$\LaTeX$ command declarations here.

In [1]:

```
from __future__ import division

# scientific
%matplotlib inline
from matplotlib import pyplot as plt;
import numpy as np;
import sklearn as skl;
import sklearn.datasets;
import sklearn.cluster;

# ipython
import IPython;

# python
import os;

#####################################################

# image processing
import PIL;

# trim and scale images
def trim(im, percent=100):
    print("trim:", percent);
    bg = PIL.Image.new(im.mode, im.size, im.getpixel((0,0)))
    diff = PIL.ImageChops.difference(im, bg)
    diff = PIL.ImageChops.add(diff, diff, 2.0, -100)
    bbox = diff.getbbox()
    if bbox:
        x = im.crop(bbox)
        return x.resize(((x.size[0]*percent)//100, (x.size[1]*pe
rcent)//100), PIL.Image.ANTIALIAS);


#####################################################

# daft (rendering PGMs)
import daft;

# set to FALSE to load PGMs from static images
RENDER_PGMS = False;

# decorator for pgm rendering
def pgm_render(pgm_func):
    def render_func(path, percent=100, render=None, *args, **kwa
rgs):
        print("render_func:", percent);
        # render
        render = render if (render is not None) else RENDER_PGM
S;

        if render:
            print("rendering");
            # render
            pgm = pgm_func(*args, **kwargs);
            pgm.render();
            pgm.figure.savefig(path, dpi=300);

            # trim
            img = trim(PIL.Image.open(path), percent);
            img.save(path, 'PNG');
        else:
            print("not rendering");

        # error
        if not os.path.isfile(path):
            raise "Error:  Graphical model image %s not found.
You may need to set RENDER_PGMS=True.";

        # display
        return IPython.display.Image(filename=path);#trim(PIL.Im
age.open(path), percent);

    return render_func;

######################################################
```

EECS 545: Machine Learning

Lecture 15: Latent Variables, d-Separation, K-Means

- Instructor: **Jacob Abernethy**
- Date: March 14, 2016

Lecture Exposition: Saket & Ben

References

- **[MLAPP]** Murphy, Kevin. *Machine Learning: A Probabilistic Perspective* (https://mitpress.mit.edu/books/machine-learning-0). 2012.
- **[PRML]** Bishop, Christopher. *Pattern Recognition and Machine Learning* (http://research.microsoft.com/en-us/um/people/cmbishop/prml/). 2006.
- **[Koller & Friedman 2009]** Koller, Daphne and Nir Friedman. *Probabilistic Graphical Models* (https://mitpress.mit.edu/books/probabilistic-graphical-models). 2009.

Outline

- Probabilistic Graphical Models
  - Latent Variable Models
  - d-separation in Bayesian Networks
- Clustering & Mixture Models
  - K-Means Clustering

Latent Variable Models

> Uses material from **[MLAPP]** §10.1-10.4, §11.1-11.2

Latent Variable Models

In general, the goal of probabilistic modeling is to

> Use what we know to make *inferences* about what we don't know.

Graphical models provide a natural framework for this problem.

- Assume unobserved variables are correlated due to the influence of unobserved **latent variables**.
- Latent variables encode beliefs about the generative process.

In a graphical model, we will often **shade in** the observed variables to distinguish them from hidden variables.

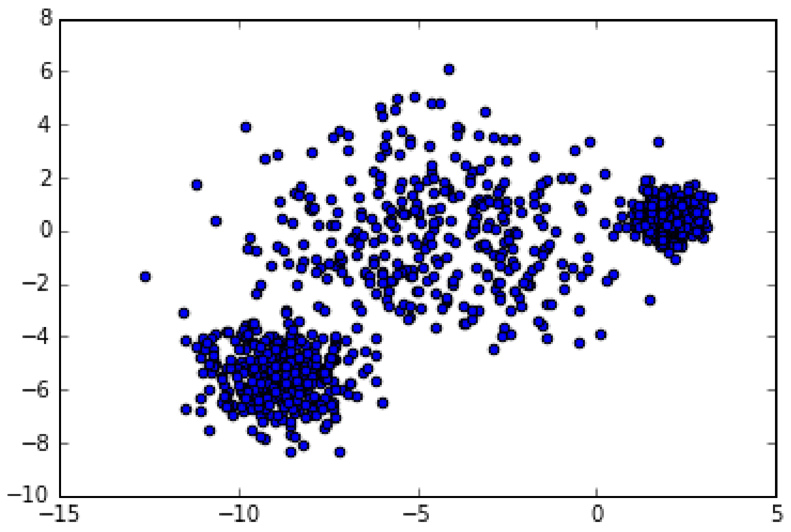
Example: Gaussian Mixture Models

This dataset is hard to explain with a single distribution.

