Graphical Models and Kernel Methods

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MLSS
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Outline

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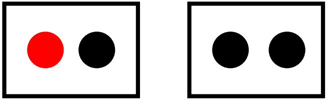
Graphical Models
- Probabilistic Inference
- Directed vs. Undirected Graphical Models
- Inference
- Parameter Estimation

Kernel Methods
- Support Vector Machines
- Kernel PCA
- Reproducing Kernel Hilbert Spaces

Outline

The envelope quiz



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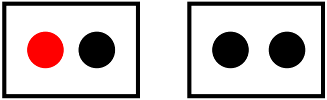

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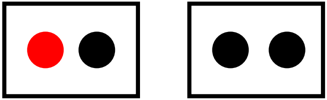

- red ball = \$\$\$
- You randomly picked an envelope, randomly took out a ball – and it was black
- Should you choose this envelope or the other envelope?

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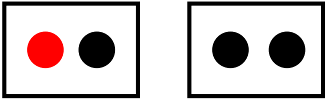

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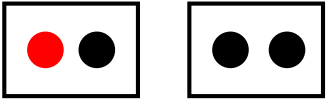

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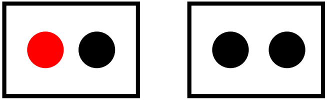

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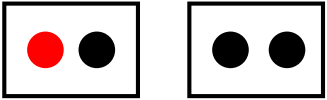

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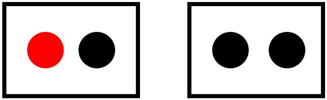

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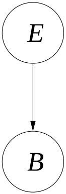

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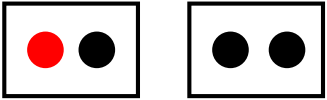

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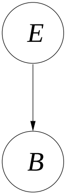

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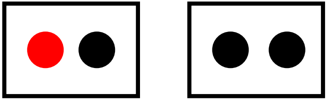

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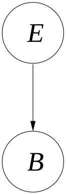

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- $P(E = 1 \mid B = b) = \frac{P(B=b|E=1)P(E=1)}{P(B=b)} = \frac{1/2 \times 1/2}{3/4} = 1/3$. Switch.

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$$p(x_d \mid x_1, \ldots, x_{d-1}) = \frac{p(x_1, \ldots, x_{d-1}, x_d)}{\sum_v p(x_1, \ldots, x_{d-1}, x_d = v)}$$

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- Learning: estimate $p(x_1, \ldots, x_d)$ from training data $X^{(1)}, \ldots, X^{(N)}$, where $X^{(i)} = (x_1^{(i)}, \ldots, x_d^{(i)})$

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- Graphical model: efficient representation, inference, and learning on $p(x_1, \ldots, x_d)$, exactly or approximately

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- If $p(x_1, \ldots, x_d)$ not given, estimate it from data
  - parameter and structure learning

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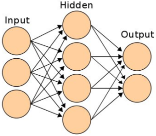
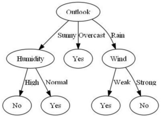
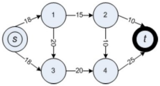
- Just because there are nodes and edges doesn't mean it's a graphical model
- These are not graphical models:



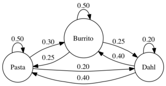
neural network



decision tree



network flow



HMM template
(but HMMs are!)

Outline

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- A cycle is a directed path $x_1 \to \ldots \to x_k$ where $x_1 = x_k$
- A directed acyclic graph (DAG) contains no cycles

Directed graphical models

- A Bayesian network on the DAG is a family of distributions satisfying

$$\{p \mid p(x_1, \ldots, x_d) = \prod_i p(x_i \mid Pa(x_i))\}$$

where $Pa(x_i)$ is the set of parents of x_i.

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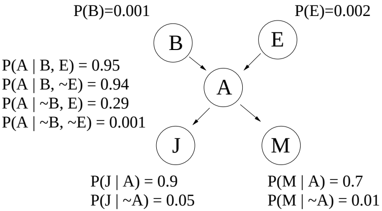
  where $Pa(x_i)$ is the set of parents of x_i.
- $p(x_i \mid Pa(x_i))$ is the conditional probability distribution (CPD) at x_i
- By specifying the CPDs for all i, we specify a joint distribution $p(x_1, \ldots, x_d)$

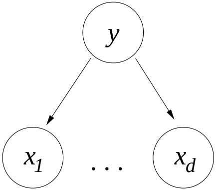
Example: Burglary, Earthquake, Alarm, John and Marry

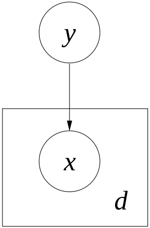
Binary variables



$$
\begin{aligned}
& P(B, \sim E, A, J, \sim M) \\
= \; & P(B)P(\sim E)P(A \mid B, \sim E)P(J \mid A)P(\sim M \mid A) \\
= \; & 0.001 \times (1 - 0.002) \times 0.94 \times 0.9 \times (1 - 0.7) \\
\approx \; & .000253
\end{aligned}
$$

Example: Naive Bayes





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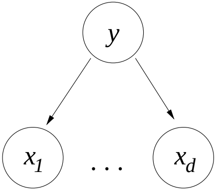

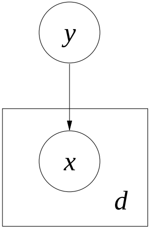

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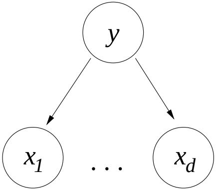

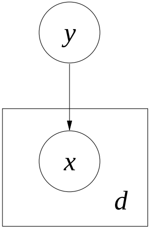

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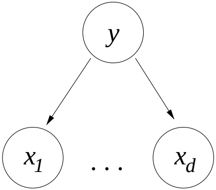

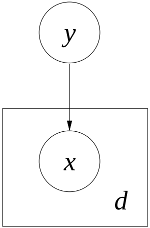

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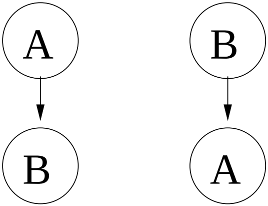
- Plate representation on the right
- $p(y)$ multinomial
- $p(x_i \mid y)$ depends on the feature type: multinomial (count x_i), Gaussian (continuous x_i), etc.

