Kernel Matrix Regression

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Outline

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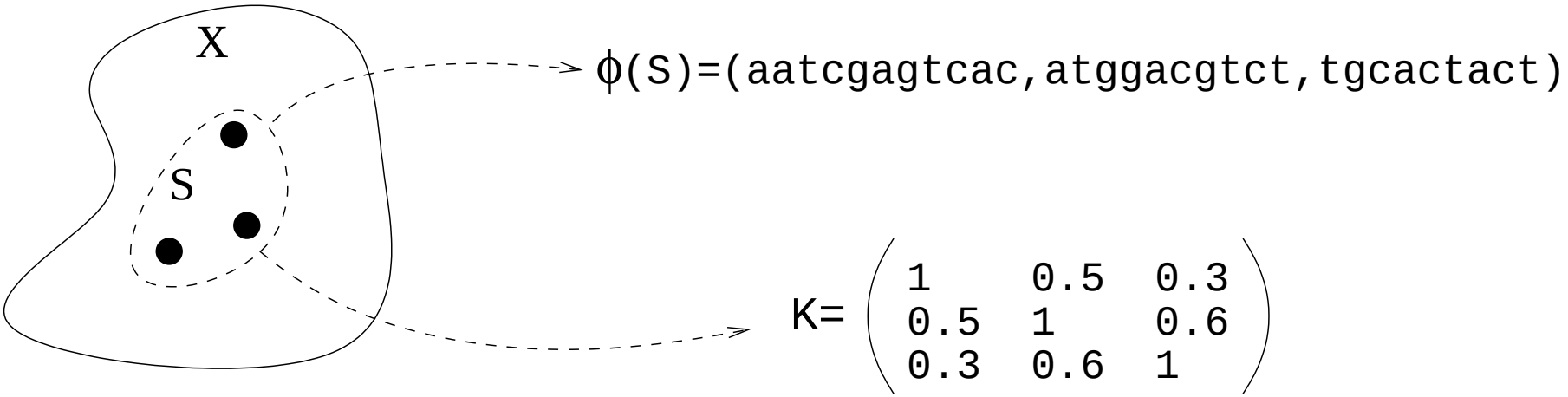
Kernel methods



- A positive definite kernel is a function $K : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$ such that any Gram matrix is positive semidefinite.
- Many algorithm for data analysis, called kernel methods, are based on p.d. kernels (SVMs, kernel PCA, kernel regression, ...)

Examples

Kernels for vectors

Classical kernels for vectors ($\mathcal{X} = \mathbb{R}^p$) include:

- The linear kernel

$$K_{lin}\left(\mathbf{x}, \mathbf{x}'\right) = \mathbf{x}^\top \mathbf{x}' \ .$$

- The polynomial kernel

$$K_{poly}\left(\mathbf{x}, \mathbf{x}'\right) = \left(\mathbf{x}^\top \mathbf{x}' + a\right)^d \ .$$

- The Gaussian RBF kernel:

$$K_{Gaussian}\left(\mathbf{x}, \mathbf{x}'\right) = \exp\left(-\frac{\| \mathbf{x} - \mathbf{x}' \|^2}{2\sigma^2}\right) \ .$$

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P.d. kernels are inner products

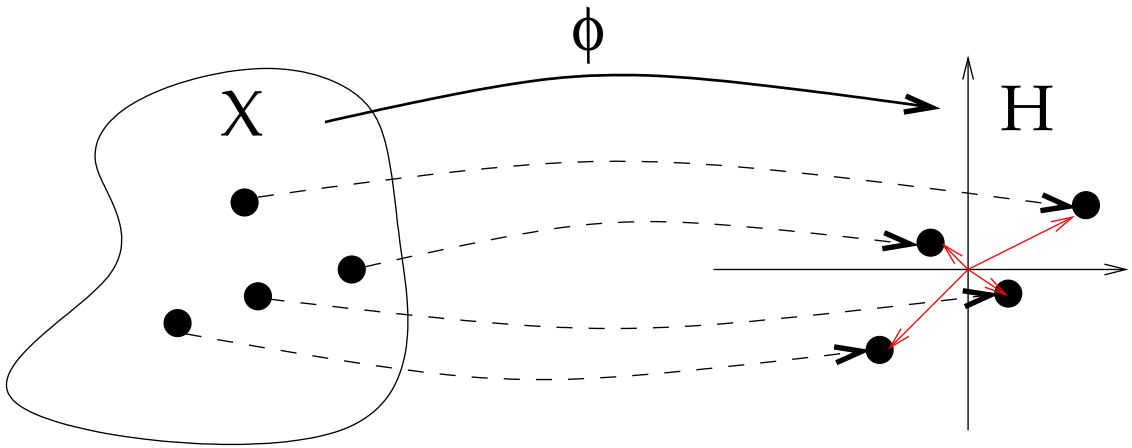
Theorem (Aronszajn, 1950)