- Underlying density is complicated overall...
- But it's clearly three Gaussians!

```
In [2]: X, y = skl.datasets.make_blobs(1000, cluster_std=[1.0, 2.5, 0.
        5], random_state=170)
        plt.scatter(X[:,0], X[:,1])
```

```
Out[2]: <matplotlib.collections.PathCollection at 0x7ff59a84b908>
```



Example: Mixture Models

Instead, introduce a latent **cluster label** $z_j \in [K]$ for each datapoint x_j,

$$\begin{aligned} z_j &\sim \mathrm{Cat}(\pi_1, \ldots, \pi_K) \qquad && \forall\, j = 1, \ldots, N \\ x_j \mid z_j &\sim \mathcal{N}(\mu_{z_j}, \Sigma_{z_j}) && \forall\, j = 1, \ldots, N \end{aligned}$$

This allows us to explain a complicated density as a **mixture** of simpler densities:

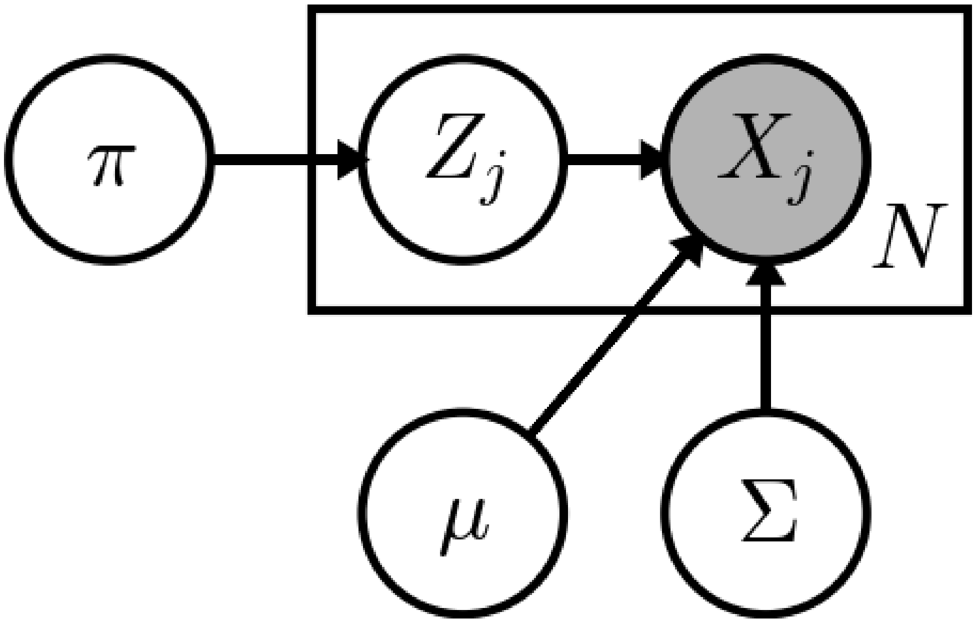
$$P(x|\mu, \Sigma) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x|\mu_k, \Sigma_k)$$

Example: Mixture Models

In [3]:
```
@pgm_render
def pgm_gmm():
    pgm = daft.PGM([4,4], origin=[-2,-1], node_unit=0.8, grid_un
it=2.0);
    # nodes
    pgm.add_node(daft.Node("pi", r"$\pi$", 0, 1));
    pgm.add_node(daft.Node("z", r"$Z_j$", 0.7, 1));
    pgm.add_node(daft.Node("x", r"$X_j$", 1.3, 1, observed=Tru
e));
    pgm.add_node(daft.Node("mu", r"$\mu$", 0.7, 0.3));
    pgm.add_node(daft.Node("sigma", r"$\Sigma$", 1.3, 0.3));

    # edges
    pgm.add_edge("pi", "z", head_length=0.08);
    pgm.add_edge("z", "x", head_length=0.08);
    pgm.add_edge("mu", "x", head_length=0.08);
    pgm.add_edge("sigma", "x", head_length=0.08);

    pgm.add_plate(daft.Plate([0.4,0.8,1.3,0.5], label=r"$\qquad
\qquad\qquad\;\; N$",
    shift=-0.1))

    return pgm;
```

```
In [4]: %%capture
        pgm_gmm("images/pgm/pgm-gmm.png")
```

Out[4]:



Example: Hidden Markov Models

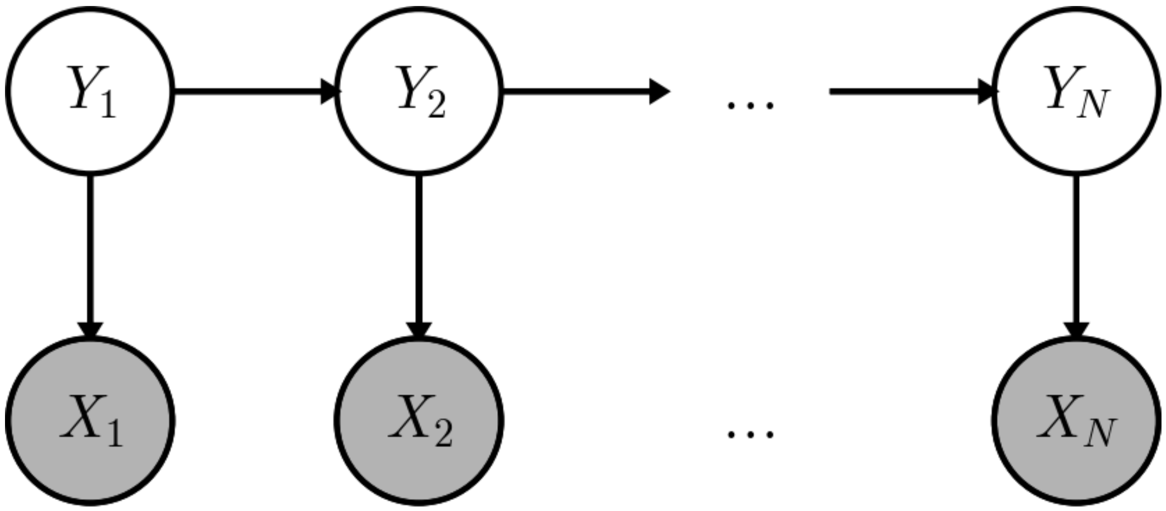
Noisy observations X_k generated from hidden Markov chain Y_k.