No Causality Whatsoever

$P(A)=a$
$P(B|A)=b$
$P(B|\sim A)=c$



$P(B)=ab+(1-a)c$
$P(A|B)=ab/(ab+(1-a)c)$
$P(A|\sim B)=a(1-b)/(1-ab-(1-a)c)$

The two BNs are equivalent in all respects

- Do not *read* causality from Bayesian networks

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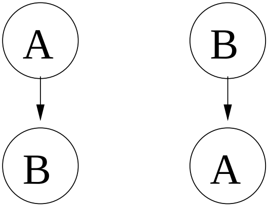

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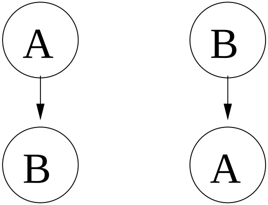

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The two BNs are equivalent in all respects

- Do not *read* causality from Bayesian networks
- They only represent correlation (joint probability distribution)
- However, it is perfectly fine to *design* BNs causally

What do we need probabilistic models for?

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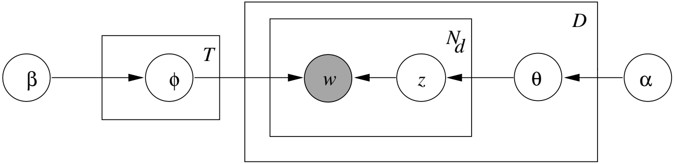
- Make predictions. $p(y \mid x)$ plus decision theory
- Interpret models. Very natural to include latent variables

Example: Latent Dirichlet Allocation (LDA)



A generative model for $p(\phi, \theta, z, w \mid \alpha, \beta)$:
For each topic t

$\phi_t \sim$ Dirichlet(β)

For each document d

$\theta \sim$ Dirichlet(α)

For each word position in d

topic $z \sim$ Multinomial(θ)

word $w \sim$ Multinomial(ϕ_z)

Inference goals: $p(z \mid w, \alpha, \beta), \operatorname{argmax}_{\phi,\theta} p(\phi, \theta \mid w, \alpha, \beta)$

Conditional Independence

- Two r.v.s A, B are independent if

$$
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- Two r.v.s A, B are conditionally independent given C if

$$
\begin{aligned}
P(A, B \mid C) &= P(A \mid C)P(B \mid C) \\
P(A \mid B, C) &= P(A \mid C) \\
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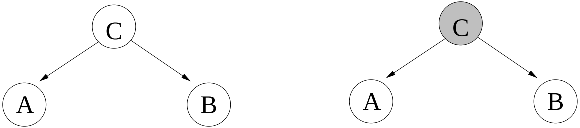
- Conditional independence in a BN is precisely specified by d-separation ("directed separation")

d-Separation Case 1: Tail-to-Tail



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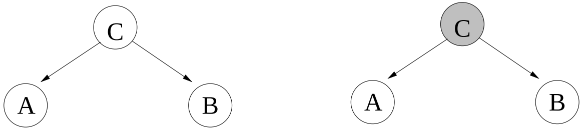

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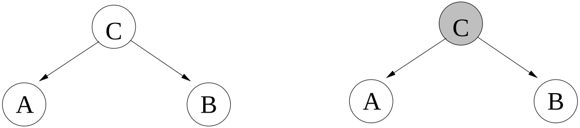

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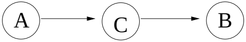

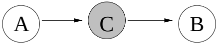

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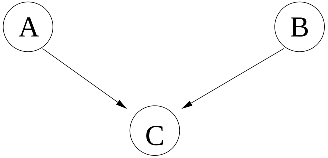

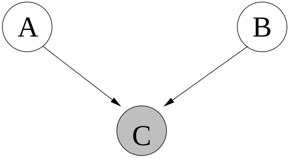

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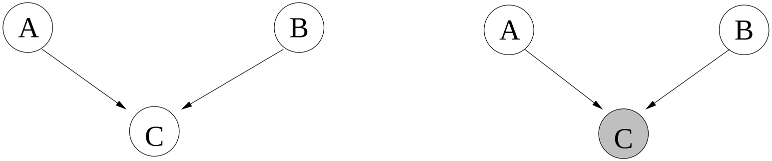

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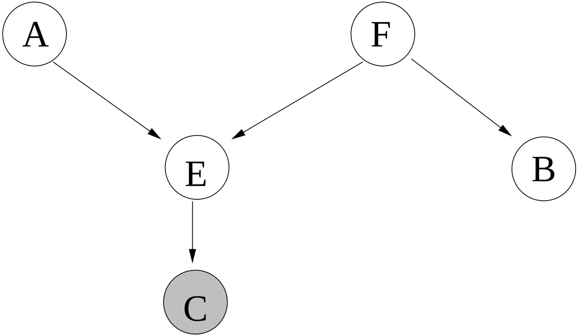
d-Separation

- Variable groups A and B are conditionally independent given C, if all undirected paths from nodes in A to nodes in B are *blocked*

d-Separation Example 1

- The undirected path from A to B is unblocked by E (because of C), and is not blocked by F



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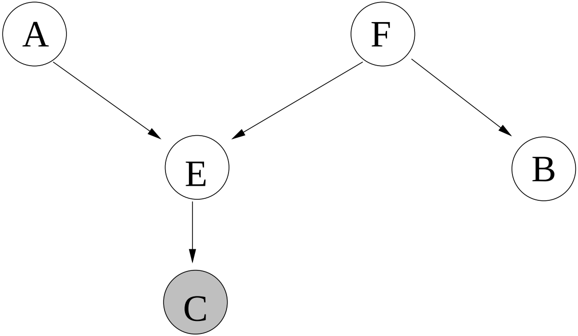

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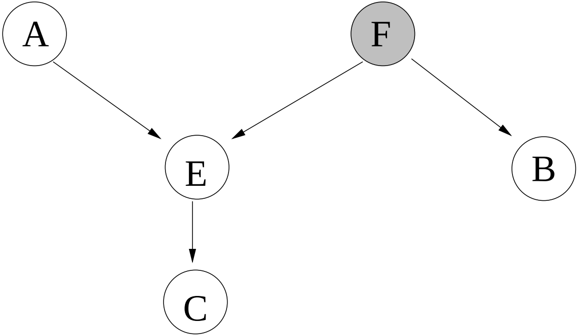

