Spectral Measures for Nearness Problems

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Nearness Problems

- Given an input matrix, find the “nearest” matrix that satisfies user constraints
- How should nearness be measured?
- Typical choices are the Frobenius norm or the spectral 2-norm
- However, these may not be appropriate for the application at hand
- Outline of talk
  - Bregman vector divergences
  - Bregman matrix divergences — offer alternate spectral measures
  - Nearness problems with von Neumann & Burg matrix divergences

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 $D_\varphi : S \times \text{relint}(S) \to \mathbb{R}$ 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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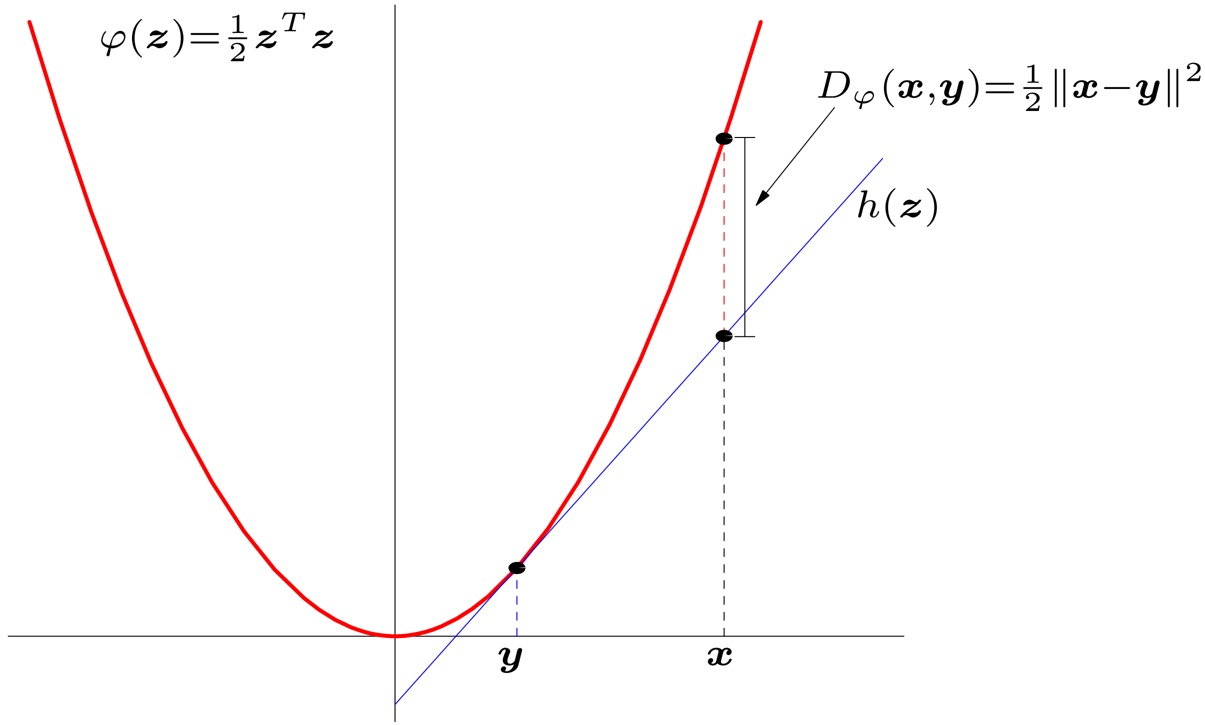

