Kernel Learning with Bregman Matrix Divergences

Inderjit S. Dhillon

The University of Texas at Austin

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Kernel Methods

Kernel methods are important for many problems in machine learning

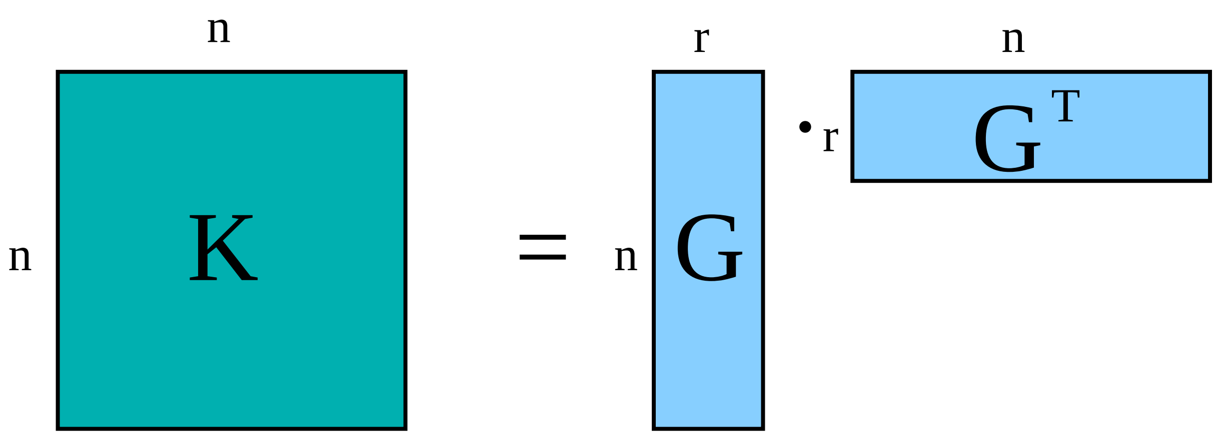
- Embed data into high-dimensional space via a mapping ψ
- Kernel function gives the inner product in the feature space:

$$\kappa(\mathbf{a}_i, \mathbf{a}_j) = \psi(\mathbf{a}_i) \cdot \psi(\mathbf{a}_j)$$

- Kernel algorithms use the kernel matrix for learning in feature space
- Kernels have been defined for various discrete structures
  - trees
  - graphs
  - strings
  - images
  - ...

Low-Rank Kernels

- A kernel matrix may not be of full rank, but rather of rank $r < n$



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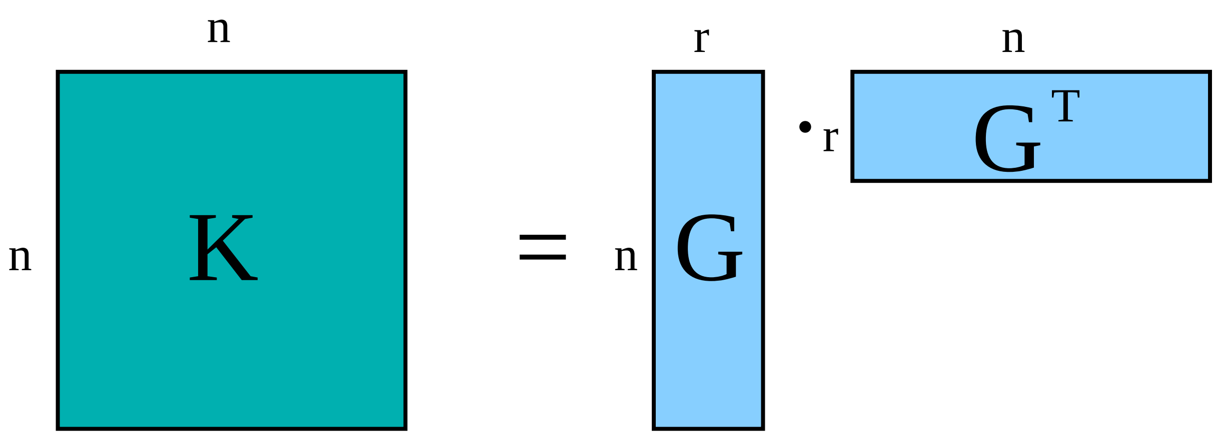