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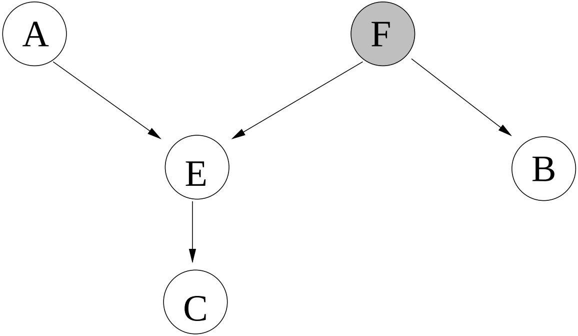

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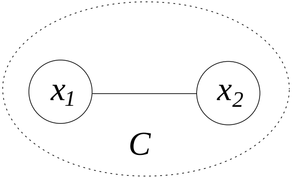
- $Z = \int \prod_C \psi_C(X_C) dX$ is the partition function

Example: A Tiny Markov Random Field



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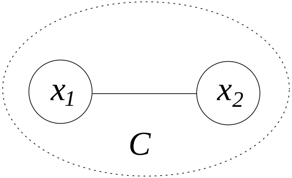

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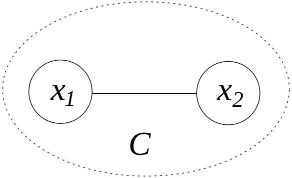

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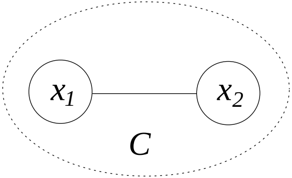

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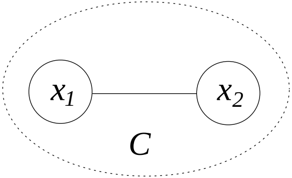

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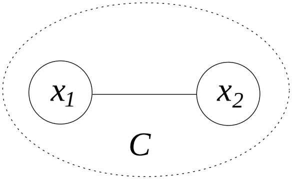

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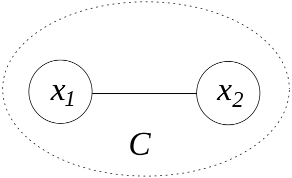

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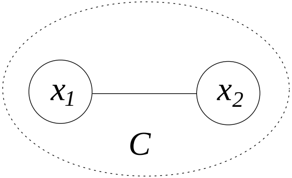

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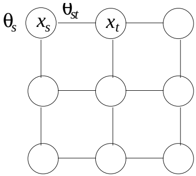
- Equivalent to MRF $p(X) = \frac{1}{Z} \prod_C \psi_C(X_C)$ with

$$\psi_C(X_C) = \exp\left(w_C f_C(X)\right)$$

Example: Ising Model

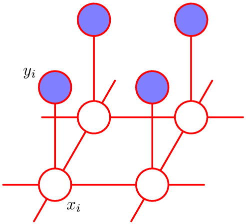


This is an undirected model with $x \in \{0, 1\}$.

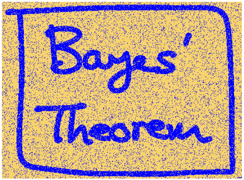
$$p_\theta(x) = \frac{1}{Z} \exp\left(\sum_{s \in V} \theta_s x_s + \sum_{(s,t) \in E} \theta_{st} x_s x_t \right)$$

- $f_s(X) = x_s$, $f_{st}(X) = x_s x_t$

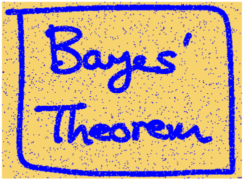
Example: Image Denoising



[From Bishop PRML]



noisy image



$\operatorname{argmax}_X P(X|Y)$

$$p_\theta(X \mid Y) = \frac{1}{Z} \exp\left(\sum_{s \in V} \theta_s x_s + \sum_{(s,t) \in E} \theta_{st} x_s x_t \right)$$

$$\theta_s = \begin{cases} c & y_s = 1 \\ -c & y_s = 0 \end{cases}, \quad \theta_{st} > 0$$

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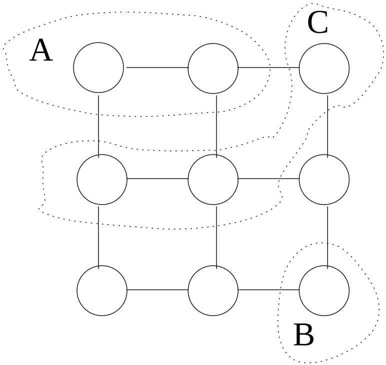
- When $\Omega_{ij} \neq 0$, there is an edge between x_i, x_j

Conditional Independence in Markov Random Fields

- Two group of variables A, B are conditionally independent given another group C, if A, B become disconnected by removing C and all edges involving C



Outline

Exact Inference

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- Unbiased (after burn-in), but can have high variance

Monte Carlo Methods

- Consider the inference problem $p(X_Q = c_Q \mid X_E)$ where $X_Q \cup X_E \subseteq \{x_1 \dots x_d\}$

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Forward Sampling

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Forward Sampling

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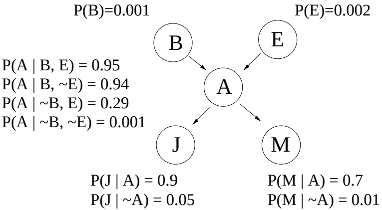
- Throw away X if it doesn't match the evidence X_E

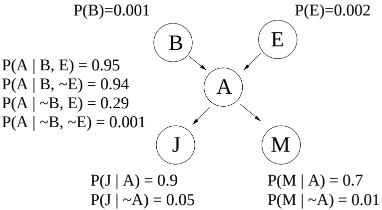
Forward Sampling: Example



To generate a sample $X = (B, E, A, J, M)$:

1. Sample $B \sim \mathrm{Ber}(0.001)$: $r \sim U(0, 1)$. If $(r < 0.001)$ then $B = 1$ else $B = 0$

Forward Sampling: Example



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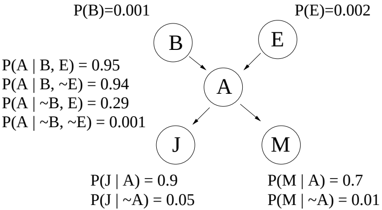