$$P(\mathbf{X},\mathbf{Y}) = P(Y_1)P(X_1 \mid Y_1)\prod_{k=2}^{N}\left(P(Y_k \mid Y_{k-1})P(X_k \mid Y_k)\right)$$

In [5]:
```
@pgm_render
def pgm_hmm():
    pgm = daft.PGM([7, 7], origin=[0, 0])

    # Nodes
    pgm.add_node(daft.Node("Y1", r"$Y_1$", 1, 3.5))
    pgm.add_node(daft.Node("Y2", r"$Y_2$", 2, 3.5))
    pgm.add_node(daft.Node("Y3", r"$\dots$", 3, 3.5, plot_params
={'ec':'none'}))
    pgm.add_node(daft.Node("Y4", r"$Y_N$", 4, 3.5))

    pgm.add_node(daft.Node("x1", r"$X_1$", 1, 2.5, observed=Tru
e))
    pgm.add_node(daft.Node("x2", r"$X_2$", 2, 2.5, observed=Tru
e))
    pgm.add_node(daft.Node("x3", r"$\dots$", 3, 2.5, plot_params
={'ec':'none'}))
    pgm.add_node(daft.Node("x4", r"$X_N$", 4, 2.5, observed=Tru
e))


    # Add in the edges.
    pgm.add_edge("Y1", "Y2", head_length=0.08)
    pgm.add_edge("Y2", "Y3", head_length=0.08)
    pgm.add_edge("Y3", "Y4", head_length=0.08)

    pgm.add_edge("Y1", "x1", head_length=0.08)
    pgm.add_edge("Y2", "x2", head_length=0.08)
    pgm.add_edge("Y4", "x4", head_length=0.08)

    return pgm;
```

In [6]:
```
%%capture
pgm_hmm("images/pgm/hmm.png");
```

Out[6]:



Example: Unsupervised Learning

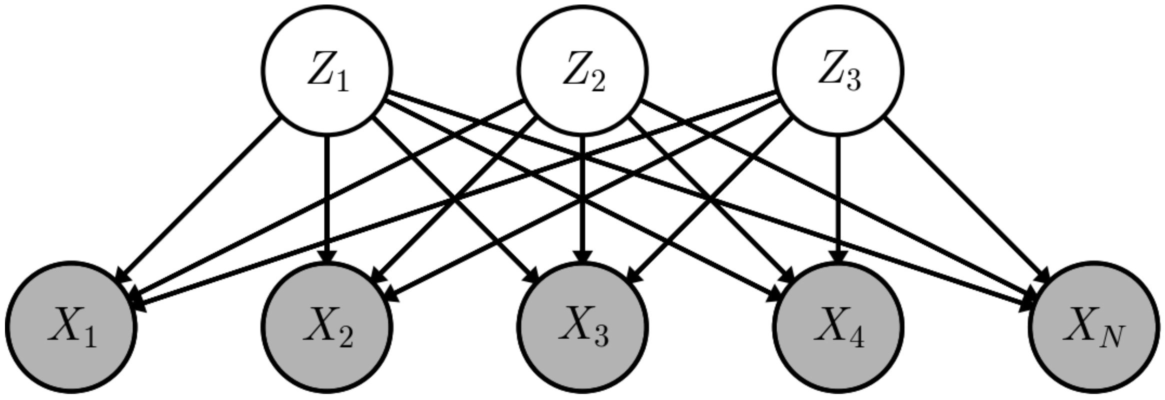
Latent variables are fundamental to unsupervised and deep learning.