K is a p.d. kernel on the set $\mathcal{X}$ if and only if there exists a Hilbert space $\mathcal{H}$ and a mapping

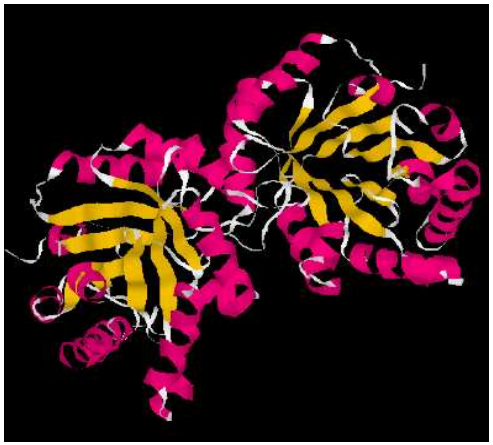
$$\Phi : \mathcal{X} \mapsto \mathcal{H} \, ,$$

such that, for any $\mathbf{x}, \mathbf{x}'$ in $\mathcal{X}$:

$$K\left(\mathbf{x}, \mathbf{x}'\right) = \left\langle \Phi\left(\mathbf{x}\right), \Phi\left(\mathbf{x}'\right) \right\rangle_{\mathcal{H}} \, .$$



Motivation 1: “expensive” vs “cheap” kernels



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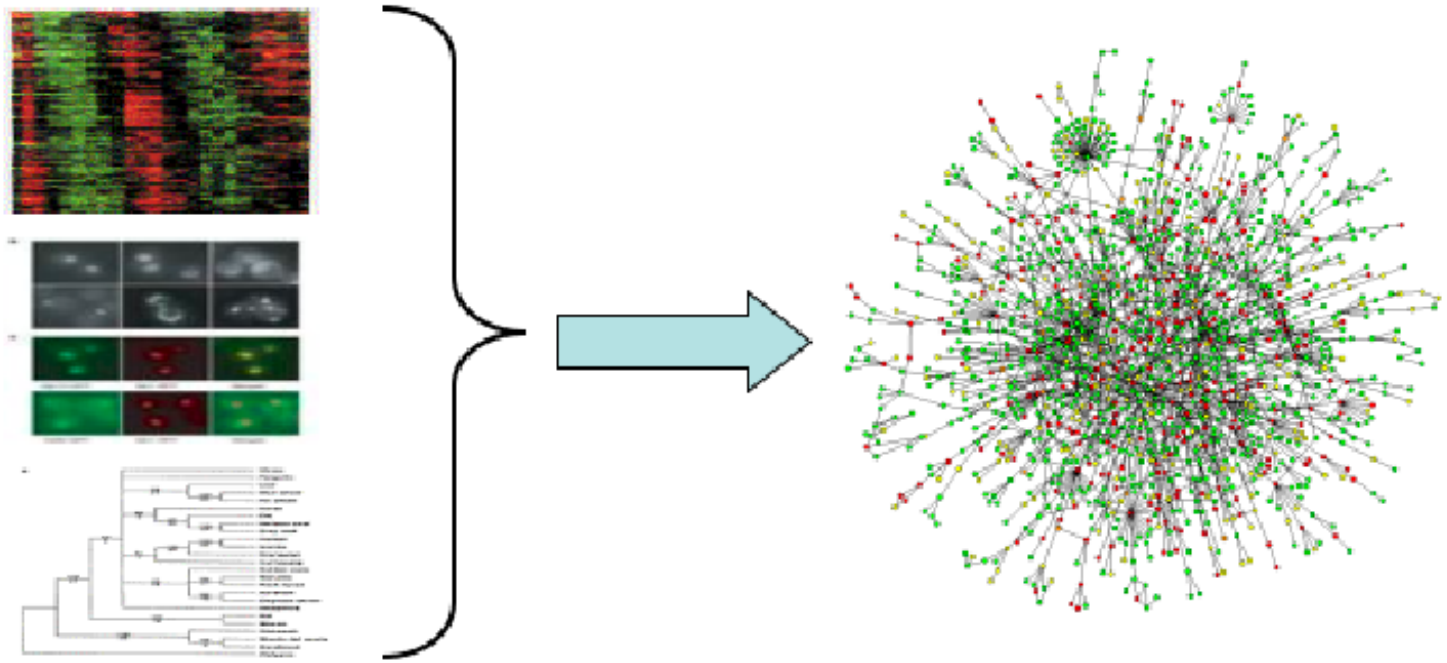
- Objective: predict the function of proteins $\Longrightarrow$ we need a kernel for proteins.
- “Cheap” kernel: all protein sequences are easily known, we easily define a kernel K_{seq} based on sequences.
- “Expensive” kernel: a few protein structures are known, we can define a kernel K_{struct} based on structures
- The problem: K_{struct} is more relevant, but not available for all proteins; K_{seq} is less relevant but known for all proteins.