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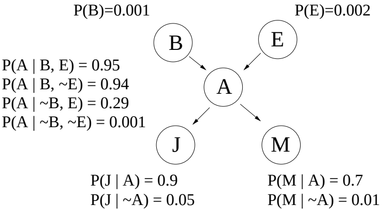

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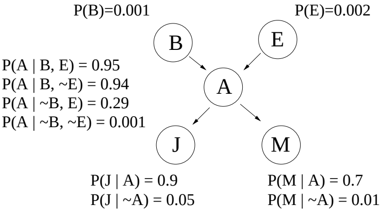

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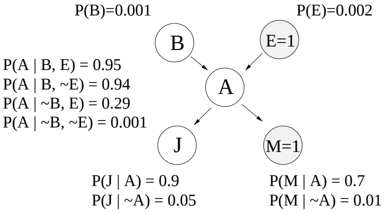

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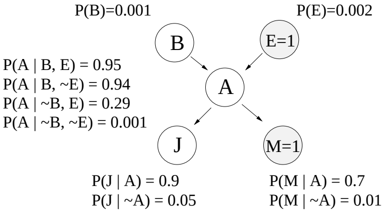

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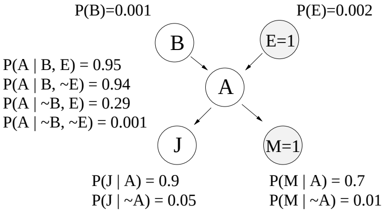

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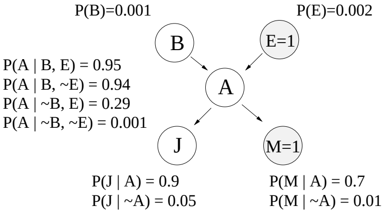

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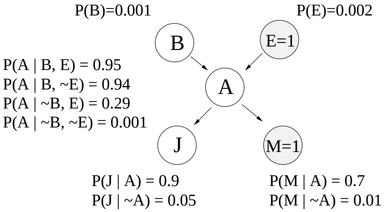

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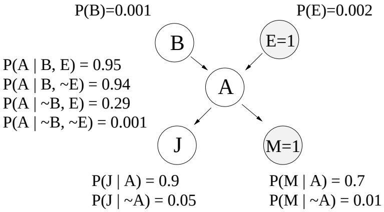

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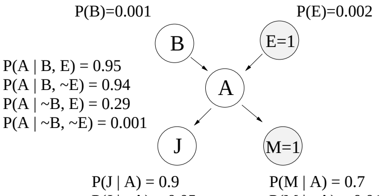

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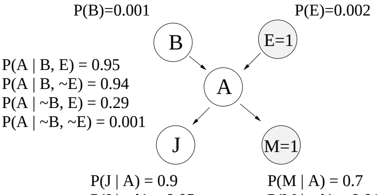

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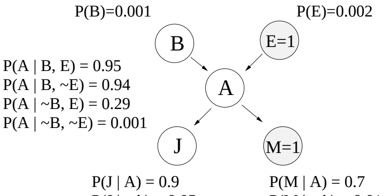
where $Pa(x)$ are the parents of x, and $C(x)$ the children of x.



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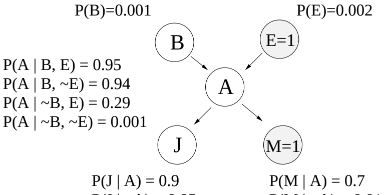

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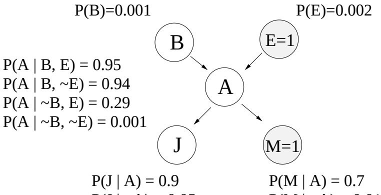
  $B \sim P(B \mid E = 1, A = 0) \propto P(B)P(A = 0 \mid B, E = 1)$



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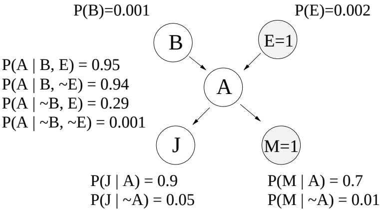

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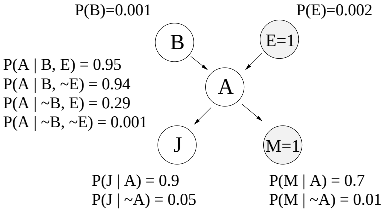

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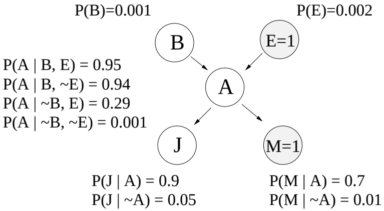

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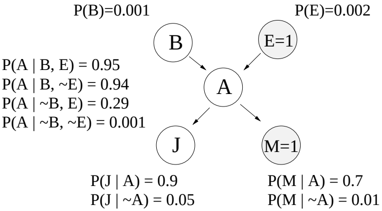
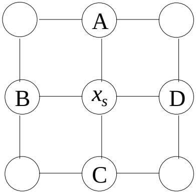
- Move on to J, then repeat $B, A, J, B, A, J \ldots$
- Keep all samples after *burn in*. $P(B = 1 \mid E = 1, M = 1)$ is the fraction of samples with $B = 1$.



Gibbs Sampling Example 2: The Ising Model



This is an undirected model with $x \in \{0, 1\}$.

$$p_\theta(x) = \frac{1}{Z} \exp \left(\sum_{s \in V} \theta_s x_s + \sum_{(s,t) \in E} \theta_{st} x_s x_t \right)$$

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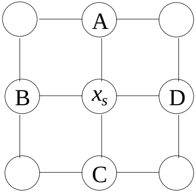

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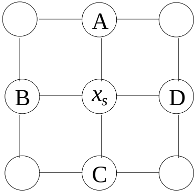

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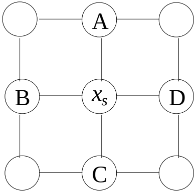

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  - Use all of $X^{(T+1)}, \ldots$ for inference (they are correlated); Do not thin

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Example: Collapsed Gibbs Sampling for LDA

Collapse θ, ϕ, Gibbs update:

$$P(z_i = j \mid \mathbf{z}_{-i}, \mathbf{w}) \propto \frac{n^{(w_i)}_{-i,j} + \beta n^{(d_i)}_{-i,j} + \alpha}{n^{(\cdot)}_{-i,j} + W\beta n^{(d_i)}_{-i,\cdot} + T\alpha}$$