- Can *decompose* the kernel as $K = GG^T$
- Several advantages to such a decomposition
  - Storage reduces from $O(n^2)$ to $O(nr)$
  - Running time of most kernel algorithms improves to linear in n
  - Example: SVM training goes from $O(n^3)$ to $O(nr^2)$

Learning Low-Rank Kernels

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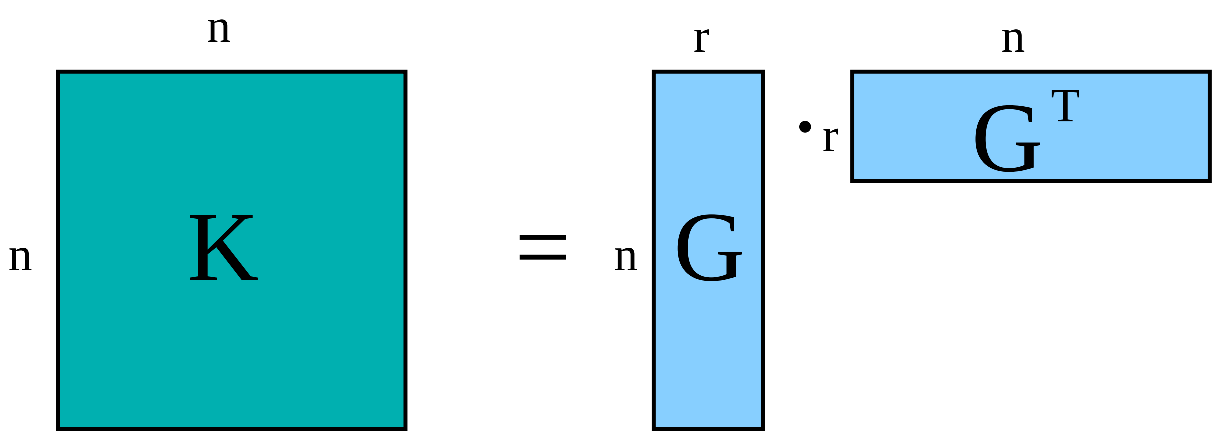

- Sometimes need to *learn* the kernel matrix
  - No kernel may be given, but other information may be available
  - An existing kernel may be given, but may want to modify the kernel to satisfy additional constraints
  - May want to combine multiple sources of data into a single kernel
- Existing methods for learning a kernel are $O(n^3)$ (or worse)
  - Semi-definite programming methods [Lanckriet et al., JMLR, 2004]
  - Projection-based methods [Tsuda et al., JMLR, 2005]
  - Hyperkernels and other methods [Ong et al, JMLR, 2005]

Bregman Divergences

- Let $\varphi : S \to \mathbb{R}$ be a differentiable, strictly convex function of "Legendre type" ($S \subseteq \mathbb{R}^d$)
- The Bregman Divergence $D_\varphi : S \times \text{ri}(S) \to \mathbb{R}$ is defined as

$$D_\varphi(\boldsymbol{x}, \boldsymbol{y}) = \varphi(\boldsymbol{x}) - \varphi(\boldsymbol{y}) - (\boldsymbol{x} - \boldsymbol{y})^T \nabla\varphi(\boldsymbol{y})$$