Motivation 2: Graph inference



- Available genomic data = K_{input}
- Graph to predict (partially known) = K_{output} (after Hilbert embedding)
- Problem: predict missing entries in K_{output} from K_{input}

The problem

$$K = \begin{pmatrix} K_{tt} & K_{pt}^\top \\ K_{pt} & K_{pp} \end{pmatrix}, \quad G = \begin{pmatrix} G_{tt} & G_{pt}^\top \\ G_{pt} & G_{pp} \end{pmatrix},$$

- K is fully known
- G_{tt} is known, but not G_{pt} nor G_{pp}
- Goal: predict G_{pt} and G_{pp} from K and G_{tt}

Outline

Direct approach

The idea

The cheap kernel could be used in place of the expensive kernel.

Solution

Use the cheap kernel as a proxy for the expensive one:

$$G_{pt} = K_{pt} \quad G_{pp} = K_{pp}.$$

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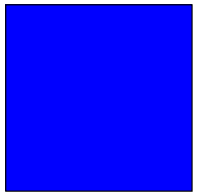
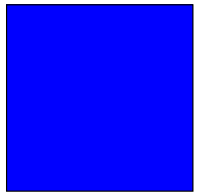
Kernel CCA approach (Y. et al., 2004)

The idea

- Consider the kernels as inner products
- Find low-dimensional projections of the t points in K_{tt} and G_{tt} with maximum correlation
- Project the last p points of K onto this subspace
- Estimate G_{tp} as the inner products in the projection from K.





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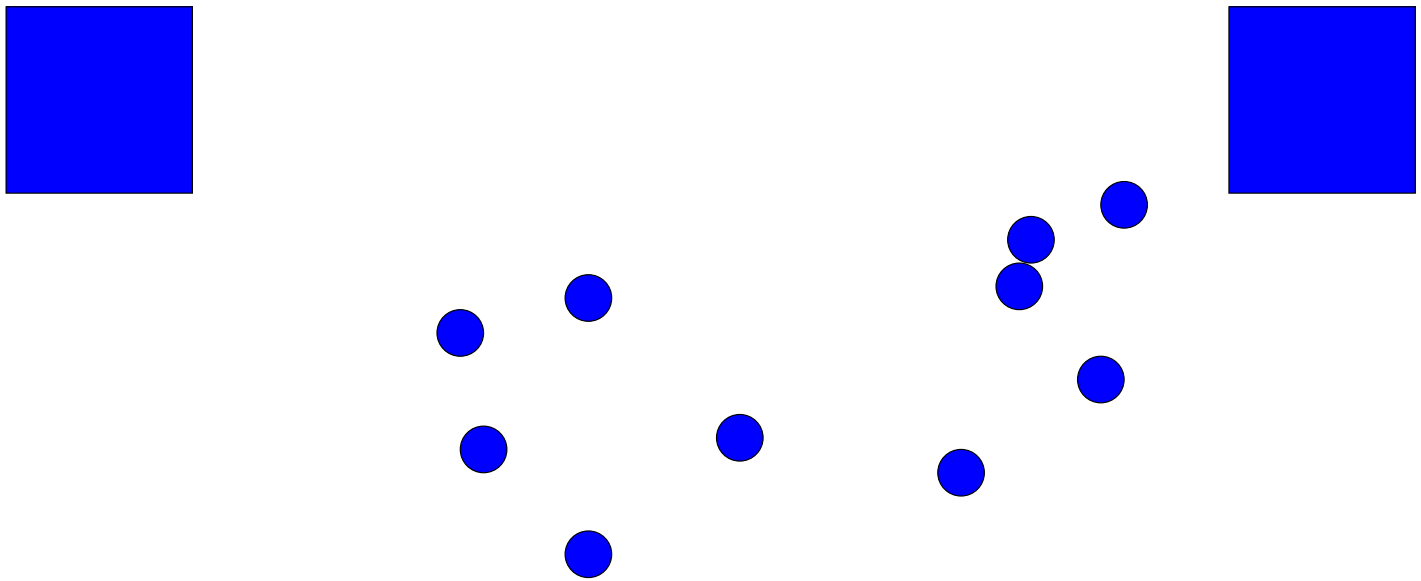