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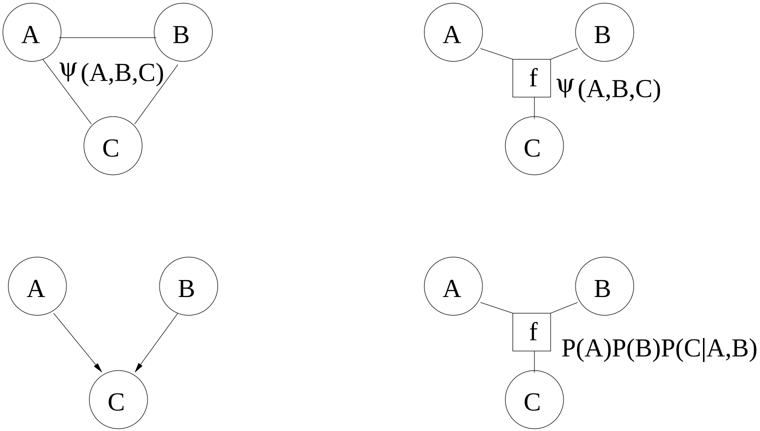
Belief Propagation

Factor Graph

- For both directed and undirected graphical models



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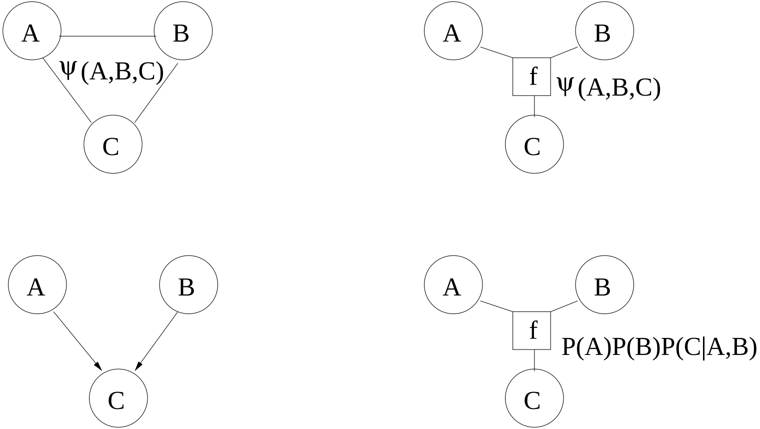
- Bipartite: edges between a variable node and a factor node



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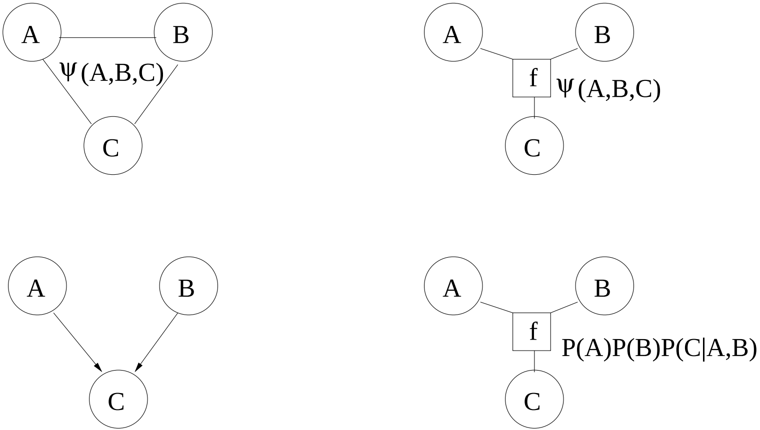
- Factors represent computation



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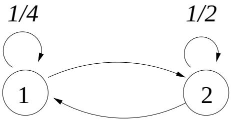
- The algorithm involves passing *messages* on the factor graph
- Alternative view: variational approximation (more later)

Example: A Simple HMM

- The Hidden Markov Model template (not a graphical model)



$P(x \mid z=1) = (1/2, 1/4, 1/4)$ — R G B

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$\pi_1 = \pi_2 = 1/2$

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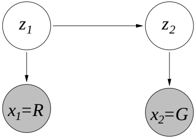
- Observing $x_1 = R, x_2 = G$, the directed graphical model



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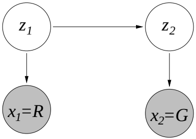

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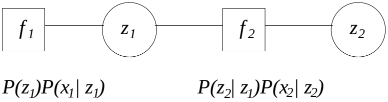

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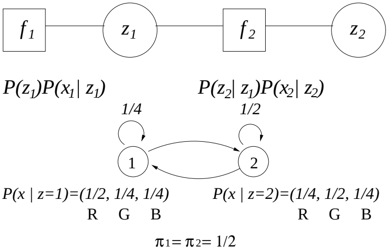
Leaf Messages

- Assume tree factor graph. Pick an arbitrary root, say z_2



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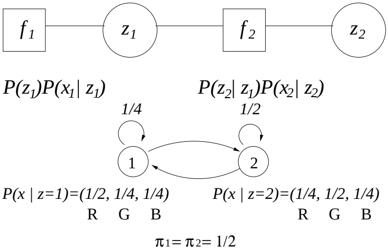

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- If a leaf is a factor node f, $\mu_{f\to x}(x) = f(x)$

$$\mu_{f_1\to z_1}(z_1 = 1) = P(z_1 = 1)P(R|z_1 = 1) = 1/2 \cdot 1/2 = 1/4$$

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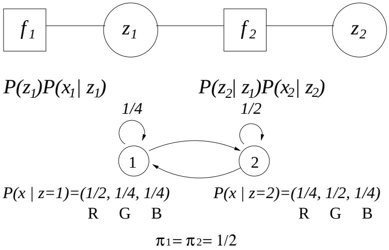

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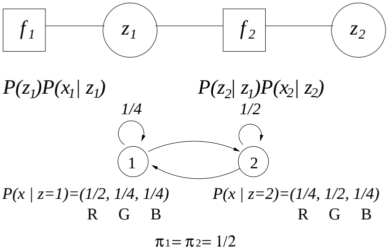
- If a leaf is a variable node x, $\mu_{x \to f}(x) = 1$