Squared Euclidean distance is a Bregman divergence

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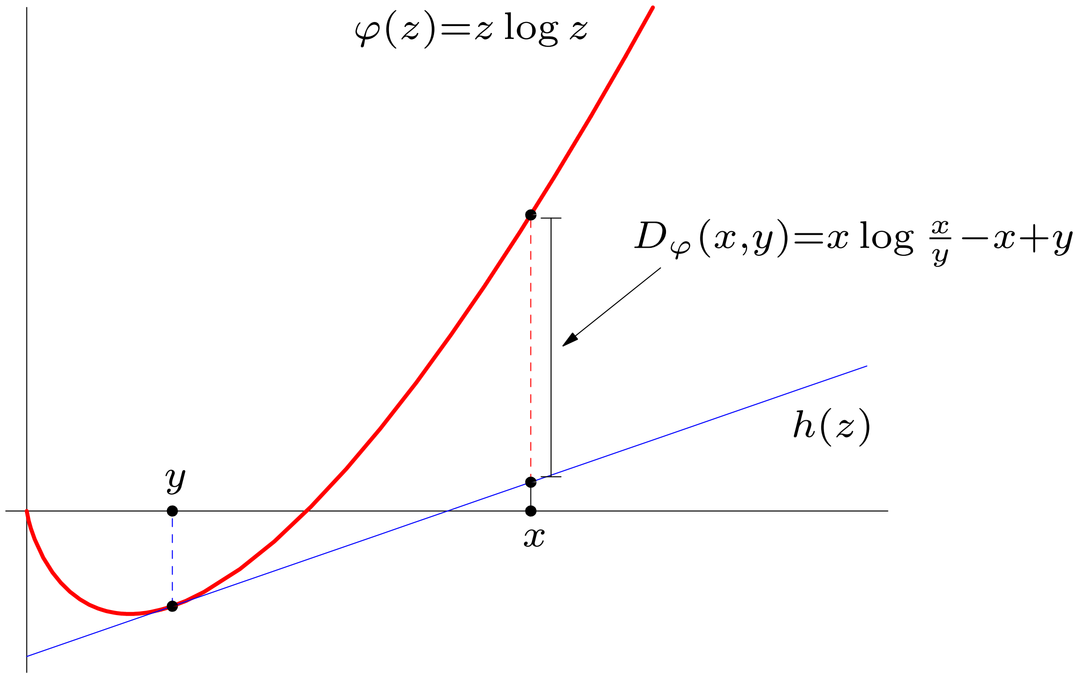

Relative Entropy (also called KL-divergence) is another Bregman divergence

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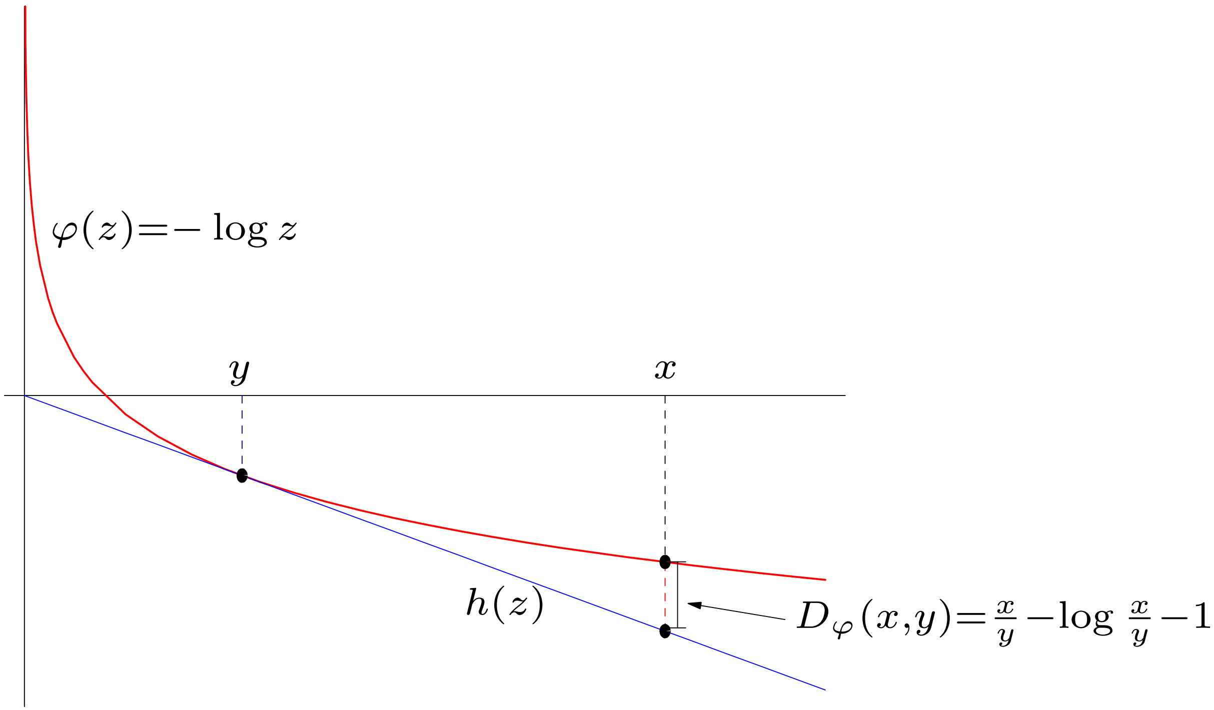