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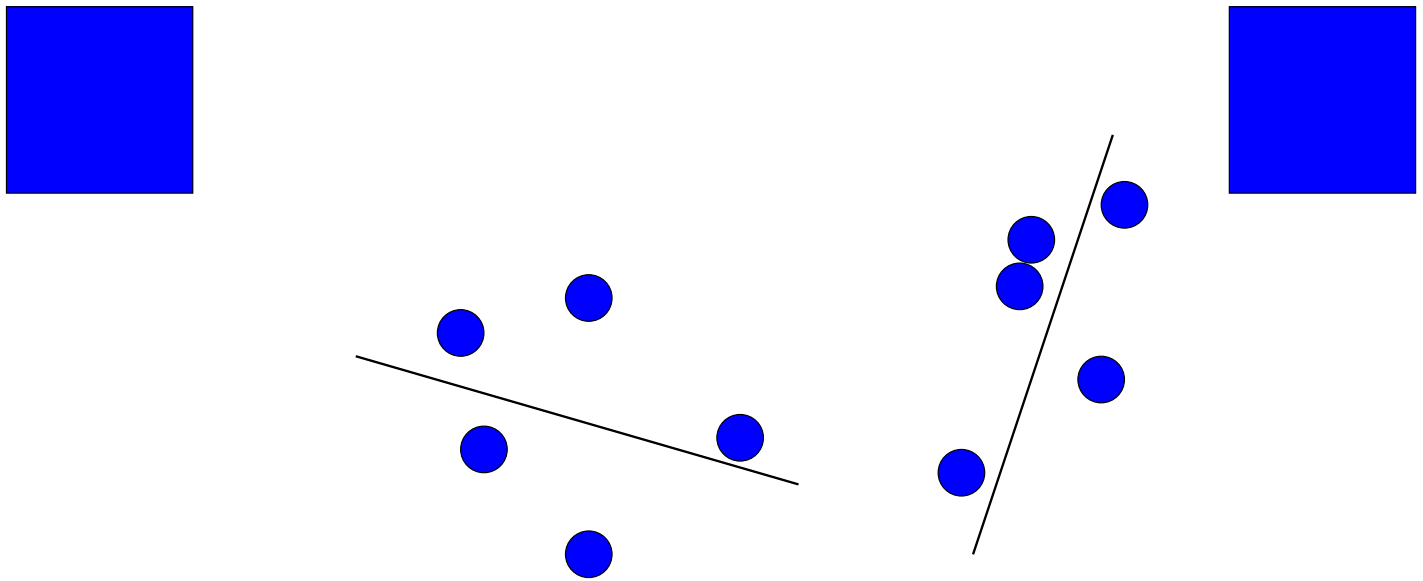