- Serve as a **bottleneck**
- Compute a **compressed** representation of data

In [7]:
```
@pgm_render
def pgm_unsupervised():
    pgm = daft.PGM([6, 6], origin=[0, 0])

    # Nodes
    pgm.add_node(daft.Node("d1", r"$Z_1$", 2, 3.5))
    pgm.add_node(daft.Node("di", r"$Z_2$", 3, 3.5))
    pgm.add_node(daft.Node("dn", r"$Z_3$", 4, 3.5))

    pgm.add_node(daft.Node("f1", r"$X_1$", 1, 2.50, observed=Tru
e))
    pgm.add_node(daft.Node("fi-1", r"$X_2$", 2, 2.5, observed=Tr
ue))
    pgm.add_node(daft.Node("fi", r"$X_3$", 3, 2.5, observed=Tru
e))
    pgm.add_node(daft.Node("fi+1", r"$X_4$", 4, 2.5, observed=Tr
ue))
    pgm.add_node(daft.Node("fm", r"$X_N$", 5, 2.5, observed=Tru
e))


    # Add in the edges.
    pgm.add_edge("d1", "f1", head_length=0.08)
    pgm.add_edge("d1", "fi-1", head_length=0.08)
    pgm.add_edge("d1", "fi", head_length=0.08)
    pgm.add_edge("d1", "fi+1", head_length=0.08)
    pgm.add_edge("d1", "fm", head_length=0.08)

    pgm.add_edge("di", "f1", head_length=0.08)
    pgm.add_edge("di", "fi-1", head_length=0.08)
    pgm.add_edge("di", "fi", head_length=0.08)
    pgm.add_edge("di", "fi+1", head_length=0.08)
    pgm.add_edge("di", "fm", head_length=0.08)

    pgm.add_edge("dn", "f1", head_length=0.08)
    pgm.add_edge("dn", "fi-1", head_length=0.08)
    pgm.add_edge("dn", "fi", head_length=0.08)
    pgm.add_edge("dn", "fi+1", head_length=0.08)
    pgm.add_edge("dn", "fm", head_length=0.08)

    return pgm
```

In [8]:
```
%%capture
pgm_unsupervised("images/pgm/unsupervised.png");
```

Out[8]:



Other Latent Variable Models

Many other models in machine learning involve latent variables:

- Neural Networks / Multilayer Perceptrons
- Restricted Boltzmann Machines
- Deep Belief Networks
- Probabilistic PCA

Latent Variable Models: Complexity

Latent variable models exhibit **emergent complexity**.

- Although each conditional distribution is simple,
- The joint distribution is capable of modeling complex interactions.

However, latent variables make learning difficult.

- Inference is challening in models with latent variables.
- They can introduce new dependencies between observed variables.

Bayesian Networks

Part II: Inference, Learning, and d-Separation

> Uses material from **[Koller & Friedman 2009]** Chapter 3, **[MLAPP]** Chapter 10, and **[PRML]** §8.2.1

Bayesian Networks: Terminology

Typically, our models will have

- Observed variables X
- Hidden variables Z
- Parameters θ

Occasionally, we will distinguish between **inference** and **learning**.

Bayesian Networks: Inference

Inference: Estimate hidden variables Z from observed variables X.

$$P(Z|X,\theta) = \frac{P(X,Z|\theta)}{P(X|\theta)}$$

- Denominator $P(X|\theta)$ is sometimes called the probability of the **evidence**.
- Occasionally we care only about a subset of the hidden variables, and marginalize out the rest.

Bayesian Networks: Learning

Learning: Estimate parameters θ from observed data X.

$$P(\theta \mid X) = \sum_{z \in Z} P(\theta, z \mid X) = \sum_{z \in Z} P(\theta \mid z, X) P(z \mid X)$$

To Bayesians, parameters *are* hidden variables, so inference and learning are equivalent.

Bayesian Networks: Probability Queries

In general, it is useful to compute $P(A|B)$ for arbitrary collections A and B of variables.

- Both inference and learning take this form.

To accomplish this, we must understand the **independence structure** of any given graphical model.

Review: Local Independencies

Every Bayesian Network $\mathcal{G}$ encodes a set $\mathcal{I}_\ell(\mathcal{G})$ of **local independence assumptions**:

> For each variable X_k, we have $(X_k \perp \mathrm{NonDesc}_{\mathcal{G}}(X_k) \mid \mathrm{Parents}_{\mathcal{G}}(X_k))$

Every node X_k is conditionally independent of its nondescendants given its parents.

> For arbitrary sets of variables, when does $(A \perp B \mid C)$ hold?

Review: I-Maps

If P satisfies the independence assertions made by $\mathcal{G}$, we say that

- $\mathcal{G}$ is an **I-Map** for P
- or that P **satisfies** $\mathcal{G}$.

Any distribution satisfying $\mathcal{G}$ shares common structure.

- We will exploit this structure in our algorithms
- This is what makes graphical models so **powerful**!