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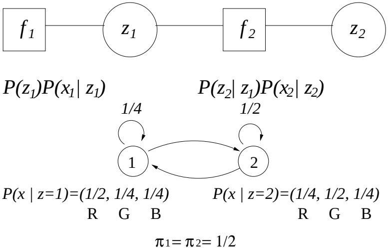
- A node (factor or variable) can send out a message if all other incoming messages have arrived



Message from Variable to Factor

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- Let x be in factor f_s. $ne(x)\backslash f_s$ are factors connected to x excluding f_s.

$$\mu_{x \to f_s}(x) = \prod_{f \in ne(x)\backslash f_s} \mu_{f \to x}(x)$$

$$\mu_{z_1 \to f_2}(z_1 = 1) = 1/4$$

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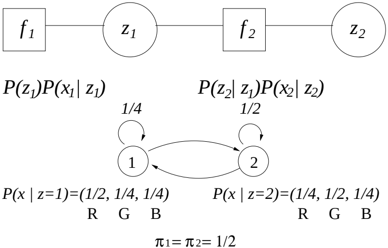

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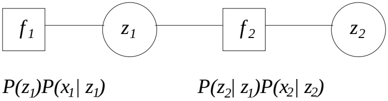
- Let x be in factor f_s. Let the other variables in f_s be $x_{1:M}$.

$$\mu_{f_s \to x}(x) = \sum_{x_1} \cdots \sum_{x_M} f_s(x, x_1, \ldots, x_M) \prod_{m=1}^{M} \mu_{x_m \to f_s}(x_m)$$



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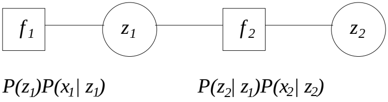
- In this example

$$\begin{aligned}
\mu_{f_2 \to z_2}(s) &= \sum_{s'=1}^{2} \mu_{z_1 \to f_2}(s') f_2(z_1 = s', z_2 = s) \\
&= 1/4 P(z_2 = s | z_1 = 1) P(x_2 = G | z_2 = s) \\
&\quad +1/8 P(z_2 = s | z_1 = 2) P(x_2 = G | z_2 = s)
\end{aligned}$$



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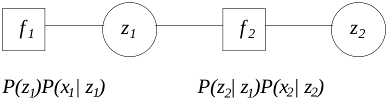
- We get $\mu_{f_2 \to z_2}(z_2 = 1) = 1/32$, $\mu_{f_2 \to z_2}(z_2 = 2) = 1/8$

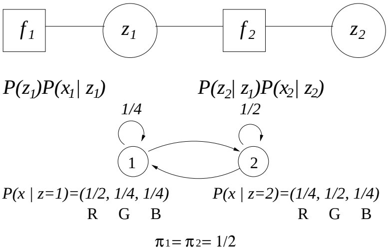


Up to Root, Back Down

- The message has reached the root, pass it back down

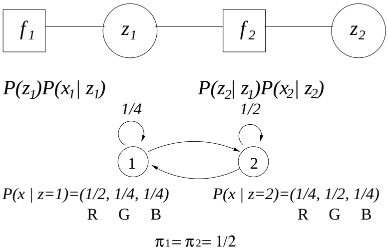
$$\mu_{z_2 \to f_2}(z_2 = 1) = 1$$

$$\mu_{z_2 \to f_2}(z_2 = 2) = 1$$



Keep Passing Down

- $\mu_{f_2 \to z_1}(s) = \sum_{s'=1}^{2} \mu_{z_2 \to f_2}(s') f_2(z_1 = s, z_2 = s')$
  $= 1P(z_2 = 1|z_1 = s)P(x_2 = G|z_2 = 1)$
  $+ 1P(z_2 = 2|z_1 = s)P(x_2 = G|z_2 = 2)$.



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  $\mu_{f_2 \to z_1}(z_1 = 1) = 7/16$
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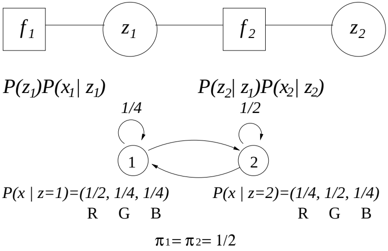

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  $P(z_2|x_1, x_2) \propto \mu_{f_2 \to z_2} = \binom{1/32}{1/8} \Rightarrow \binom{0.2}{0.8}$
- One can also compute the marginal of the *set of* variables x_s involved in a factor f_s

$$p(x_s) \propto f_s(x_s) \prod_{x \in ne(f)} \mu_{x \to f}(x)$$

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  - The conditional is easily obtained by normalization

$$p(x|X_E) = \frac{p(x, X_E)}{\sum_{x'} p(x', X_E)}$$

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- Loopy BP may not convergence, but “works” in many cases

Outline

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  - The EM algorithm finds a local maximum

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- M and θ treated separately; combinatorial search over M

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- Equivalently, x_i, x_j are conditionally independent given other variables

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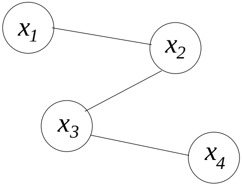
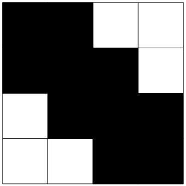
- The corresponding graphical model structure is





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- The log likelihood is $\frac{n}{2} \log |\Omega| - \frac{1}{2} \sum_{i=1}^{n} (X^{(i)} - \mu)^\top \Omega (X^{(i)} - \mu)$

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- S^{-1} is not a good estimate of Ω when n is small

Structure Learning for Gaussian Random Fields

- For centered data, minimize a regularized problem instead:

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- Known as GLASSO

Outline

Kernel methods

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- Precise definition: Reproducing Kernel Hilbert Space (RKHS)

Outline

The Linearly Separable Case

- $x \in R^d$, $y \in \{-1, 1\}$

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- linear decision boundary $\{x \in \mathbb{R}^d \mid f(x) = 0\}$ orthogonal to w

The Linearly Separable Case

- Distance between a correctly classified x and the decision boundary:
$$\frac{yf(x)}{\|w\|}$$

The Linearly Separable Case

- Training task: given $\{(x, y)_{1:n}\}$, find a decision boundary w, b to maximize the distance to the closest point

$$\max_{w,b} \min_{i=1}^{n} \frac{y_i(w^\top x_i + b)}{\|w\|}$$

The Linearly Separable Case

- Equivalently,

$$\max_{w,b} \quad \frac{1}{\|w\|}$$
$$s.t. \quad y_i(w^\top x_i + b) \geq 1 \;\; i = 1 \dots n$$