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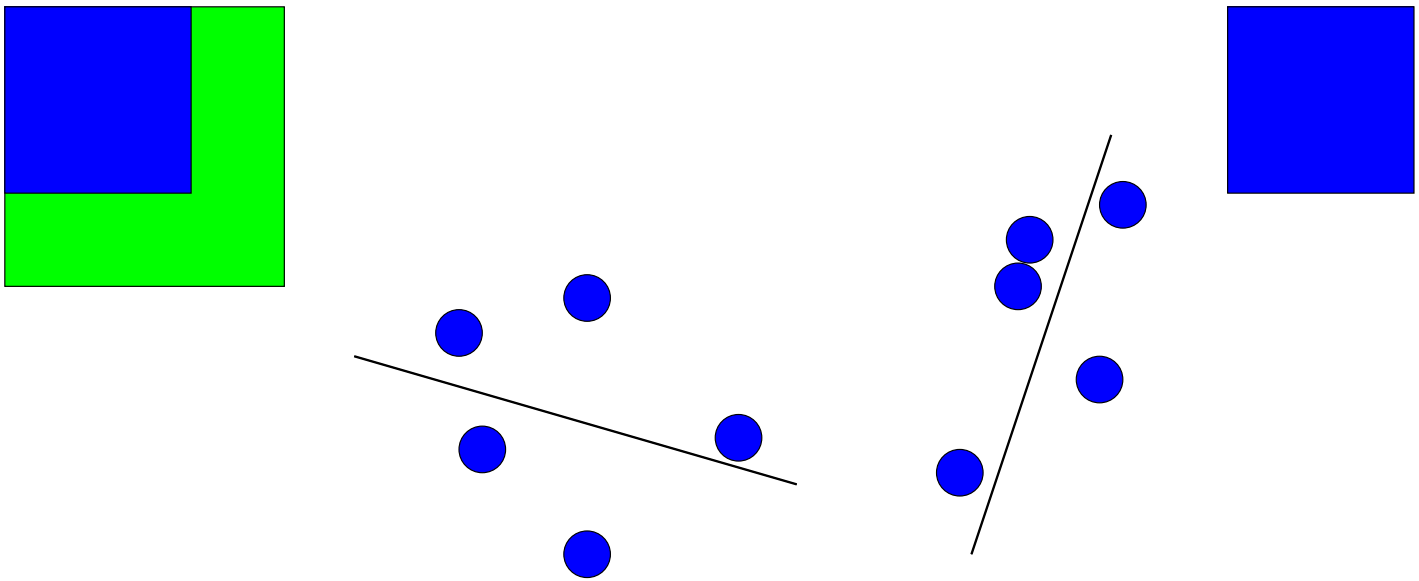

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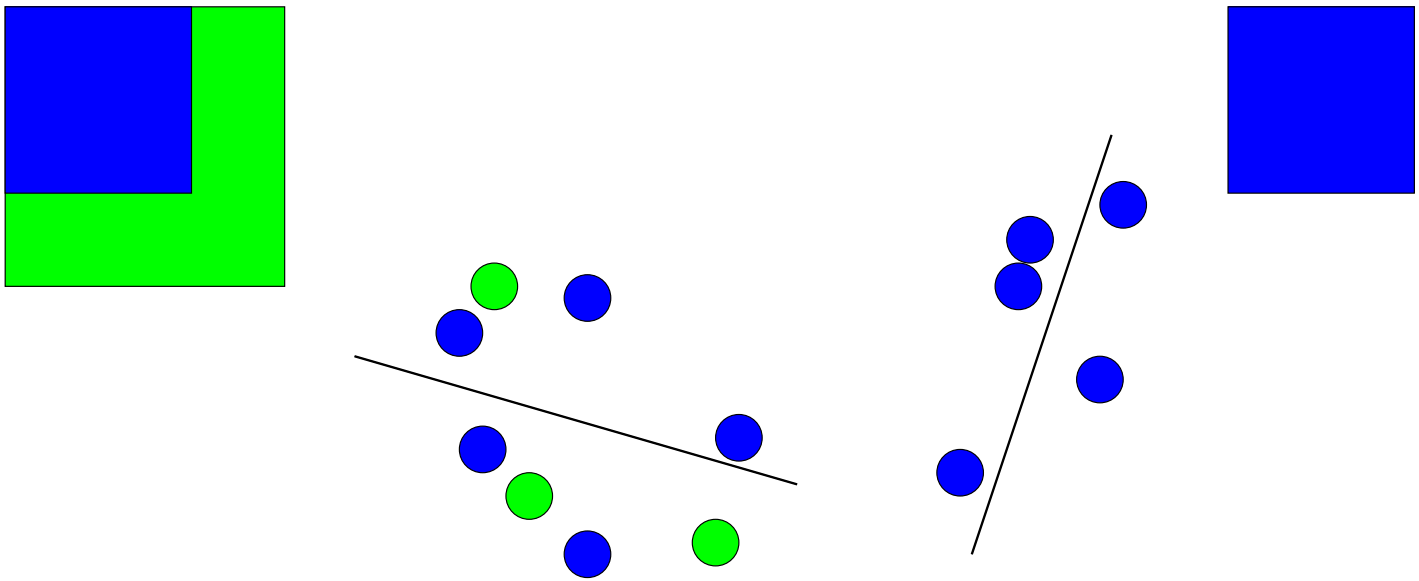