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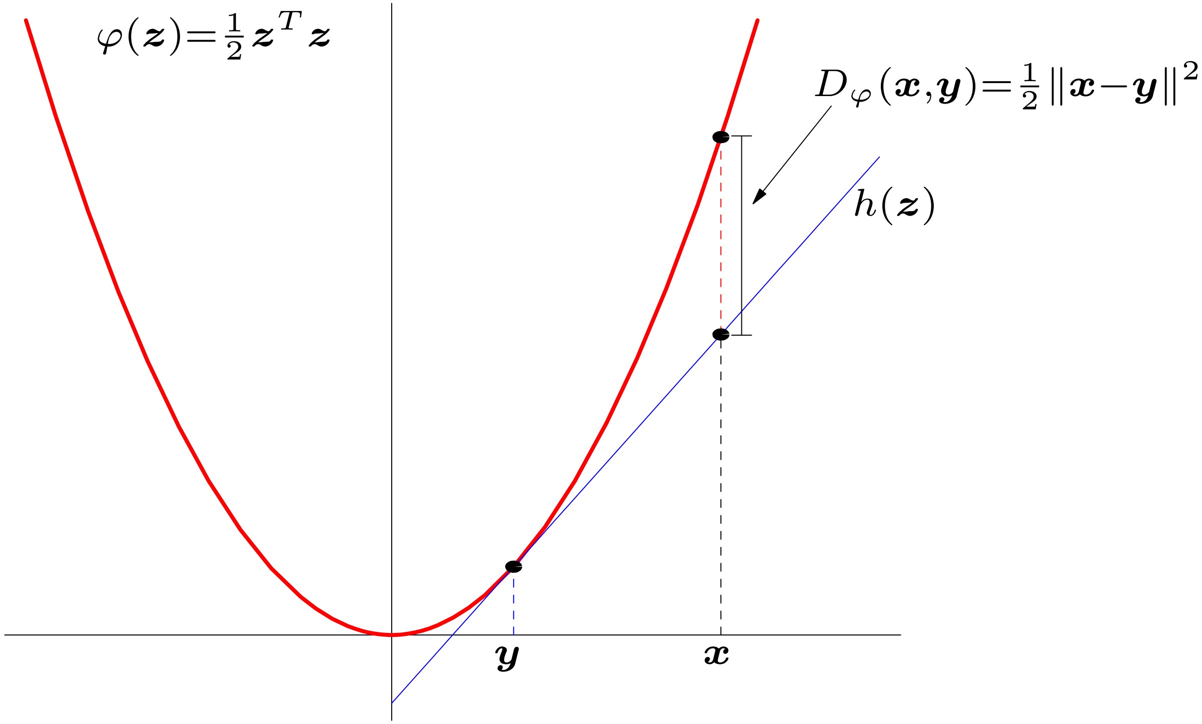

Squared Euclidean distance is a Bregman divergence

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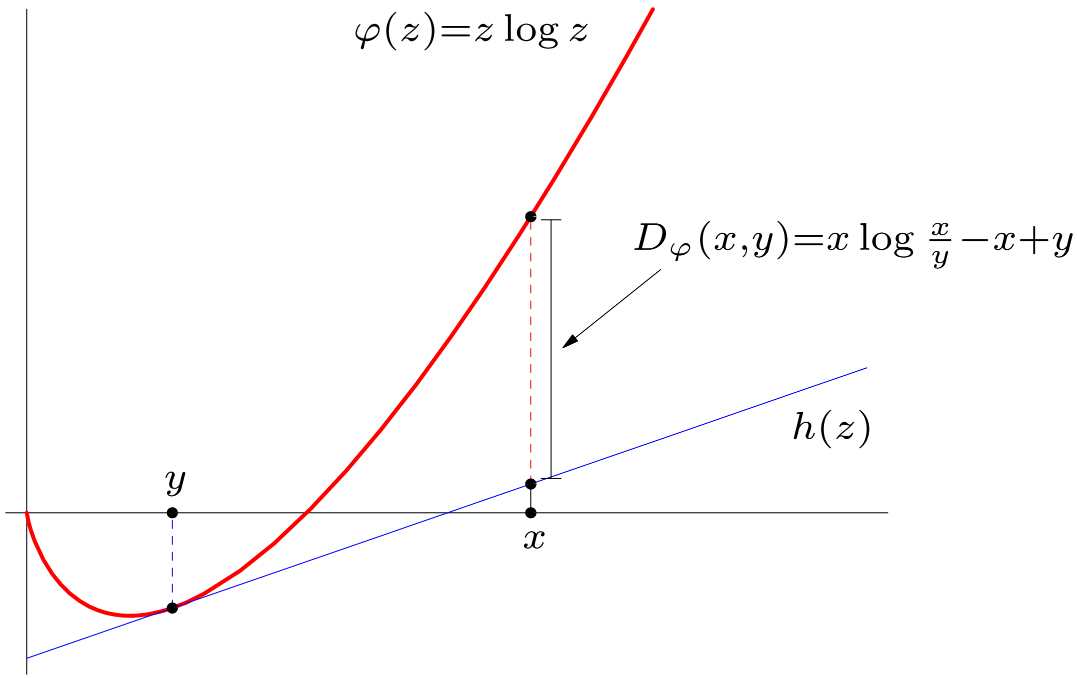