Itakura-Saito Distance (used in signal processing) is another Bregman divergence

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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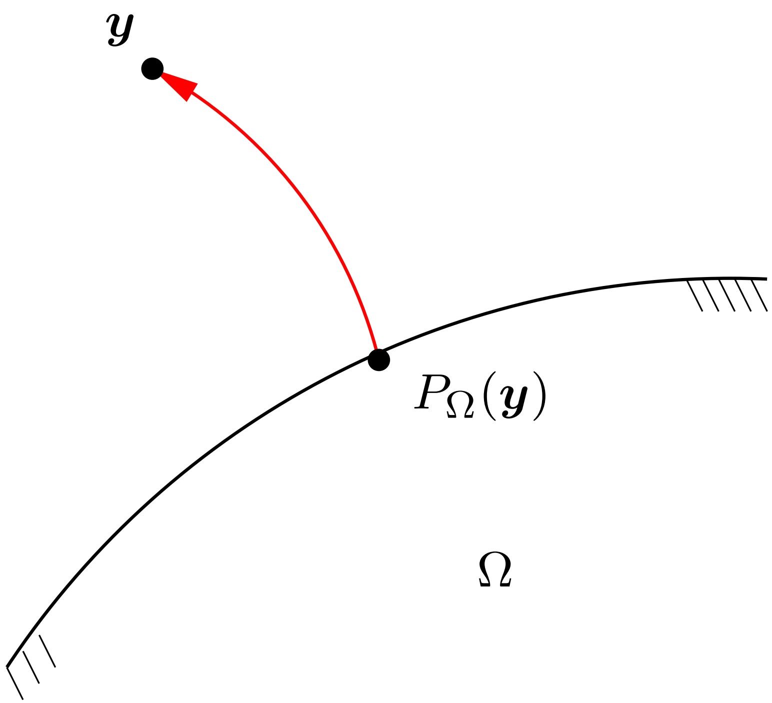

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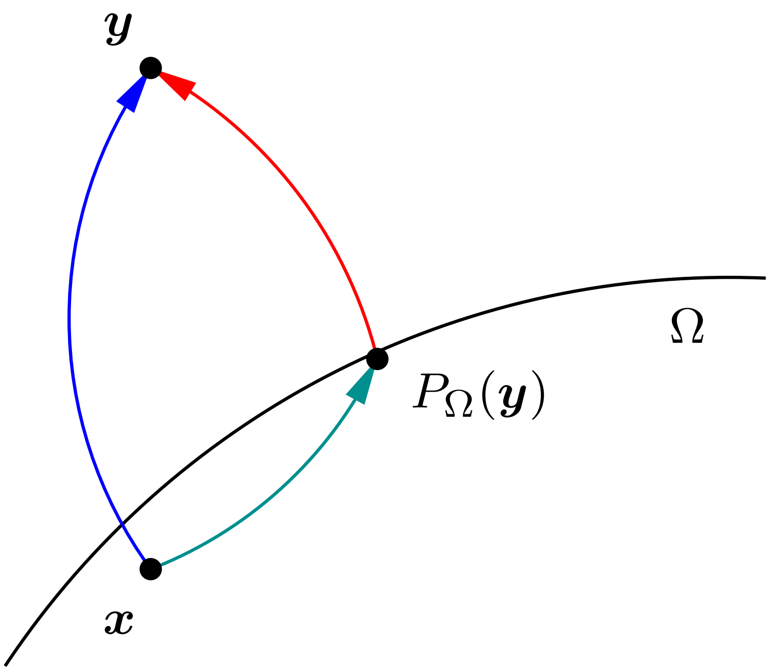

- Generalized Pythagoras Theorem:

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

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

Bregman Matrix Divergences

- Generalizes the notion of divergence to matrices
- Let φ be a real-valued convex function over matrices
- Leads to Bregman matrix divergences:

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

- For example, $\varphi(\boldsymbol{X}) = \|\boldsymbol{X}\|_F^2$ leads to

$$D_\varphi(\boldsymbol{X}, \boldsymbol{Y}) = \|\boldsymbol{X} - \boldsymbol{Y}\|_F^2$$

