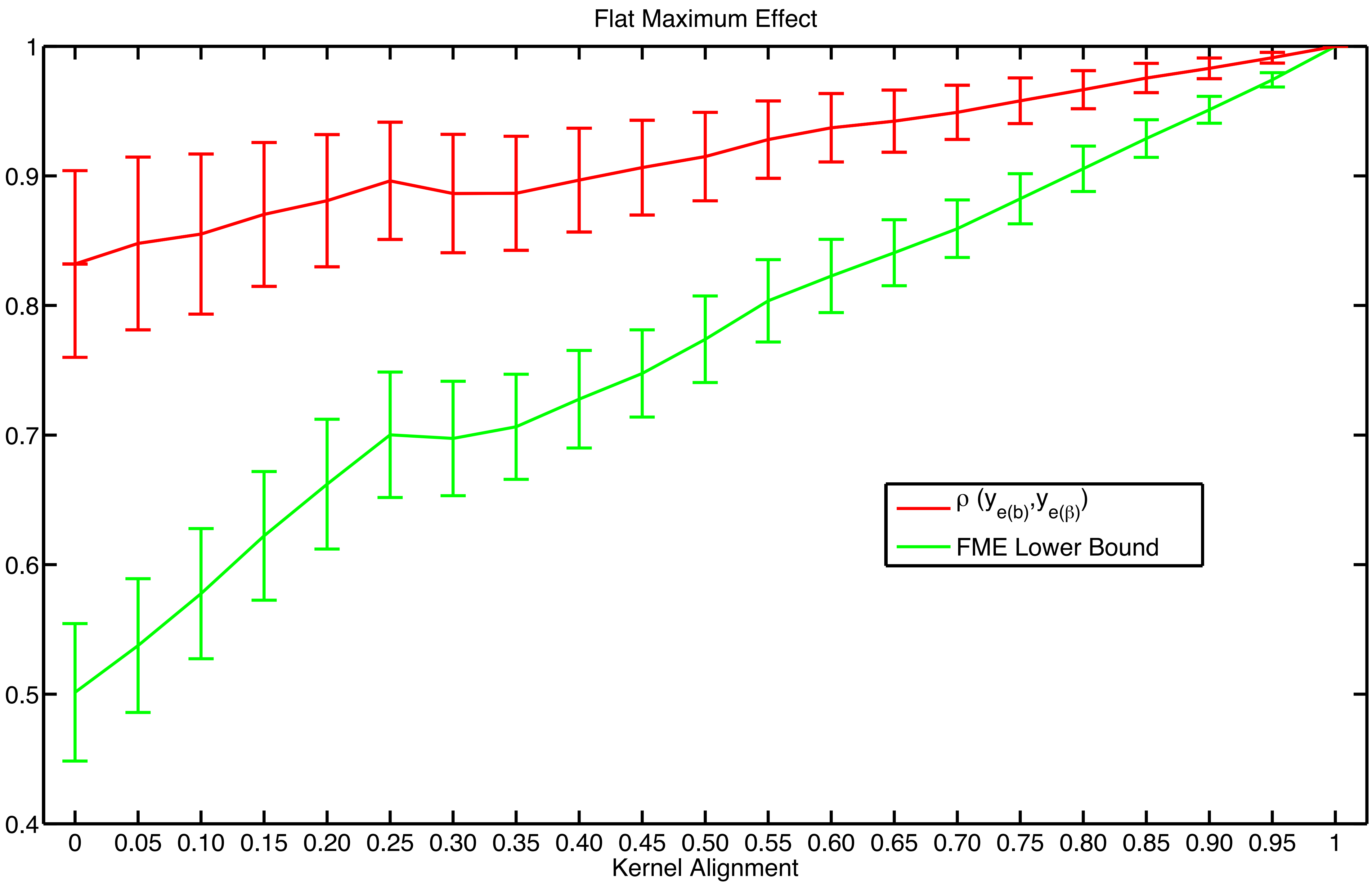
$$\mathbf{y}_{e_{(\boldsymbol{b})}} = \sum_{j=1}^{N} w_j \sum_{s=1}^{S} b_s k_s(\mathbf{x}_i, \mathbf{x}_j) = \sum_{s=1}^{S} b_s \mathbf{y}_s \qquad \mathbf{y}_{e_{(\boldsymbol{\beta})}} = \sum_{j=1}^{N} w_j \sum_{\sigma=1}^{S} \beta_\sigma k_\sigma(\mathbf{x}_i, \mathbf{x}_j) = \sum_{\sigma=1}^{S} \beta_\sigma \mathbf{y}_\sigma$$