Review: Factorization Theorem

Last time, we proved that for any P satisfying $\mathcal{G}$,

$$P(X_1, \dots, X_N) = \prod_{k=1}^{N} P(X_k \mid \mathbf{Parents}_{\mathcal{G}}(X_k))$$

If we understand independence structure, we can factorize arbitrary conditional distributions:

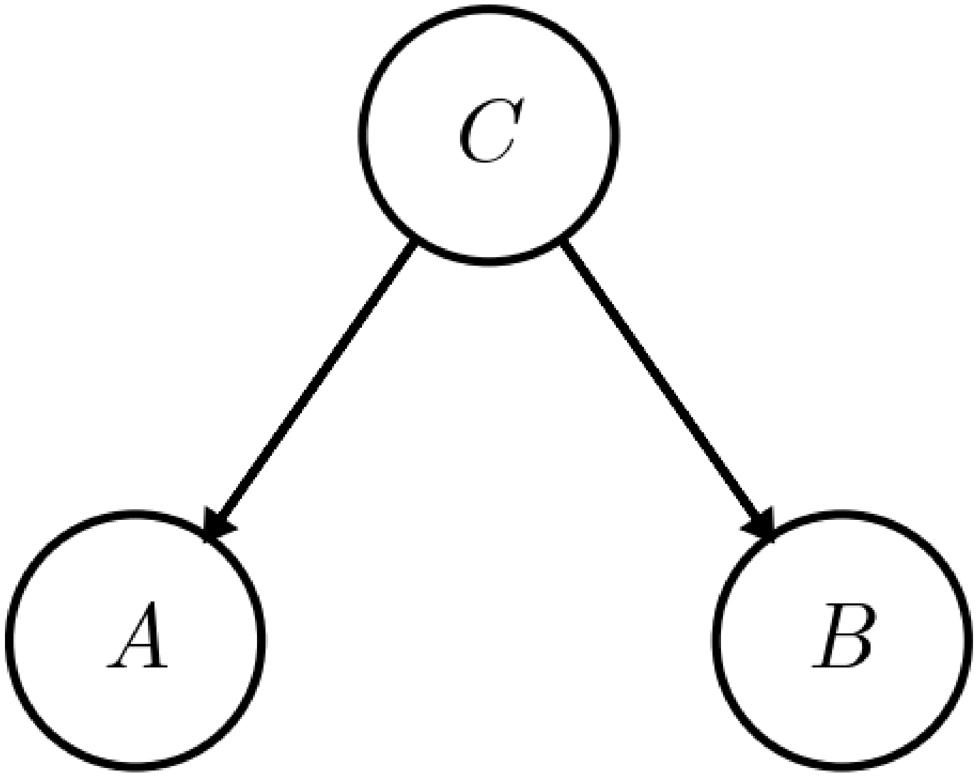
$$P(A_1, \dots, A_n \mid B_1, \dots, B_m) = ?$$

Question 1: Is $(A \perp B)$?

In [9]:
```
@pgm_render
def pgm_question1():
    pgm = daft.PGM([4, 4], origin=[0, 0])

    # Nodes
    pgm.add_node(daft.Node("c", r"$C$", 2, 3.5))
    pgm.add_node(daft.Node("a", r"$A$", 1.3, 2.5))
    pgm.add_node(daft.Node("b", r"$B$", 2.7, 2.5))

    # Add in the edges.
    pgm.add_edge("c", "a", head_length=0.08)
    pgm.add_edge("c", "b", head_length=0.08)

    return pgm;
```

In [10]:
```
%%capture
pgm_question1("images/pgm/question1.png")
```

Out[10]:



Answer 1: No!

No! A and B are not marginally independent.

- Note C is not shaded, so we don't observe it.

In general,

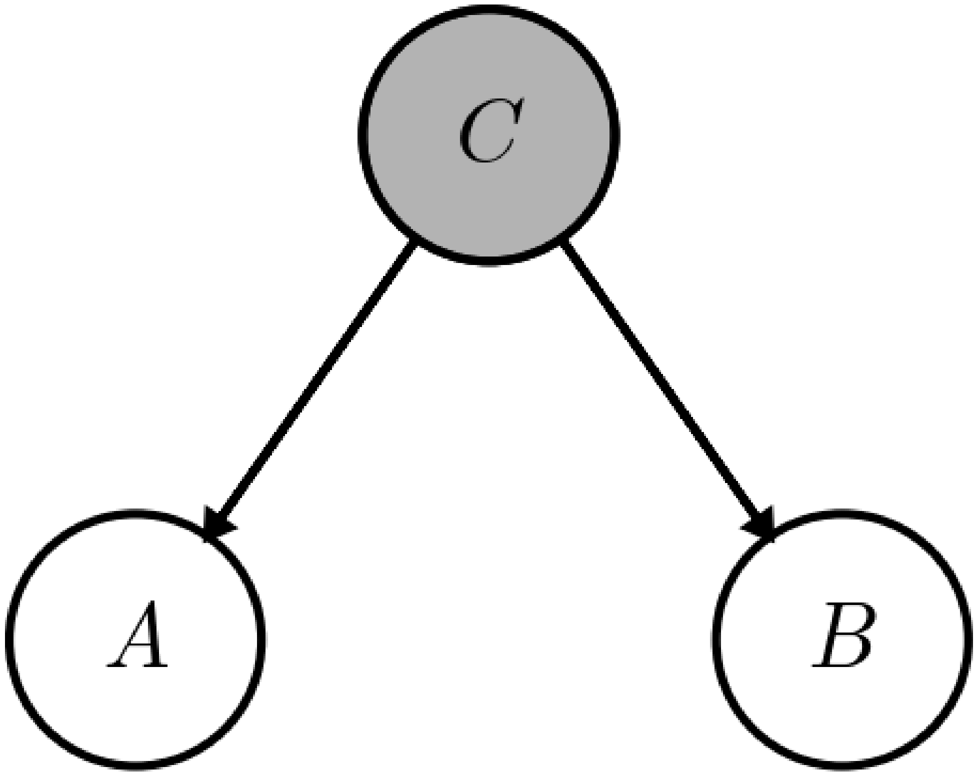
$$P(A,B) = \sum_{c \in C} P(A,B,c) = \sum_{c \in C} P(A|C)P(B|C)P(C) \neq P(A)P(B)$$

Question 2: Is $(A \perp B \mid C)$?