Squared Euclidean Distance	$\longleftrightarrow$	Squared Frobenius Distance
Relative Entropy	$\longleftrightarrow$	von Neumann Divergence (Quantum Relative Entropy)
Itakura-Saito Divergence	$\longleftrightarrow$	Burg Divergence (LogDet Divergence)

Von Neumann Matrix Divergence

- Let $\boldsymbol{X} = \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^T$ be a positive definite matrix
- Consider negative entropy of the eigenvalues (von Neumann entropy):

$$\varphi(\boldsymbol{X}) = \sum_i (\lambda_i \log \lambda_i - \lambda_i) = \mathrm{tr}(\boldsymbol{X} \log \boldsymbol{X} - \boldsymbol{X})$$

- Yields the von Neumann matrix divergence (quantum relative entropy):

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

- In terms of the spectrum of $\boldsymbol{X}$ and $\boldsymbol{Y}$ ($\boldsymbol{X} = \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^T$, $\boldsymbol{Y} = \boldsymbol{U}\boldsymbol{\Theta}\boldsymbol{U}^T$):

$$D_{vN}(\boldsymbol{X}, \boldsymbol{Y}) = \sum_i \lambda_i \log \lambda_i - \sum_i \sum_j (\boldsymbol{v}_i^T \boldsymbol{u}_j)^2 \lambda_i \log \theta_j - \sum_i (\lambda_i - \theta_i)$$

- Definition can be extended to semi-definite matrices
- Divergence is finite iff $\mathrm{range}(\boldsymbol{X}) \subseteq \mathrm{range}(\boldsymbol{Y})$

Burg Matrix Divergence

- Let $\boldsymbol{X} = \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^T$ be an $N \times N$ positive definite matrix
- Consider Burg entropy of the eigenvalues:

$$\varphi(\boldsymbol{X}) = -\sum_i \log \lambda_i = -\log\det \boldsymbol{X}$$

- Yields the Burg (or LogDet) matrix divergence:

$$D_{Burg}(\boldsymbol{X}, \boldsymbol{Y}) = \mathrm{tr}(\boldsymbol{X}\boldsymbol{Y}^{-1}) - \log\det(\boldsymbol{X}\boldsymbol{Y}^{-1}) - N$$

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- Divergence is finite iff $\mathrm{range}(\boldsymbol{X}) = \mathrm{range}(\boldsymbol{Y})$

Nearness Problem with Matrix Divergences

- Nearness with respect to linear constraints

$$\min_{\boldsymbol{X} \in S} \quad d(\boldsymbol{X}, \boldsymbol{X}_0)$$
$$\text{subject to} \quad \operatorname{tr}(\boldsymbol{X}\boldsymbol{A}_i) \leq b_i$$

Nearness Problem with Matrix Divergences

- Nearness with respect to linear constraints

$$\begin{aligned} \min_{\boldsymbol{X}} \quad & D_{\varphi}(\boldsymbol{X}, \boldsymbol{X}_0) \\ \text{subject to} \quad & \operatorname{tr}(\boldsymbol{X}\boldsymbol{A}_i) \le b_i \\ & \boldsymbol{X} \succeq 0 \end{aligned}$$

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- Arises in various applications:
  - Nearest correlation matrix (Higham, 2002)
  - Kernel learning (Tsuda et al, 2004; Kulis et al 2006)
  - ...

Rank-Constrained Nearness Problem

- Nearness with respect to linear and rank constraints

$$\begin{aligned} \min_{\boldsymbol{X}} \quad & D_\varphi(\boldsymbol{X}, \boldsymbol{X}_0) \\ \text{subject to} \quad & \operatorname{tr}(\boldsymbol{X}\boldsymbol{A}_i) \le b_i \\ & \boldsymbol{X} \succeq 0 \\ & \operatorname{rank}(\boldsymbol{X}) \le r \end{aligned}$$

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- In general, the above problem is non-convex
- Turns out to be convex if:
  - $\operatorname{rank}(\boldsymbol{X}_0) \le r$, and
  - D_φ is the von Neumann or Burg divergence

Rank-Constrained Nearness Problem

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- In general, the above problem is non-convex
- Turns out to be convex if:
  - $\operatorname{rank}(\boldsymbol{X}_0) \leq r$, and
  - D_φ is the von Neumann or Burg divergence
- Thus, in this case, the last two constraints can be “dropped”:

$$\begin{aligned} \min_{\boldsymbol{X}} \quad & D_\varphi(\boldsymbol{X}, \boldsymbol{X}_0) \\ \text{subject to} \quad & \operatorname{tr}(\boldsymbol{X}\boldsymbol{A}_i) \leq b_i \end{aligned}$$