Relative Entropy (also called KL-divergence)

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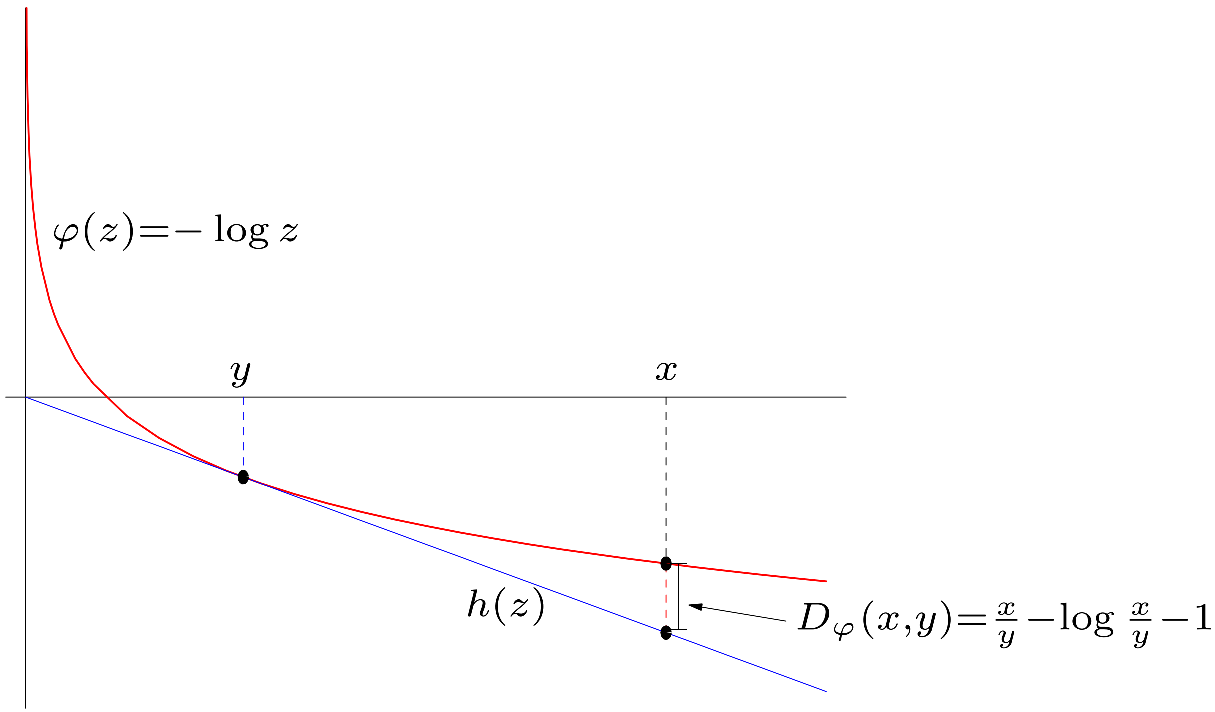

Itakura-Saito Distance (or Burg divergence)—used in signal processing

Properties of Bregman Divergences

- $D_\varphi(\boldsymbol{x}, \boldsymbol{y}) \geq 0$, and equals 0 iff $\boldsymbol{x} = \boldsymbol{y}$
- Not a metric (symmetry, triangle inequality do not hold)
- Strictly convex in the first argument, but not convex (in general) in the second argument
- Three-point property generalizes the “Law of cosines”:

$$D_\varphi(\boldsymbol{x}, \boldsymbol{y}) = D_\varphi(\boldsymbol{x}, \boldsymbol{z}) + D_\varphi(\boldsymbol{z}, \boldsymbol{y}) - (\boldsymbol{x} - \boldsymbol{z})^T (\nabla\varphi(\boldsymbol{y}) - \nabla\varphi(\boldsymbol{z}))$$