Flat Maximum Lower Bound

$$\boxed{\rho(\mathbf{y}_{e_{(\boldsymbol{b})}}, \mathbf{y}_{e_{(\boldsymbol{\beta})}}) \geq \sum_{s,\sigma=1}^{S} b_s \beta_\sigma \rho(\mathbf{y}_s, \mathbf{y}_\sigma)}$$

The correlation between any two weighted kernel combination responses is lower bounded by a function of the correlation between base kernel responses.

- Sample Kernels - Sample Kernel Combination Parameters - Sample Regression Coefficients



- Ensemble response correlation increases as kernel alignment increases.
- Little or no benefit in parameterized (global) kernel combinations for highly aligned base kernels.

Decompositions of the Loss

Ambiguity

$$\underbrace{(\mathbf{y}_e-\mathbf{y})^T(\mathbf{y}_e-\mathbf{y})}_{\text{Composite Error}} = \underbrace{\sum_{s=1}^{S}\beta_s(\mathbf{y}_s-\mathbf{y})^T(\mathbf{y}_s-\mathbf{y})}_{\text{Weighted Ind. Error}} - \underbrace{\sum_{s=1}^{S}\beta_s(\mathbf{y}_s-\mathbf{y}_e)^T(\mathbf{y}_s-\mathbf{y}_e)}_{\text{Ambiguity}}$$

Brown & Wyatt
ICML '03

- Need for accurate (Weighted Ind. Error) but diverse (Ambiguity) base kernels.