Method of cyclic projections

- Consider the convex optimization problem:

$$\begin{aligned} \min_{\boldsymbol{x}} \quad & \varphi(\boldsymbol{x}) \\ \text{subject to} \quad & \boldsymbol{a}_i^T \boldsymbol{x} = b_i, \quad i = 0, \ldots, m-1 \end{aligned}$$

- Bregman's cyclic projection method:
  1. Start with $\boldsymbol{x}^0$ that satisfies $\nabla\varphi(\boldsymbol{x}^0) = -A^T\boldsymbol{\pi}$. Set $t = 0$.
  2. Let $j = t \mod m$. Compute $\boldsymbol{x}^{t+1}$ to be the Bregman projection of $\boldsymbol{x}^t$ onto the j-th hyperplane, i.e., $\boldsymbol{x}^{t+1}$ is the solution of

$$\begin{aligned} \min_{\boldsymbol{x}} \quad & D_\varphi(\boldsymbol{x}, \boldsymbol{x}^t) \\ \text{subject to} \quad & \boldsymbol{a}_j^T \boldsymbol{x} = b_j \end{aligned}$$

  3. Set $t = t + 1$ and repeat.
- Converges to globally optimal solution (Bregman, 1967)
- Can be extended to halfspace and convex constraints — each projection needs to be followed by a correction

Cyclic Projection Step

- At step t of the cyclic projection algorithm, we need to solve:

$$\begin{array}{rl} \min_{\boldsymbol{X}} & D_\varphi(\boldsymbol{X}, \boldsymbol{X}_t) \\ \text{subject to} & \operatorname{tr}(\boldsymbol{X}\boldsymbol{A}_i) = b_i \end{array}$$

- Lagrange dual:

$$L(\boldsymbol{X}, \alpha) = \min_{\boldsymbol{X}} \; D_\varphi(\boldsymbol{X}, \boldsymbol{X}_t) + \alpha(\operatorname{tr}(\boldsymbol{X}\boldsymbol{A_i}) - b_i)$$

- Need to solve for X_{t+1} and α:

$$\begin{aligned} \nabla\varphi(\boldsymbol{X}_{t+1}) &= \nabla\varphi(\boldsymbol{X}_t) + \alpha \boldsymbol{A}_i \\ \operatorname{tr}(\boldsymbol{X}_{t+1}\boldsymbol{A}_i) &= b_i \end{aligned}$$

Burg Update

- Burg Divergence

$$D_{Burg}(\boldsymbol{X}, \boldsymbol{X}_t) = \mathrm{tr}(\boldsymbol{X}\boldsymbol{X}_t^{-1}) - \log\det(\boldsymbol{X}\boldsymbol{X}_t^{-1}) - N$$

- Gradient is

$$\nabla D_{Burg}(\boldsymbol{X}, \boldsymbol{X}_t) = -\boldsymbol{X}^{-1} + \boldsymbol{X}_t^{-1}$$

- The Burg projection update becomes:

$$\begin{aligned} \nabla\varphi(\boldsymbol{X}_{t+1}) &= \nabla\varphi(\boldsymbol{X}_t) + \alpha\boldsymbol{A}_i \\ \Longrightarrow \qquad \boldsymbol{X}_{t+1} &= (\boldsymbol{X}_t^{-1} - \alpha\boldsymbol{A}_i)^{-1} \end{aligned}$$

- The update is often rank-one, $\boldsymbol{A}_i = \boldsymbol{z}_i\boldsymbol{z}_i^T$
  - Correlation matrix
  - Distance constraints in kernel learning

Projection Parameter—Burg Divergence

- Burg update:

$$
\begin{aligned}
\boldsymbol{X}_{t+1} &= (\boldsymbol{X}_t^{-1} - \alpha \boldsymbol{z}\boldsymbol{z}^T)^{-1} \\
\boldsymbol{z}^T \boldsymbol{X}_{t+1} \boldsymbol{z} &= b
\end{aligned}
$$