Bregman Projections

- Nearness in Bregman divergence: the "Bregman" projection of $\boldsymbol{y}$ onto a convex set Ω,

$$P_\Omega(\boldsymbol{y}) = \operatorname*{argmin}_{\boldsymbol{\omega} \in \Omega} D_\varphi(\boldsymbol{\omega}, \boldsymbol{y})$$

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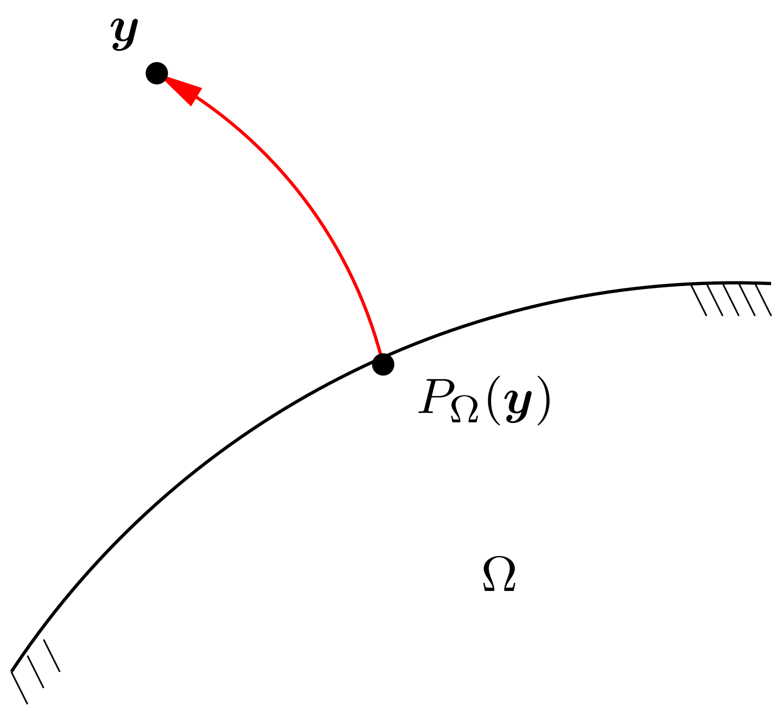

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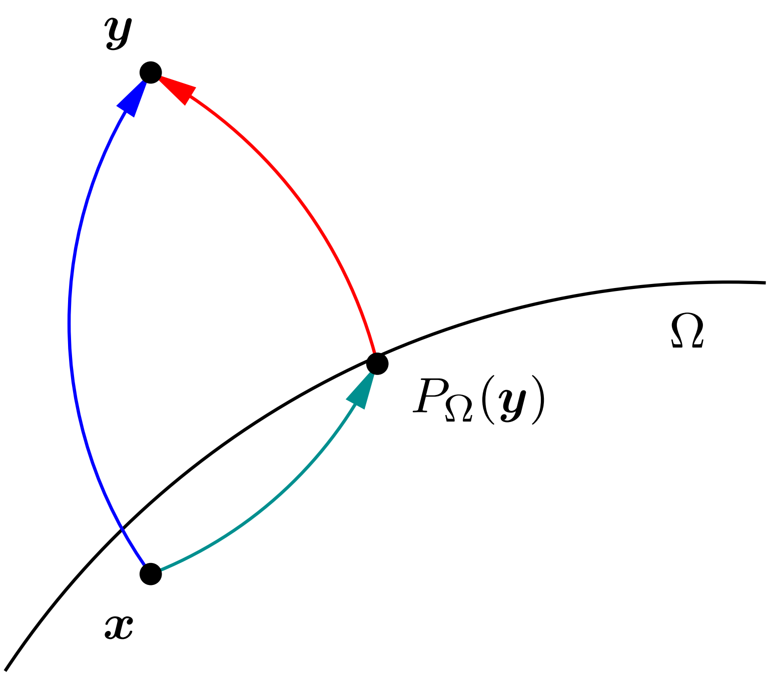

- Generalized Pythagoras Theorem:

$$D_\varphi(\boldsymbol{x}, \boldsymbol{y}) \geq D_\varphi(\boldsymbol{x}, P_\Omega(\boldsymbol{y})) + D_\varphi(P_\Omega(\boldsymbol{y}), \boldsymbol{y})$$