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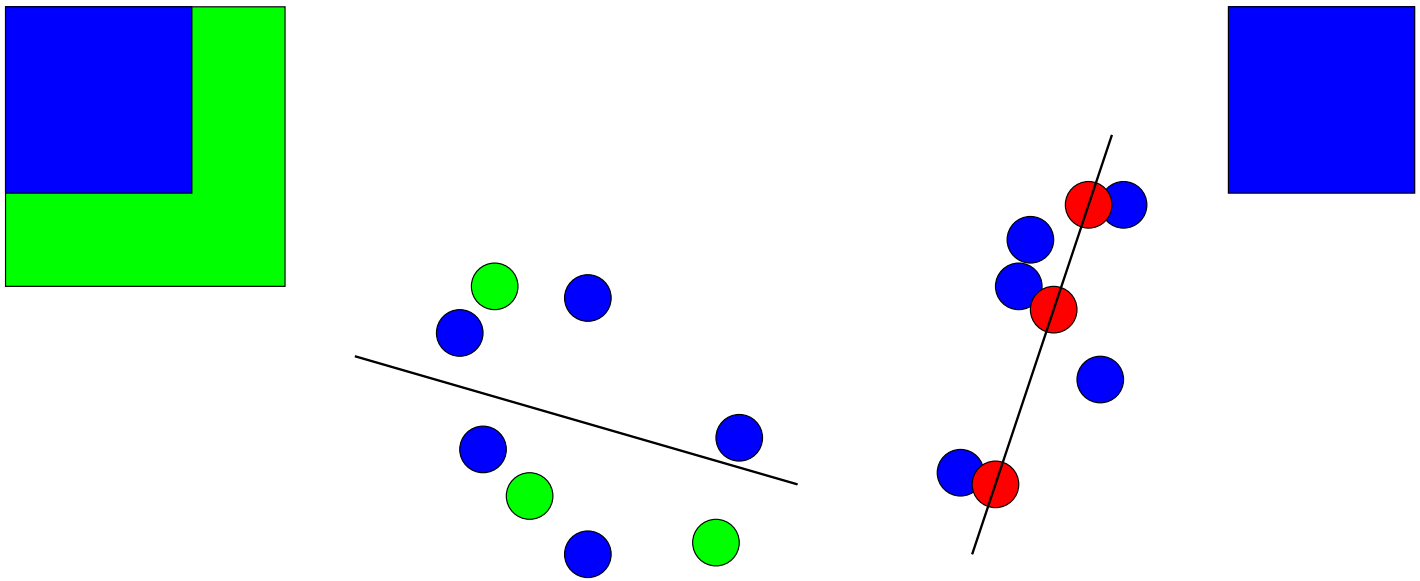