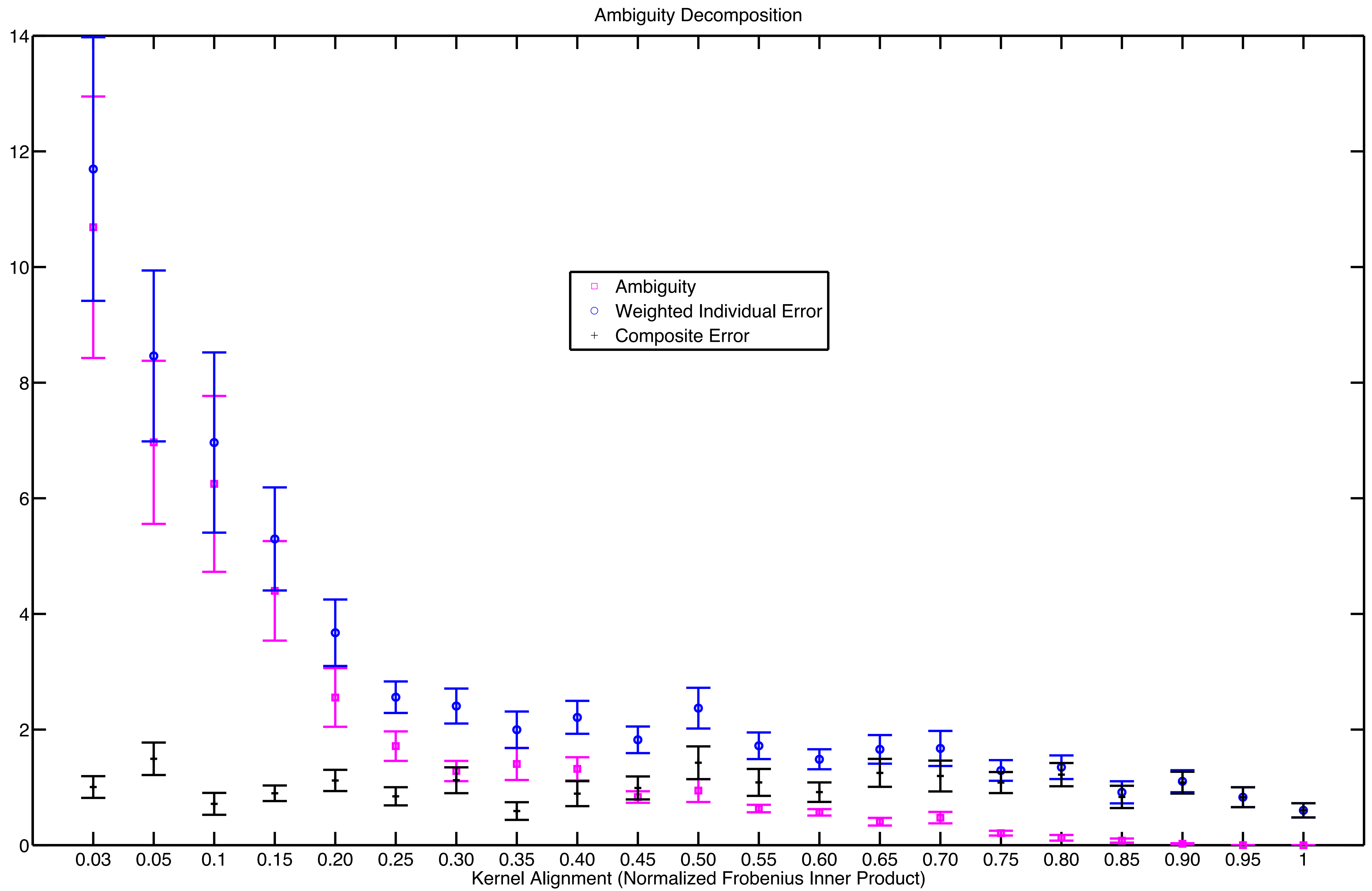
Bias
vs
Variance
vs
Covariance

$$\mathbb{E}\left\{(\mathbf{y}_e-\mathbf{y})^{\mathrm{T}}((\mathbf{y}_e-\mathbf{y})\right\} = \sum_{s,\sigma=1}^{S}\beta_s\beta_\sigma\underbrace{(\mathbb{E}\{\mathbf{y}_s\}-\mathbf{y})^{\mathrm{T}}(\mathbb{E}\{\mathbf{y}_\sigma\}-\mathbf{y})}_{\mathrm{Bias}^{\mathrm{T}}\mathrm{Bias}}$$
$$+\sum_{s=1}^{S}\beta_s^2\underbrace{\mathbb{E}\left\{(\mathbf{y}_s-\mathbb{E}\{\mathbf{y}_s\})^{\mathrm{T}}(\mathbf{y}_s-\mathbb{E}\{\mathbf{y}_s\})\right\}}_{\text{Variance}} + \sum_{s=1,\sigma\neq s}^{S}\beta_s\beta_\sigma\underbrace{\mathbb{E}\left\{(\mathbf{y}_s-\mathbb{E}\{\mathbf{y}_s\})^{\mathrm{T}}(\mathbf{y}_\sigma-\mathbb{E}\{\mathbf{y}_\sigma\})\right\}}_{\text{Covariance}}$$