In [11]:
```
@pgm_render
def pgm_question2():
    pgm = daft.PGM([4, 4], origin=[0, 0])

    # Nodes
    pgm.add_node(daft.Node("c", r"$C$", 2, 3.5,
                           observed=True))
    pgm.add_node(daft.Node("a", r"$A$", 1.3, 2.5))
    pgm.add_node(daft.Node("b", r"$B$", 2.7, 2.5))

    # Add in the edges.
    pgm.add_edge("c", "a", head_length=0.08)
    pgm.add_edge("c", "b", head_length=0.08)

    return pgm
```

In [12]:
```
%%capture
pgm_question2("images/pgm/question2.png")
```

Out[12]:



Answer 2: Yes!

Yes! $(A \perp B | C)$ follows from the local independence properties of Bayesian networks.

> Every variable is conditionally independent of its nondescendants given its parents.

Observing $C$ *blocks* the path of influence from $A$ to $B$. Or, using factorization theorem:

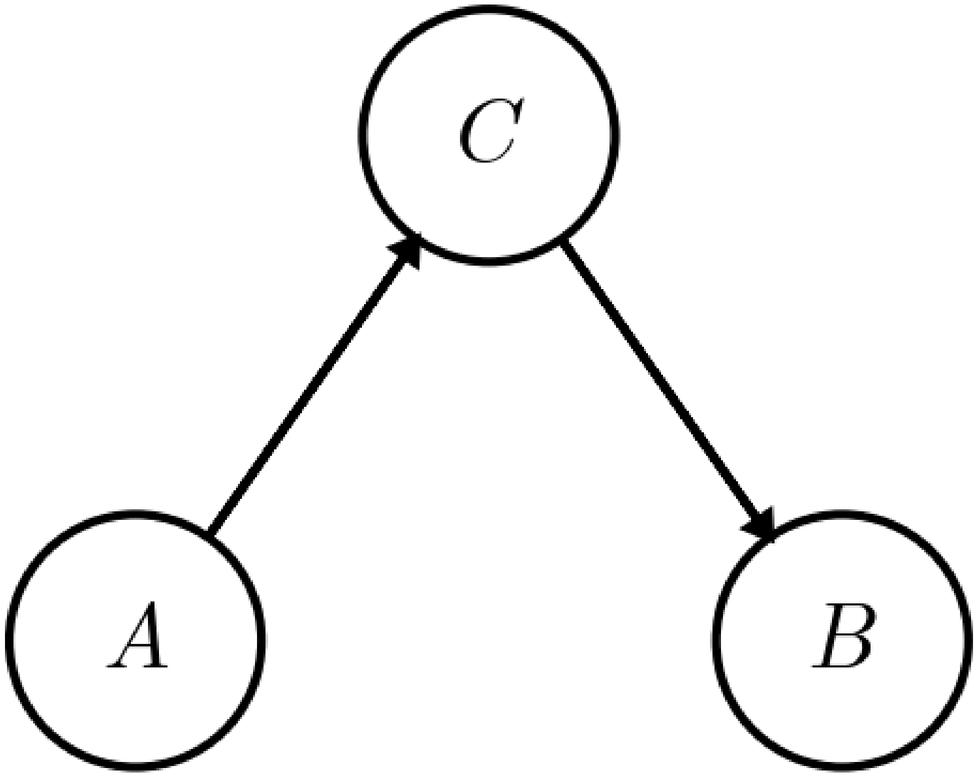
$$\begin{aligned} P(A, B|C) &= \frac{P(A, B, C)}{P(C)} \\ &= \frac{P(C)P(A|C)P(B|C)}{P(C)} \\ &= P(A|C)P(B|C) \end{aligned}$$

Question 3: Is $(A \perp B)$?

In [13]:
```
@pgm_render
def pgm_question3():
    pgm = daft.PGM([4, 4], origin=[0, 0])

    # Nodes
    pgm.add_node(daft.Node("c", r"$C$", 2, 3.5))
    pgm.add_node(daft.Node("a", r"$A$", 1.3, 2.5))
    pgm.add_node(daft.Node("b", r"$B$", 2.7, 2.5))

    # Add in the edges.
    pgm.add_edge("a", "c", head_length=0.08)
    pgm.add_edge("c", "b", head_length=0.08)

    return pgm
```

In [14]:
```
%%capture
pgm_question3("images/pgm/question3.png")
```

Out[14]:



Answer 3: No!