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- Primal problem, uses feature vectors $x_i \in \mathbb{R}^d$
- The equivalent dual problem will involve only inner products $x_i^\top x_j$

The Linearly Separable Case

- The dual problem

$$\begin{array}{ll} \max\limits_{\alpha} & -\frac{1}{2}\sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j x_i^\top x_j + \sum_{i=1}^{n} \alpha_i \\ s.t. & \alpha_i \geq 0 \;\; i = 1 \ldots n \\ & \sum_{i=1}^{n} \alpha_i y_i = 0 \end{array}$$

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- $d+1$ primal variables w, b
- n dual variables α (interesting when $d \gg n$)

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- primal discriminant function $f(x) = w^\top x + b$

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- another inner-product

Support vectors

- The Karush-Kuhn-Tucker complementarity condition:
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- $\alpha_i \neq 0$ (x_i is support vector) $\Rightarrow y_i(w^\top x_i + b) = 1$ (x_i on the margin)

The Non-Separable Case

- Relax margin constraints

$$y_i(w^\top x_i + b) \geq 1 - \xi_i$$

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- Large enough ξ_i allows x_i on the wrong side of the decision boundary

The Non-Separable Case

- Primal problem

$$\begin{aligned}
\min_{w,b,\xi} \quad & \tfrac{1}{2}\|w\|^2 + C\textstyle\sum_{i=1}^n \xi_i \\
s.t. \quad & y_i(w^\top x_i + b) \geq 1 - \xi_i \;\; i = 1 \ldots n \\
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\end{aligned}$$

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$$
\begin{array}{ll}
\max\limits_{\alpha} & -\frac{1}{2}\sum_{i,j=1}^{n}\alpha_i\alpha_j y_i y_j x_i^\top x_j + \sum_{i=1}^{n}\alpha_i \\
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  - $\alpha = C \Rightarrow x_i$ inside the margin if $\xi \le 1$, or on the wrong side of the decision boundary if $\xi > 1$

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- Inner product again

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- K_n positive semi-definite if $\forall \mathbf{z} = (z_1, \dots, z_n)^\top \in \mathbb{R}^n$,

$$\mathbf{z}^\top K_n \mathbf{z} \geq 0$$

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P.d. K examples:

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- Radial Basis Function (RBF) kernel

$$k(x_i, x_j) = \exp\left(-\frac{\|x_i - x_j\|^2}{2\sigma^2}\right)$$

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- What does the kernel trick buy us?

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- Equivalently, we used a kernel

$$K(x_i, x_j) = \phi(x_i)^\top \phi(x_j) = (1 + x_i x_j)^2$$

  in *linear* SVM without slack variables.

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The Kernel Trick is not just for SVMs

Summary of the kernel trick:

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- many algorithms can be kernelized

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  where $\bar{x} = \frac{1}{n} \sum_j x_j$
- $d \times d$ sample covariance matrix

$$C = \frac{1}{n} \sum_i x_i x_i^\top$$

PCA

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$$C = U\Lambda U^\top = \sum_{j=1}^{d} \lambda_j u_j u_j^\top$$

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- $u_1 \ldots u_d$ orthonormal basis of $\mathbb{R}^d$, rotated axes

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- U_k minimizes training set ℓ_2-error among rank-k projections

$$\sum_{i=1}^{n} \|x_i - U_k^\top x_i\|_2^2$$

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- U_k the first k columns of $U = [u_1 \mid u_2 \mid \dots \mid u_d]$
- $x \in \mathbb{R}^d$ projected to $\mathbb{R}^k$ by

$$U_k^\top x = \begin{bmatrix} u_1^\top x \\ \vdots \\ u_k^\top x \end{bmatrix}$$

- U_k minimizes training set ℓ_2-error among rank-k projections

$$\sum_{i=1}^{n} \|x_i - U_k^\top x_i\|_2^2$$

- So far PCA with feature vectors in $\mathbb{R}^d$. Next: PCA with inner products

PCA with inner products

- For $j = 1 \dots d$

$$\begin{aligned} Cu_j &= \lambda_j u_j \\ \frac{1}{n}\sum_{i=1}^{n} x_i x_i^\top u_j &= \lambda_j u_j \\ \sum_{i=1}^{n} \frac{(x_i^\top u_j)}{n\lambda_j} x_i &= u_j \end{aligned}$$

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- $\alpha_{ji} \in \mathbb{R}$, value not obvious (involving u_j)

PCA with inner products

- $n \times n$ matrix K with $K_{ij} = x_i^\top x_j$

PCA with inner products

- $n \times n$ matrix K with $K_{ij} = x_i^\top x_j$
- $\alpha_j = (\alpha_{j1}, \ldots, \alpha_{jn})^\top$ satisfy the eigenvalue equation

$$K\alpha_j = n\lambda_j\alpha_j$$

Why?

$$
\begin{aligned}
Cu_j &= \lambda_j u_j \\
x_i^\top C u_j &= x_i^\top \lambda_j u_j, \quad i = 1 \ldots n \\
x_i^\top \left(\frac{1}{n} \sum_{k=1}^{n} x_k x_k^\top \right) \left(\sum_{m=1}^{n} \alpha_{jm} x_m \right) &= x_i^\top \lambda_j \sum_{m=1}^{n} \alpha_{jm} x_m \\
\frac{1}{n} \sum_{k=1}^{n} \sum_{m=1}^{n} \alpha_{jm} x_i^\top x_k x_k^\top x_m &= \sum_{m=1}^{n} \lambda_j \alpha_{jm} x_i^\top x_m \\
\frac{1}{n} \sum_{k=1}^{n} \sum_{m=1}^{n} \alpha_{jm} K_{ik} K_{km} &= \sum_{m=1}^{n} \lambda_j \alpha_{jm} K_{im} \\
\frac{1}{n} K_{i.} K \alpha_j &= \lambda_j K_{i.} \alpha_j, \quad i = 1 \ldots n \\
\frac{1}{n} K K \alpha_j &= \lambda_j K \alpha_j \\
K \alpha_j &= n \lambda_j \alpha_j
\end{aligned}
$$

assuming $n \leq d$ and K invertible

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- Norm of α_j is also fixed:
$$\begin{aligned}
\|u_j\| &= 1 \\
u_j^\top u_j &= 1 \\
\sum_{k,m=1}^{n} \alpha_{jk} x_k^\top x_m \alpha_{jm} &= 1 \\
\sum_{k,m=1}^{n} \alpha_{jk} K_{km} \alpha_{jm} &= 1 \\
\alpha_j^\top K \alpha_j &= 1 \\
\alpha_j^\top n\lambda_j \alpha_j &= 1 \\
\|\alpha_j\| &= \sqrt{\frac{1}{n\lambda_j}}
\end{aligned}$$