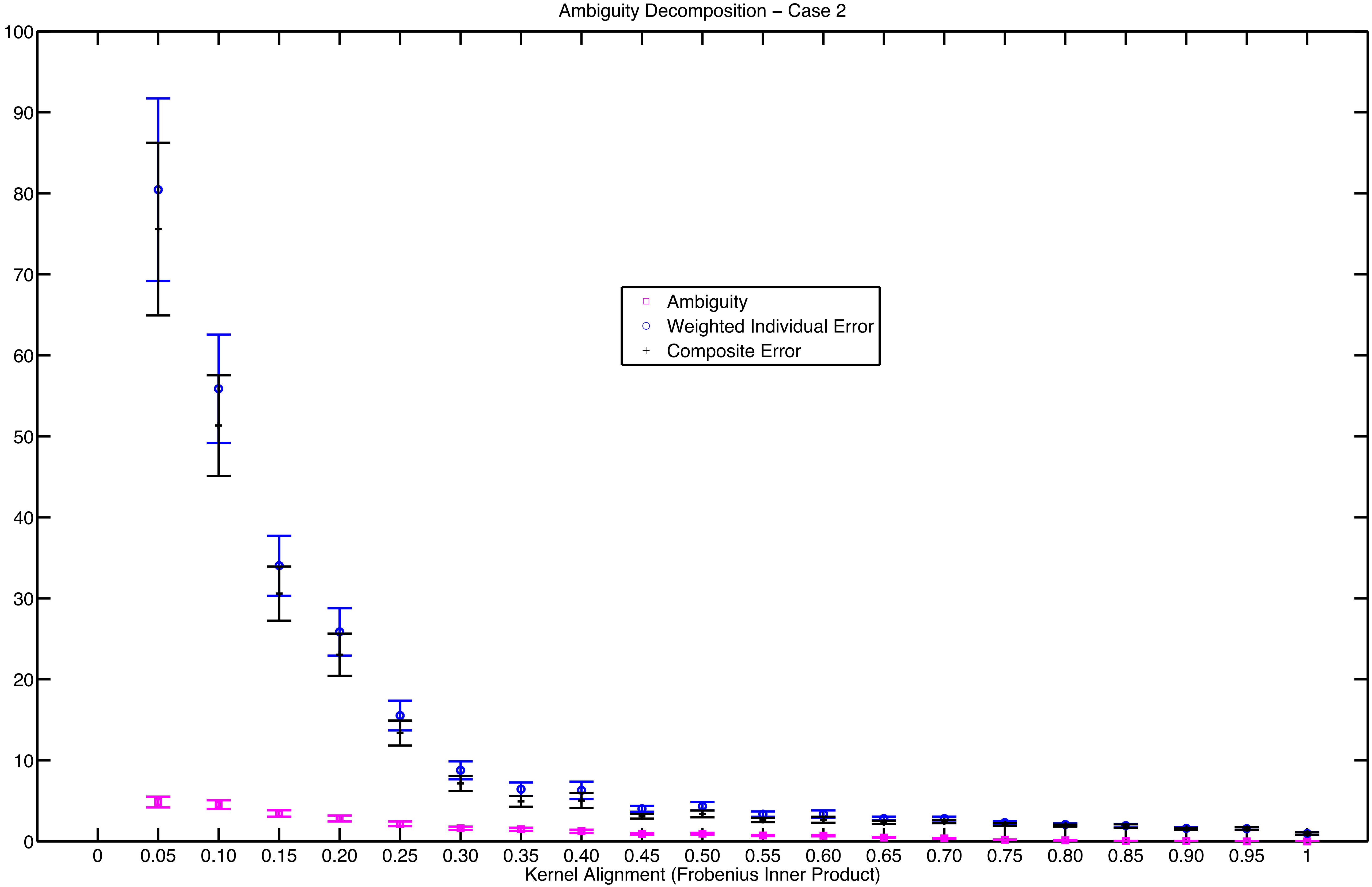
Ueda & Nakano
ICNN '96

- Fitting (Bias) versus Generalisation (Variance) versus Diversity (Covariance).

- Sample data from ensemble response.
- Quantifying the need for accurate and diverse base kernels.



- Sampling data from single base kernel response.
- Varying composite error - high individual error - diverse but not accurate.



Design of Experiments

- MKL as an Experimental Design problem [R. A. Fisher, The Design of Experiments,1935]
- Maximize the information offered for the model parameters with respect to the evidence observed

$$\mathbf{F}(\boldsymbol{\theta}) = -\mathbb{E}\left\{\frac{\partial^2 \mathcal{L}}{\partial\boldsymbol{\theta}\partial\boldsymbol{\theta}^{\mathrm{T}}}\right\}$$