When Ω is an affine set, the above holds with equality

Bregman Matrix Divergences

- Extend Bregman divergences over vectors to divergences over real, symmetric matrices:

$$D_\varphi(X,Y) = \varphi(X) - \varphi(Y) - \mathrm{trace}((\nabla\varphi(Y))^T(X-Y))$$

- Squared Frobenius norm: $\varphi(X) = \frac{1}{2}\text{tr}(X^TX)$. Then

$$D_{Frob}(X,Y) = \frac{1}{2}\|X-Y\|_F^2$$

- von Neumann Divergence: $\varphi(X) = \text{tr}(X\log X - X)$ (negative entropy of the eigenvalues). Then

$$D_{vN}(X,Y) = \mathrm{trace}(X\log X - X\log Y - X + Y)$$

- Burg Matrix Divergence (LogDet divergence): $\varphi(X) = -\log\text{det}X$ (Burg entropy of the eigenvalues). Then

$$D_{Burg}(X,Y) = \mathrm{trace}(XY^{-1}) - \log\text{det}(XY^{-1}) - n$$

Optimization Framework

- Optimization problem:

$$\begin{array}{rl} \text{minimize} & D_\varphi(K, K_0) \\ \text{subject to} & \mathrm{tr}(KA_i) \leq b_i, \ 1 \leq i \leq c \\ & \mathrm{rank}(K) \leq r \\ & K \succeq 0. \end{array}$$

- Problem is non-convex due to the rank constraint
- Standard convex optimization techniques do not seem to apply here

Rank-Preserving Matrix Divergences

- Rewrite the Von Neumann divergence and Burg divergence using the eigendecompositions
- Given matrices X and Y, let $X = V\Lambda V^T$ and $Y = U\Theta U^T$
- von Neumann:

$$
\begin{aligned}
D_{vN}(X,Y) &= \text{tr}(X\log X - X\log Y - X + Y) \\
&= \sum_i \lambda_i \log\lambda_i - \sum_{i,j}(\mathbf{v}_i^T\mathbf{u}_j)^2\lambda_i\log\theta_j - \sum_i(\lambda_i - \theta_i)
\end{aligned}
$$

- Important Implication: $D_{vN}(X,Y)$ is finite iff range$(X) \subseteq$ range(Y)

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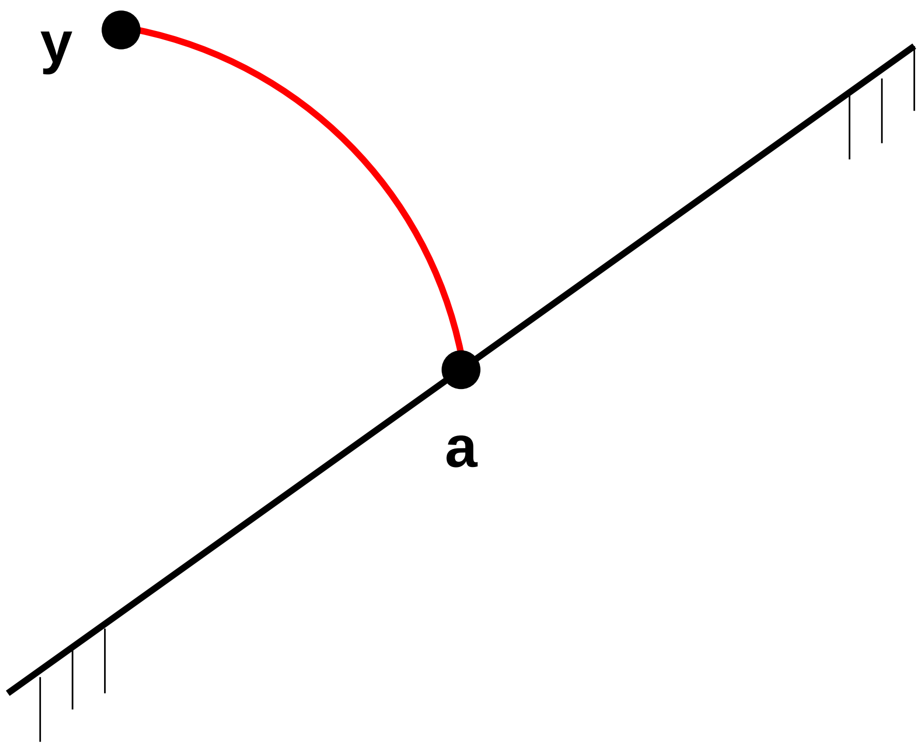
- Important Implication: $D_{Burg}(X, Y)$ is finite iff range$(X) =$ range(Y)
- Optimization problem:
  - Satisfies rank$(K) \leq$ rank(K_0) in vN divergence
  - Satisfies rank$(K) =$ rank(K_0) in Burg divergence
  - Implicitly maintains rank and positive semi-definite constraints
  - Is convex when rank$(K_0) \leq r$