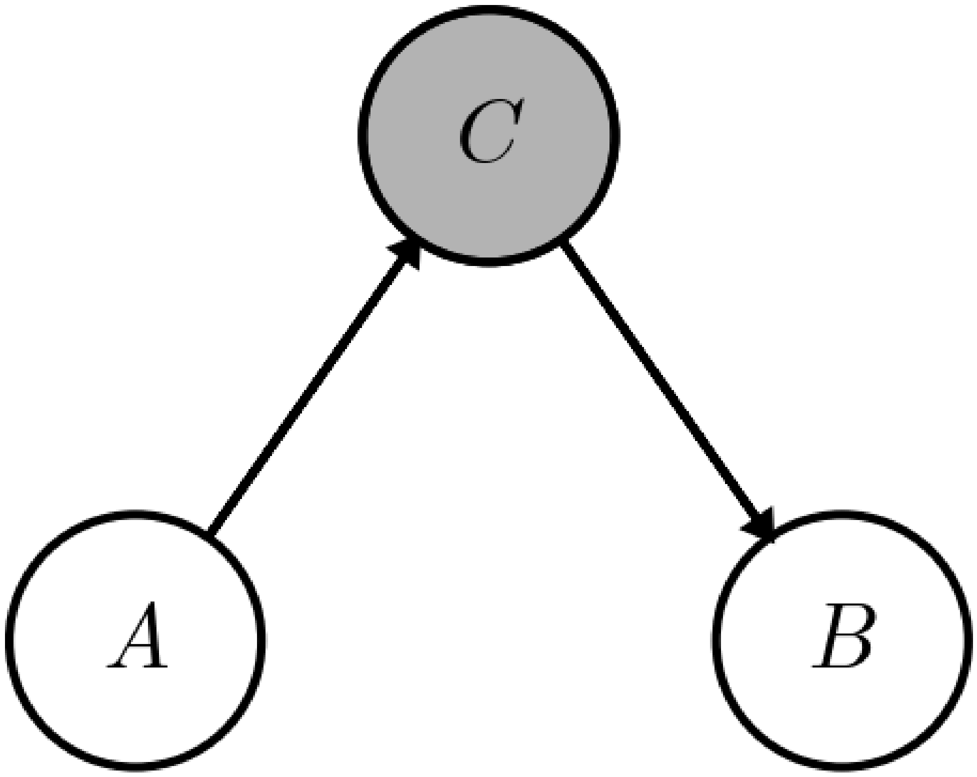
Again, $C$ is not given, so $A$ and $B$ are dependent.

Question 4: Is $(A \perp B \mid C)$?

In [15]:
```
@pgm_render
def pgm_question4():
    pgm = daft.PGM([4, 4], origin=[0, 0])

    # Nodes
    pgm.add_node(daft.Node("c", r"$C$", 2, 3.5, observed=True))
    pgm.add_node(daft.Node("a", r"$A$", 1.3, 2.5))
    pgm.add_node(daft.Node("b", r"$B$", 2.7, 2.5))

    # Add in the edges.
    pgm.add_edge("a", "c", head_length=0.08)
    pgm.add_edge("c", "b", head_length=0.08)

    return pgm
```

In [16]:
```
%%capture
pgm_question4("images/pgm/question4.png")
```

Out[16]:



Answer 4: Yes!

Again, observing C *blocks* influence from A to B.

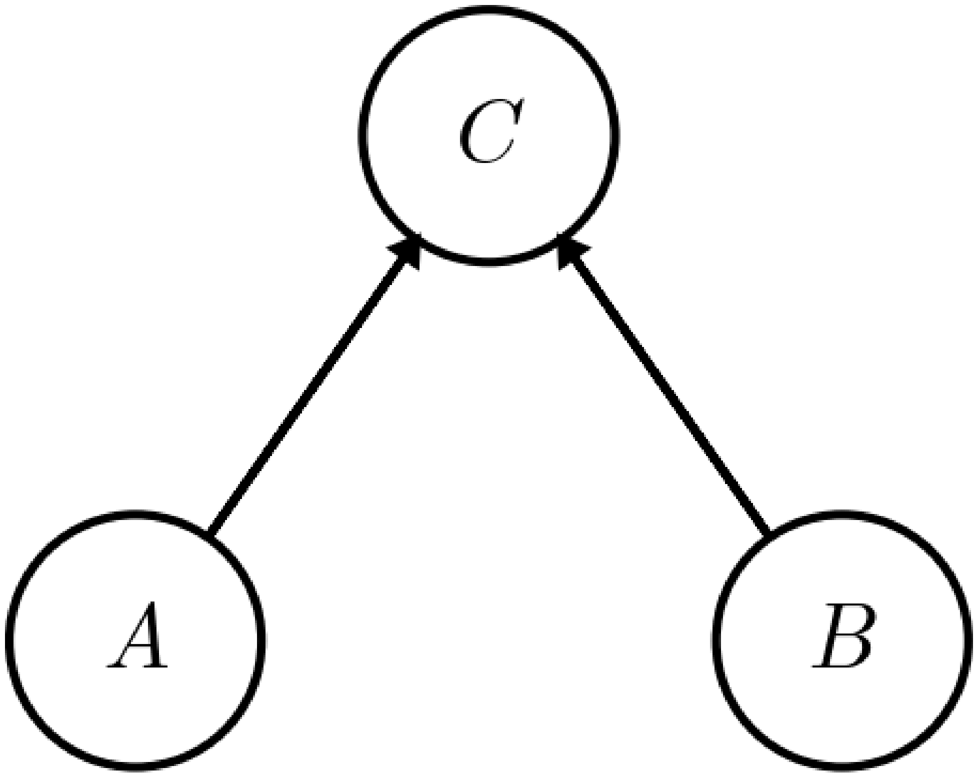
> Every variable is conditionally independent of its nondescendants given its parents.