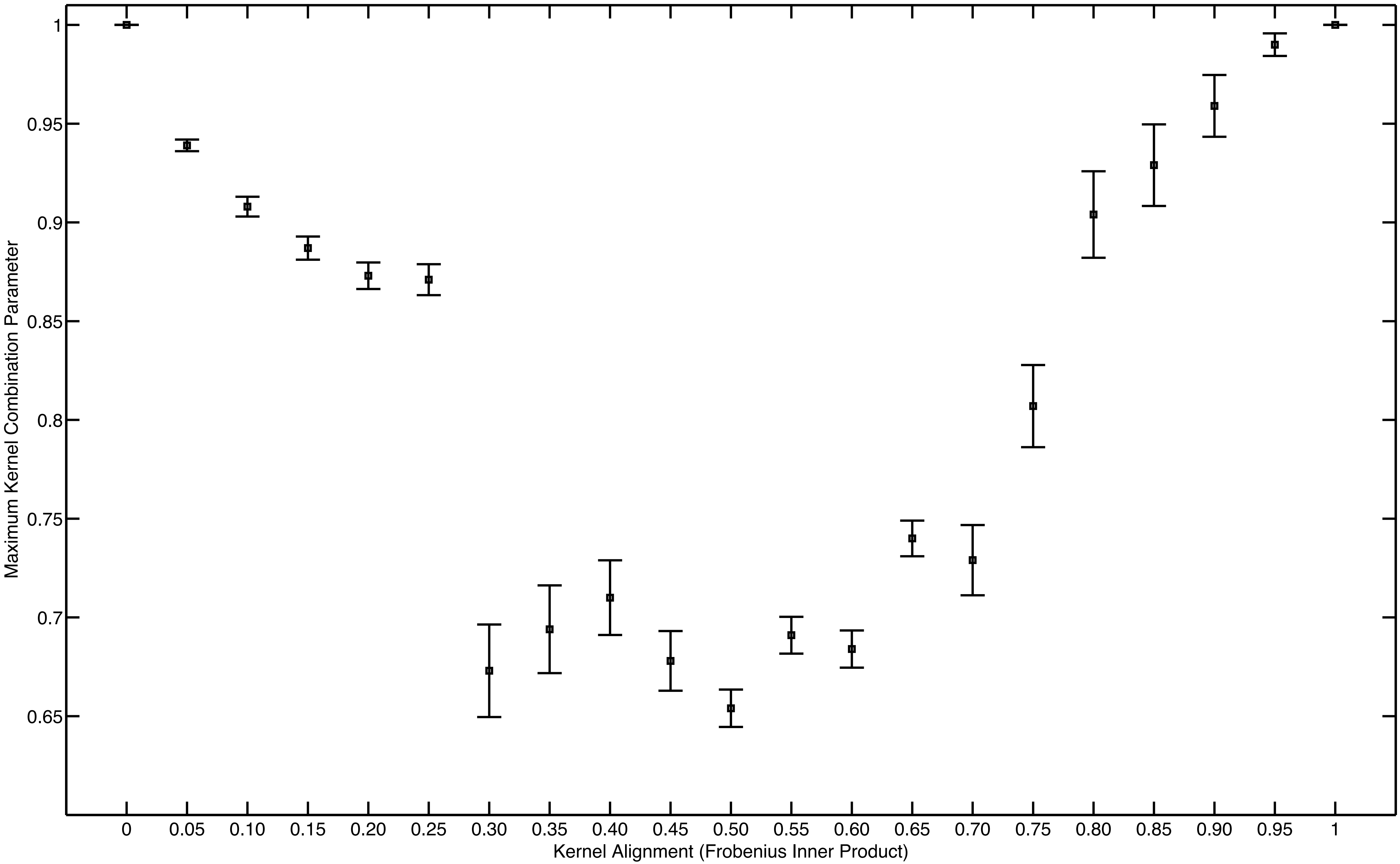
$$\mathcal{L} = \left(\mathbf{y}^{\mathrm{T}}\sum_{s=1}^{S}\beta_s\mathbf{K}_s\mathbf{w} - \frac{1}{2}\mathbf{w}^{\mathrm{T}}\sum_{s,\sigma=1}^{S}\beta_s\beta_\sigma\mathbf{K}_s\mathbf{K}_\sigma\mathbf{w}\right)$$

$$\mathbf{F}_{s\sigma}(\boldsymbol{\beta}) = \mathbf{w}^{\mathrm{T}}\mathbf{K}_s^{\mathrm{T}}\mathbf{K}_\sigma\mathbf{w} \qquad \mathbf{F}(\mathbf{w}) = \mathbf{K}_{\boldsymbol{\beta}}^{\mathrm{T}}\mathbf{K}_{\boldsymbol{\beta}}$$

- Information Optimality Criteria: Maximize Information by minimizing variance of estimator.
- D-optimality :

$$\beta \leftarrow \underset{\beta}{\operatorname{argmin}}\left\{-2\log|\mathbf{K}_\beta|\right\}$$

- Maximum value of kernel combination parameter while varying alignment.
- Fisher MKL approach and an area of “learning”.



Conclusions

- FME and a lower bound for correlation of MKL responses - flat maxima.
- Ambiguity and BVC decompositions - accuracy & diversity.
- DoE approach for simple linear regression MKL case - Fisher information.

What's next

- Fisher MKL for Classification.
- Analyzing the effect of sparsity (prior-regularization) and "localized" MKL?

Code

- www.dcs.gla.ac.uk/inference/pMKL (Variational Bayes & Sparse models)

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Thank you for your attention

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