Method of Cyclic Projections

- Use the "Bregman" projection of $\boldsymbol{y}$ onto affine set $\mathcal{H}$,

$$P_{\mathcal{H}}(\boldsymbol{y}) = \underset{\boldsymbol{a}\in\mathcal{H}}{\operatorname{argmin}}\, D_{\varphi}(\boldsymbol{a}, \boldsymbol{y})$$



- Method projects onto each constraint, one at a time, and applies appropriate "correction"—provably converges to the optimal solution

Projections with rank-preserving Bregman divergences

- Solve smaller optimization problem to get projection onto constraint i

$$\begin{array}{rl} \text{minimize} & D_\varphi(K_{t+1}, K_t) \\ \text{subject to} & \text{tr}(K_{t+1}A_i) \le b_i \end{array}$$

- For both divergences, projections can be calculated in $O(r^2)$ time
- Requires all operations to be done on a suitable factored form of the kernel matrices

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- Burg divergence update:

$$\begin{array}{rcl} K_{t+1} & = & (K_t^\dagger - \alpha A_i^T)^\dagger \\ \text{such that} \quad \mathrm{tr}(K_{t+1}A_i) & \leq & b_i \end{array}$$

  - Distance constraints expressed as $A_i = \boldsymbol{z}_i \boldsymbol{z}_i^T$
  - Projection parameter α *has a closed form solution*
  - $O(r^2)$ projection achieved using factored form of K_t

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  - Requires the fast multipole method to achieve $O(r^2)$ projection
  - We have designed a custom non-linear solver to compute the projection parameter α

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- End Result: Algorithms are linear in $n + c$, quadratic in r

Special Cases and Related Work

- Full-rank case with von Neumann divergence, $b_i = 0 \forall i$, obtain DefiniteBoost optimization problem [Tsuda et al., JMLR, 2005]
  - Improve the running time from $O(n^3)$ to $O(n^2)$ per projection
  - Allow arbitrary linear constraints, both equality and inequality

- For constraints $K_{ii} = 1 \forall i$, obtain the nearest correlation matrix problem [Higham, IMA J. Numerical Analysis, 2002]
  - Arises in financial applications
  - New efficient methods for finding low-rank correlation matrices

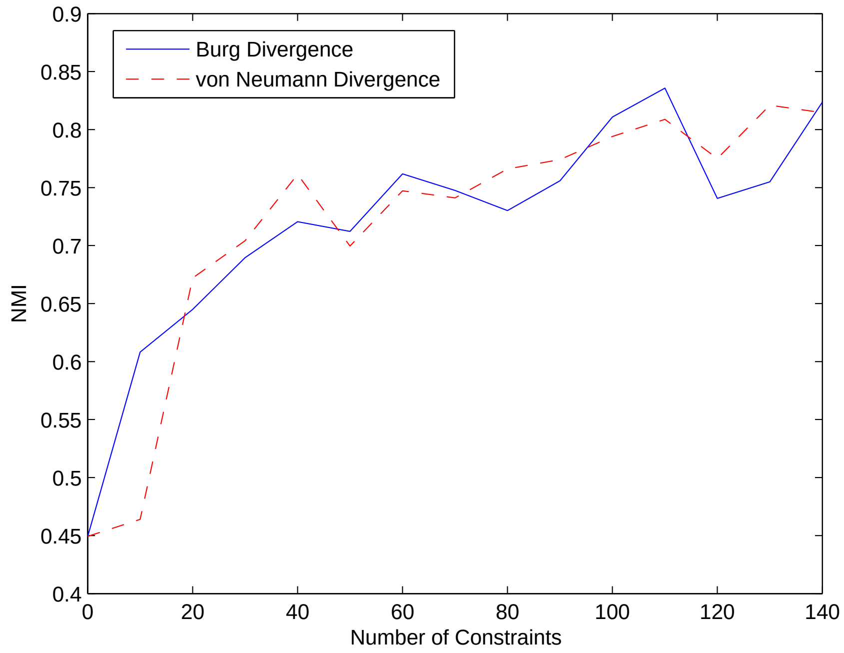
- Can be used for nonlinear dimensionality reduction
  - Isometry constraints are linear
  - [Weinberger et al., ICML, 2004] maximize trace(X) (by semi-definite programming)