- A closed form solution exists!
- Sherman-Morrison-Woodbury formula leads to:

$$
\begin{aligned}
p &= \boldsymbol{z}^T \boldsymbol{X}_t \boldsymbol{z} \\
\alpha &= \frac{1}{p} - \frac{1}{b} \\
\beta &= \alpha/(1 - \alpha p) \\
\boldsymbol{X}_{t+1} &= \boldsymbol{X}_t + \beta \boldsymbol{X}_t \boldsymbol{z}\boldsymbol{z}^T \boldsymbol{X}_t
\end{aligned}
$$

- Allows extension to the rank-deficient case

Burg Update—Efficiency

- Burg update:

$$\boldsymbol{X}_{t+1} = \boldsymbol{X}_t + \beta \boldsymbol{X}_t \boldsymbol{z}\boldsymbol{z}^T \boldsymbol{X}_t$$

- Using $\boldsymbol{X}_t = \boldsymbol{G}_t \boldsymbol{G}_t^T$, the Cholesky factor $\boldsymbol{G}_t$ needs to be updated:

$$\begin{aligned} I + \beta(\boldsymbol{G}_t^T \boldsymbol{z})(\boldsymbol{G}_t^T \boldsymbol{z})^T &= \boldsymbol{L}\boldsymbol{L}^T \\ \boldsymbol{G}_{t+1} &= \boldsymbol{G}_t \boldsymbol{L} \end{aligned}$$

- Note that $I + \beta(\boldsymbol{G}_t^T \boldsymbol{z})(\boldsymbol{G}_t^T \boldsymbol{z})^T$ is an $r \times r$ matrix
- Multiplication with $\boldsymbol{L}$ appears to be the most expensive operation
- Special structure of $\boldsymbol{L}$ allows an $O(r^2)$ algorithm

Burg Update using Eigendecomposition

- Burg update:

$$\boldsymbol{X}_{t+1} = (\boldsymbol{X}_t^{-1} - \alpha \boldsymbol{z}\boldsymbol{z}^T)^{-1}$$

- Maintain alternate factored form: $\boldsymbol{X}_t = \boldsymbol{V}_t \boldsymbol{\Lambda}_t \boldsymbol{V}_t^T$

$$\begin{aligned} \boldsymbol{X}_{t+1} &= (\boldsymbol{V}_t \boldsymbol{\Lambda}_t^{-1} \boldsymbol{V}_t^T - \alpha \boldsymbol{z}\boldsymbol{z}^T)^{-1} \\ &= \boldsymbol{V}_t (\boldsymbol{\Lambda}_t^{-1} - \alpha \boldsymbol{V}_t^T \boldsymbol{z}\boldsymbol{z}^T \boldsymbol{V}_t)^{-1} \boldsymbol{V}_t^T \end{aligned}$$

- Eigenvalue problem for a diagonal plus rank-one matrix:

$$\boldsymbol{\Lambda}_t^{-1} - \alpha (\boldsymbol{V}_t^T \boldsymbol{z})(\boldsymbol{V}_t^T \boldsymbol{z})^T = \boldsymbol{U}\boldsymbol{\Theta}\boldsymbol{U}^T$$

- Update the factored form:

$$\boldsymbol{V}_{t+1} = \boldsymbol{V}_t \boldsymbol{U}, \; \boldsymbol{\Lambda}_{t+1} = \boldsymbol{\Theta}^{-1}$$

Von Neumann Update

- Von Neumann divergence:

$$D_{vN}(\boldsymbol{X}, \boldsymbol{X}_t) = \mathrm{tr}(\boldsymbol{X} \log \boldsymbol{X} - \boldsymbol{X} \log \boldsymbol{X}_t - \boldsymbol{X} + \boldsymbol{X}_t)$$

- Gradient is:

$$\nabla D_{vN}(\boldsymbol{X}, \boldsymbol{X}_t) = \log \boldsymbol{X} - \log \boldsymbol{X}_t$$

- The von Neumann projection update becomes:

$$\begin{aligned} \nabla\varphi(\boldsymbol{X}_{t+1}) &= \nabla\varphi(\boldsymbol{X}_t) + \alpha \boldsymbol{A}_i \\ \Longrightarrow \quad \boldsymbol{X}_{t+1} &= \exp(\log(\boldsymbol{X}_t) + \alpha \boldsymbol{A}_i) \end{aligned}$$