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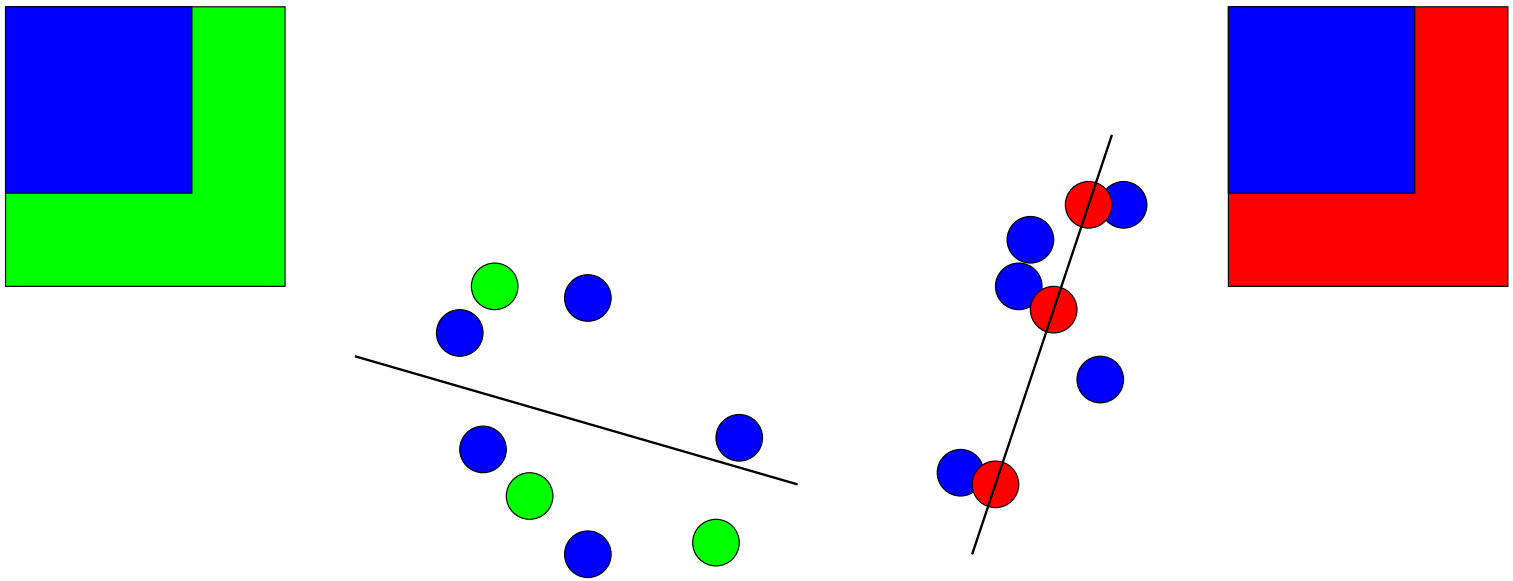


Kernel matrix regression

The idea

- Directly try to predict the expensive kernel G from K, using the know part as training set.
- In order to learn a p.d. function we impose the model:

$$G(x, y) = \sum_i u_i(x) u_i(y) + \epsilon \,,$$

  for $u_i : \mathcal{X} \to \mathbb{R}$.
- We minimize the L_2 (Frobenius) norm of ϵ over the training set.

Kernel matrix regression

Solution

- We look for u_i in the RKHS of K:

$$u_i(x) = \sum_{i=1}^{n} \alpha_j^i K(x_j, x)\,.$$

- Minimization over the α's of

$$\| G_{tt} - K_{tt} A A^\top K_{tt} \|_{Fro}^2$$

gives:

$$A A^\top = K_{tt}^{-1} G_{tt} K_{tt}^{-1}\,,$$

and therefore:

$$G_{pt} = K_{pt} K_{tt}^{-1} G_{tt} \quad G_{pp} = K_{pt} K_{tt}^{-1} G_{tt} K_{tt}^{-1} K_{pt}^\top.$$

Regularized kernel matrix regression

Minimization over the α's of

$$\| G_{tt} - K_{tt} A A^\top K_{tt} \|^2_{Fro} + 2\lambda \sum_i \| u_i \|^2_{RKHS}$$

gives:

$$A A^\top = K_{tt}^{-1} \left(G_{tt} - \lambda K_{tt}^{-1} \right) K_{tt}^{-1} ,$$

and therefore:

$$G_{pt} = K_{pt} K_{tt}^{-1} \left(G_{tt} - \lambda K_{tt}^{-1} \right) \quad G_{pp} = K_{pt} K_{tt}^{-1} \left(G_{tt} - \lambda K_{tt}^{-1} \right) K_{tt}^{-1} K_{pt}^\top .$$