Experiments

- Digits data: 317 digits, 3 classes
  - Given a rank-16 kernel for 317 digits
  - Randomly create constraints:

$$d(i_1, i_2) \leq (1 - \epsilon) b_i$$
$$d(i_1, i_2) \geq (1 + \epsilon) b_i$$

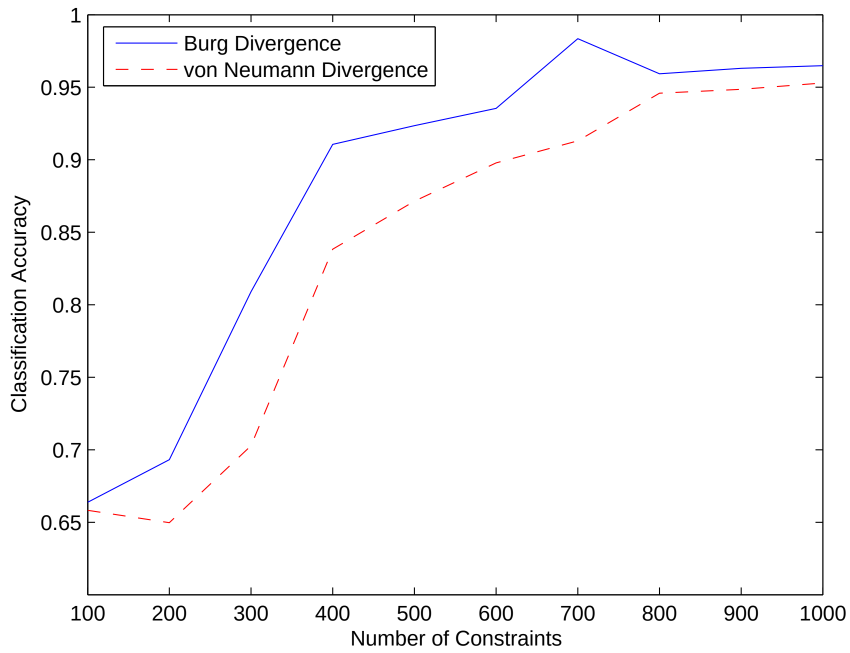
  - Attempt to learn a "better" rank-16 kernel



- Clustering: use kernel k-means with random initialization, compute accuracy using normalized mutual information

Experiments

- GyrB protein data: 52 proteins, 3 classes
  - Given *only* constraints
  - Want to learn a kernel based on constraints
  - Constraints generated from target kernel matrix
  - Attempt to learn a full-rank kernel



- Classification: use k-nearest neighbor, $k = 5$, 50/50 training/test split, 2-fold cross validation averaged over 20 runs

Relevant Papers

- [Dhillon & Tropp] "Matrix Nearness Problems with Bregman Divergences", submitted to the SIAM Journal on Matrix Analysis and Applications, 2006.
- [Kulis, Sustik & Dhillon] "Low-Rank Kernel Learning", International Conference on Machine Learning, 2006 (to appear).

Conclusions

- Low-rank kernel matrices can be learnt efficiently using appropriate Bregman matrix divergences
  - Burg divergence and von Neumann divergence
  - Implicitly maintain rank and positive semi-definiteness constraints
- Algorithms scale linearly with n and quadratically with r
- Future Work
  - Further investigate the gains of preserving range space
  - Apply to varied applications
  - Improvement over cyclic projection methods