PCA with inner products

- Compute $\alpha_1, \ldots, \alpha_k$ by solving the eigenvalue equation (k largest eigenvalues)

PCA with inner products

- Compute $\alpha_1, \ldots, \alpha_k$ by solving the eigenvalue equation (k largest eigenvalues)
- Project (new) point x to top $k \leq n$ directions

$$\begin{bmatrix} u_1^\top x \\ \vdots \\ u_k^\top x \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^n \alpha_{1i} x_i^\top x \\ \vdots \\ \sum_{i=1}^n \alpha_{ki} x_i^\top x \end{bmatrix} = \begin{bmatrix} \alpha_1^\top K_x \\ \vdots \\ \alpha_k^\top K_x \end{bmatrix}$$

where $K_x = (K(x_1, x), \ldots, K(x_n, x))^\top$ and $K(x_i, x) = x_i^\top x$

Kernel PCA

Perhaps replacing $K_{ij} = x_i^\top x_j$ with any kernel $K(x_i, x_j)$?

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- Need to center K

Centering the kernel for training

$$
\begin{aligned}
\phi'(x_i) &= \phi(x_i) - \frac{1}{n}\sum_{k=1}^{n}\phi(x_k) \\
\phi'(x_i)^\top \phi'(x_j) &= \left(\phi(x_i) - \frac{1}{n}\sum_{k=1}^{n}\phi(x_k)\right)^\top \left(\phi(x_j) - \frac{1}{n}\sum_{k=1}^{n}\phi(x_k)\right) \\
K'_{ij} &= K_{ij} - \frac{1}{n}\sum_{k=1}^{n} K_{jk} - \frac{1}{n}\sum_{k=1}^{n} K_{ik} + \frac{1}{n^2}\sum_{k,m=1}^{n} K_{km}
\end{aligned}
$$

Finding α_j by solving the eigenvalue problem

$$
K'\alpha_j = n\lambda_j\alpha_j
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$$K'(x_i, x) = K(x_i, x) - \frac{1}{n} \sum_{k=1}^{n} K(x_k, x) - \frac{1}{n} \sum_{k=1}^{n} K_{ik} + \frac{1}{n^2} \sum_{k,m=1}^{n} K_{km}$$

Outline

Norm

Let $\mathcal{F}$ be a vector space over $\mathbb{R}$. A function $\|\cdot\|_{\mathcal{F}} : \mathcal{F} \mapsto \mathbb{R}_{\geq 0}$ is a norm if

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- $\|f+g\|_{\mathcal{F}} \leq \|f\|_{\mathcal{F}} + \|g\|_{\mathcal{F}}$ (triangle inequality)

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- $\|f\|_p = \left(\int_{\mathcal{X}} |f(x)|^p d\mu \right)^{\frac{1}{p}}$ is a norm

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- $\{f_n(x)\}$ is Cauchy, but not convergent (limit $\notin C[0,1]$)

Banach space

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  $L_p(\mathcal{X}, \mu) = \left\{ f : \mathcal{X} \mapsto \mathbb{R} \text{ measurable} \mid \int_{\mathcal{X}} |f(x)|^p d\mu < \infty \right\}$
  with norm $\|f\|_p = \left(\int_{\mathcal{X}} |f(x)|^p d\mu \right)^{\frac{1}{p}}$ is a Banach space

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  - $\langle f, f\rangle_{\mathcal{F}} \geq 0$ with 0 iff $f = 0$
- An inner product space is a normed space with $\|f\| = \sqrt{\langle f, f\rangle}$

Hilbert space

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- Example: $L_2(\mathcal{X}, \mu)$ is a Hilbert space with inner product

$$\langle f, g \rangle = \int_{\mathcal{X}} f(x)g(x)d\mu$$

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- When $\mathcal{G} = \mathbb{R}$, A is a linear functional
- Example: For a fixed $h \in \mathcal{F}$,

$$A_h(f) = \langle f, h \rangle_{\mathcal{F}}$$

is a linear functional

Continuity

- $A : \mathcal{F} \mapsto \mathcal{G}$ is continuous at $f_0 \in \mathcal{F}$, if for every $\epsilon > 0$, $\exists \delta$ s.t.

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- A is continuous on $\mathcal{F}$ if it is continuous at all $f \in F$

Riesz representation

In a Hilbert space $\mathcal{F}$, all continuous linear functionals are of the form $\langle \cdot, g \rangle_{\mathcal{F}}$, for some $g \in \mathcal{F}$.

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Reproducing Kernel Hilbert Space

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- $\mathcal{H}$ is an RKHS (i.e. its evaluation functionals δ_x are continuous) iff $\mathcal{H}$ has a reproducing kernel

Positive definiteness

- A symmetric function $h : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$ is positive definite if $\forall n, \forall a \in \mathbb{R}^n, \forall x_1 \dots x_n \in \mathcal{X}$,

$$a^\top H a \geq 0$$

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- A symmetric function $h : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$ is positive definite if $\forall n, \forall a \in \mathbb{R}^n, \forall x_1 \ldots x_n \in \mathcal{X}$,

$$a^\top H a \geq 0$$

  where H is the $n \times n$ matrix with $H_{ij} = h(x_i, x_j)$
- Reproducing kernels are positive definite
- Let $k : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$ be positive definite. There is a unique RKHS $\mathcal{H} = \{f : \mathcal{X} \mapsto \mathbb{R}\}$ with reproducing kernel k [Moore-Aronszajn]

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- Let the empirical risk function $\hat{R}$ be arbitrary
- Any minimizer

$$\operatorname*{argmin}_{f \in \mathcal{H}_k} \hat{R}((x_1, y_1, f(x_1)), \ldots, (x_n, y_n, f(x_n))) + \Omega(\|f\|)$$

admits the form

$$\sum_{i=1}^{n} \alpha_i k(\cdot, x_i)$$

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