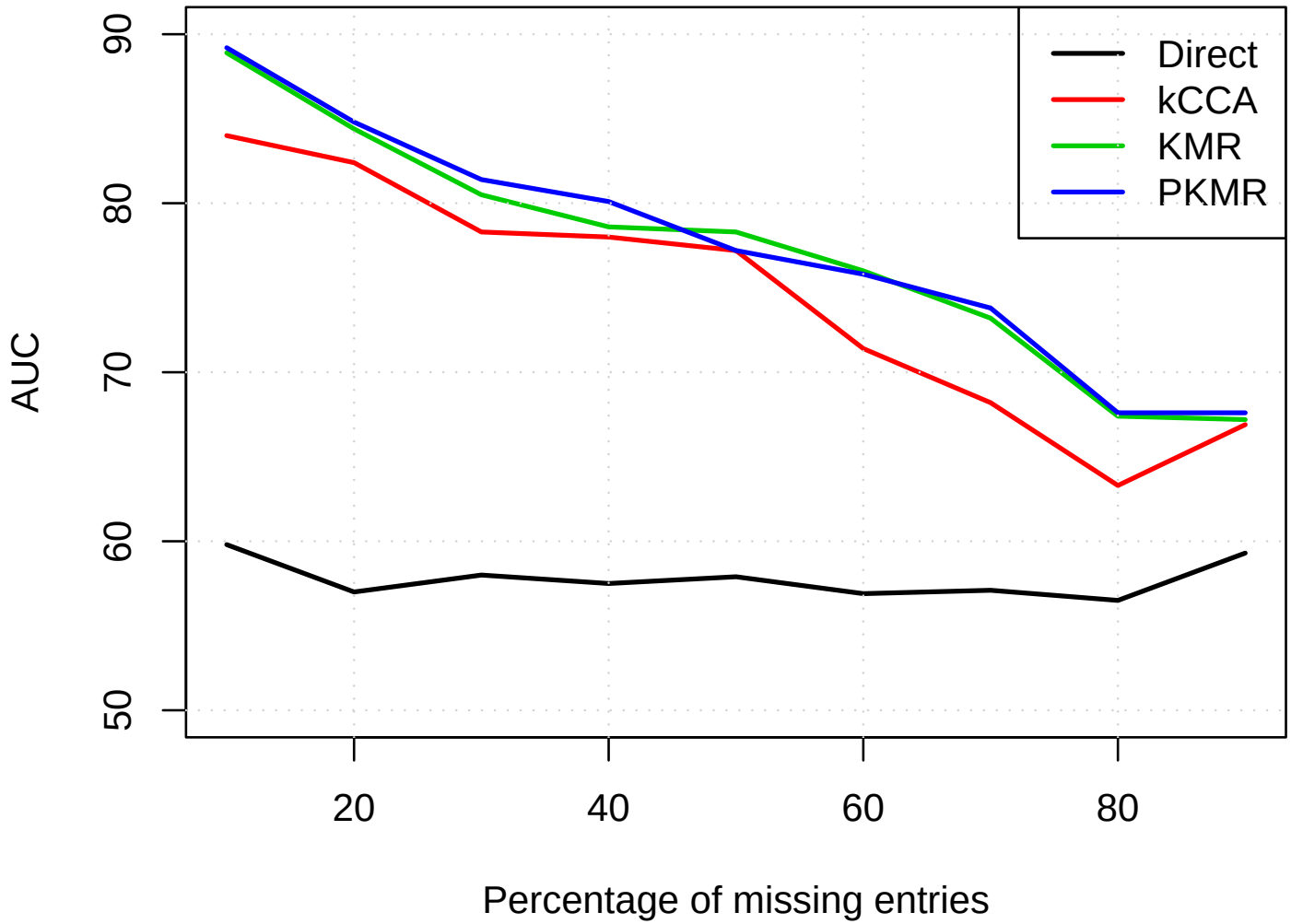
Outline

Biological network inference

Data

- Reconstruct the metabolic gene network, a biological network with 769 genes as vertices
- Use a kernel over genes deduced from gene expression data, phylogenetic profiles, cellular localization.
- The graph is embedded to a Hilbert space using a diffusion kernel
- 5-fold cross-validation, measure average AUC.

Biological network inference: Results



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Conclusion

- A method to predict missing entries in a kernel Gram matrix using side information from another Gram matrix
- Objective function and regularization more adapted to the problem than kernel CCA