- For rank-one updates: $\boldsymbol{A}_i = \boldsymbol{z}_i \boldsymbol{z}_i^T$

Von Neumann Update

- Von Neumann Update:

$$\begin{aligned} \boldsymbol{X}_{t+1} &= \exp(\log(\boldsymbol{X}_t) + \alpha \boldsymbol{z}\boldsymbol{z}^T) \\ \boldsymbol{z}^T \boldsymbol{X}_{t+1} \boldsymbol{z} &= b \end{aligned}$$

- Maintain factored form for efficiency: $\boldsymbol{X}_t = \boldsymbol{V}_t \boldsymbol{\Lambda}_t \boldsymbol{V}_t^T$

$$\begin{aligned} \boldsymbol{X}_{t+1} &= \exp(\boldsymbol{V}_t \log(\boldsymbol{\Lambda}_t) \boldsymbol{V}_t^T + \alpha \boldsymbol{z}\boldsymbol{z}^T) \\ &= \boldsymbol{V}_t \exp(\log(\boldsymbol{\Lambda}_t) + \alpha \boldsymbol{V}_t^T \boldsymbol{z}\boldsymbol{z}^T \boldsymbol{V}_t) \boldsymbol{V}_t^T \end{aligned}$$

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$$\log(\boldsymbol{\Lambda}_t) + \alpha (\boldsymbol{V}_t^T \boldsymbol{z})(\boldsymbol{V}_t^T \boldsymbol{z})^T = \boldsymbol{U} \boldsymbol{\Theta} \boldsymbol{U}^T$$

- Update in factored form:

$$\boldsymbol{V}_{t+1} = \boldsymbol{V}_t \boldsymbol{U}, \;\; \boldsymbol{\Lambda}_{t+1} = \exp(\boldsymbol{\Theta})$$

Von Neumann Update—Efficiency

- Von Neumann update in factored form:

$$\log(\mathbf{\Lambda}_t) + \alpha(\boldsymbol{V}_t^T \boldsymbol{z})(\boldsymbol{V}_t^T \boldsymbol{z})^T = \boldsymbol{U}\boldsymbol{\Theta}\boldsymbol{U}^T$$

$$\boldsymbol{V}_{t+1} = \boldsymbol{V}_t \boldsymbol{U}, \ \mathbf{\Lambda}_{t+1} = \exp(\boldsymbol{\Theta})$$

- Note that $\log(\mathbf{\Lambda}_t) + \alpha(\boldsymbol{V}_t^T \boldsymbol{z})(\boldsymbol{V}_t^T \boldsymbol{z})^T$ is an $r \times r$ matrix
- The most expensive operation appears to be the $\boldsymbol{V}_t \boldsymbol{U}$ multiplication
- The Fast Multipole Method can exploit the structure of U (Greengard & Rokhlin, 1987)
- The multiplication can be performed in $O(r^2)$ time

Projection Parameter—Von Neumann Update

- Von Neumann Update:

$$\begin{aligned} \boldsymbol{X}_{t+1} &= \exp(\log(\boldsymbol{X}_t) + \alpha \boldsymbol{z}\boldsymbol{z}^T) \\ \boldsymbol{z}^T \boldsymbol{X}_{t+1} \boldsymbol{z} &= b \end{aligned}$$

- Set $\boldsymbol{w} = \boldsymbol{V}_t^T \boldsymbol{z}$. We need to solve the following for α:

$$\boldsymbol{w}^T \exp(\log(\boldsymbol{\Lambda}_t) + \alpha \boldsymbol{w}\boldsymbol{w}^T)\boldsymbol{w} = b$$

- The left hand side is a monotone function of α
- Ordinary bisection converges linearly (>50 iterations)
- Custom non-linear solver rarely needs more than 6 evaluations

Projection Parameter—Von Neumann Divergence

- We exploit the fact that

$$g(\alpha) = \boldsymbol{w}^T \exp(\log(\boldsymbol{\Lambda}_t) + \alpha \boldsymbol{w}\boldsymbol{w}^T)\boldsymbol{w} - b$$

  is similar to an exponential function
- Like Newton's method, but fit exponentials instead of straight lines
- Set $\alpha_0 = 0$, $\alpha_1 = 1$. At the i-th step let $g_1(\alpha) = \exp(p\alpha + q) - b$ such that:

$$g_1(\alpha_{i-1}) = g(\alpha_{i-1}), \;\; g_1(\alpha_i) = g(\alpha_i)$$

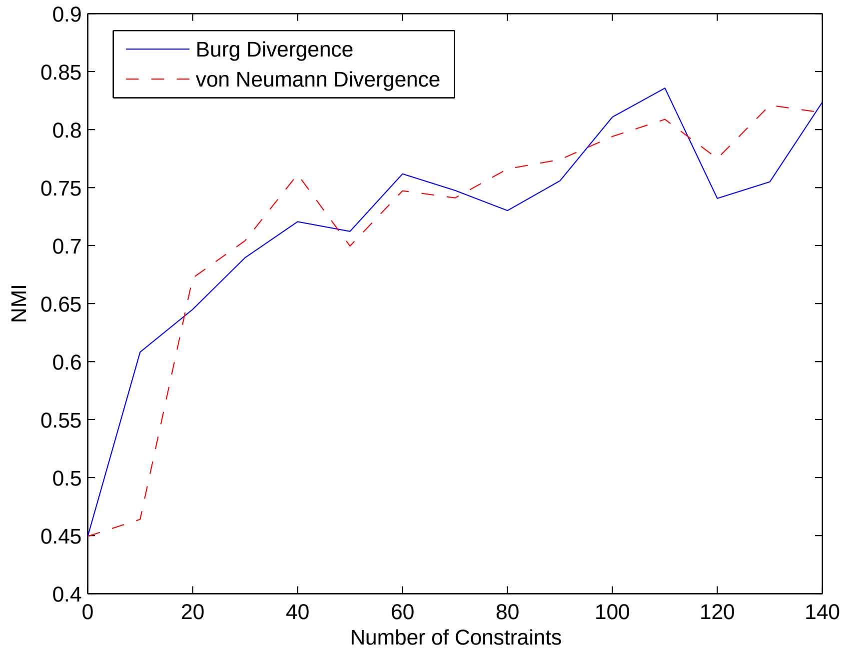
- Set α_{i+1} to be the solution of $g_1(\alpha) = 0$.
- Each iteration involves the solution of a secular equation

Experiments

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

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

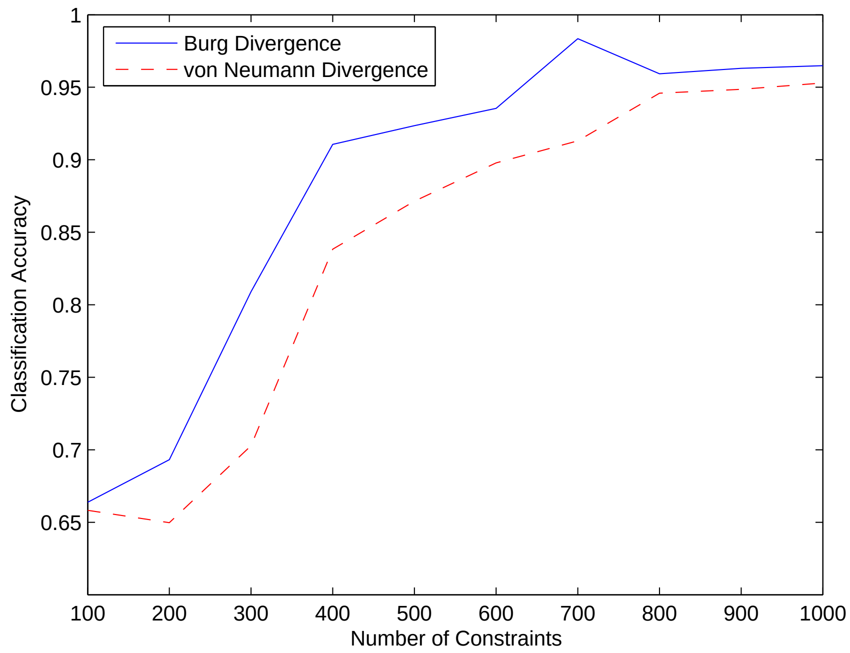
  - Attempt to learn a "better" rank-16 kernel



- 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

Conclusions & Future Work

- Bregman matrix divergences lead to intriguing nearness problems
- Nearness problems with von Neumann & Burg matrix divergences
  - Very useful if rank & null space need to be preserved
- Future Work:
  - Characterize usefulness of preserving null space
  - Detailed investigations into:
    - Nearest correlation matrix problem
    - Kernel learning problem
  - Improvement over cyclic projection methods