Question 5: Is $(A \perp B)$?

In [17]:
```
@pgm_render
def pgm_question5():
    pgm = daft.PGM([4, 4], origin=[0, 0])

    # Nodes
    pgm.add_node(daft.Node("c", r"$C$", 2, 3.5))
    pgm.add_node(daft.Node("a", r"$A$", 1.3, 2.5))
    pgm.add_node(daft.Node("b", r"$B$", 2.7, 2.5))

    # Add in the edges.
    pgm.add_edge("a", "c", head_length=0.08)
    pgm.add_edge("b", "c", head_length=0.08)

    return pgm
```

In [18]:
```
%%capture
pgm_question5("images/pgm/question5.png")
```

Out[18]:



Answer 5: Yes!

Using the factorization rule,

$$P(A,B,C) = P(A)P(B)P(C \mid A,B)$$

Therefore, marginalizing out $C$,

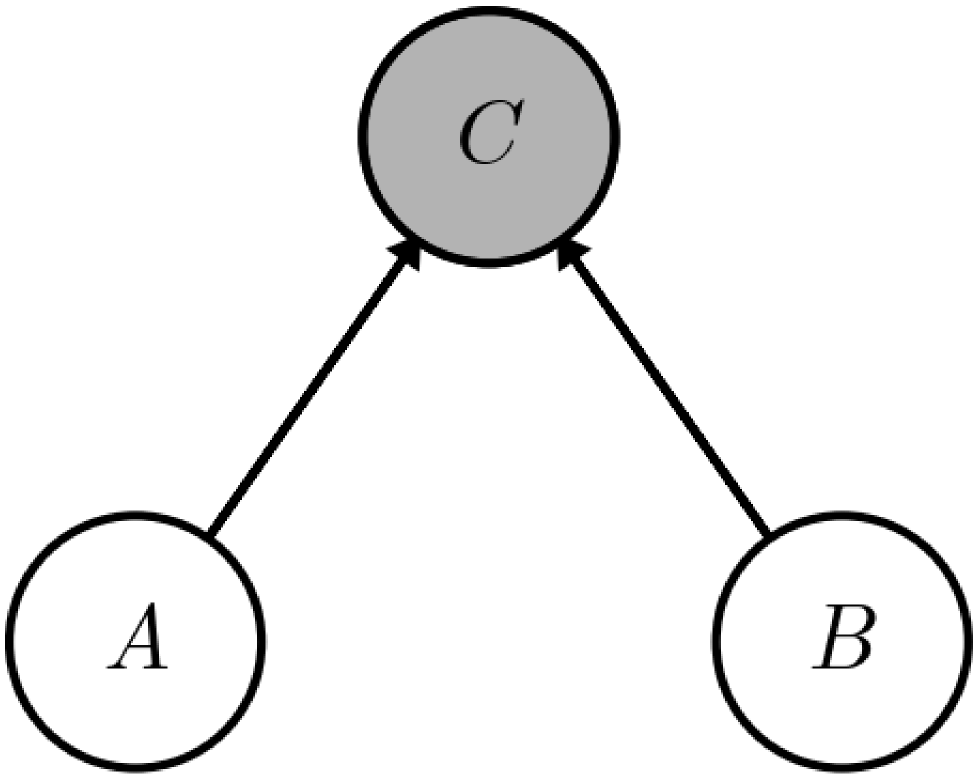
$$\begin{aligned} P(A,B) &= \sum_{c \in C} P(A,B,c) \\ &= \sum_{c \in C} P(A)P(B)P(c \mid A,B) \\ &= P(A)P(B)\sum_{c \in C} P(c \mid A,B) = P(A)P(B) \end{aligned}$$

Question 6: Is $P(A \perp B \mid C)$?

In [19]:
```
@pgm_render
def pgm_question6():
    pgm = daft.PGM([4, 4], origin=[0, 0])

    # Nodes
    pgm.add_node(daft.Node("c", r"$C$", 2, 3.5, observed=True))
    pgm.add_node(daft.Node("a", r"$A$", 1.3, 2.5))
    pgm.add_node(daft.Node("b", r"$B$", 2.7, 2.5))

    # Add in the edges.
    pgm.add_edge("a", "c", head_length=0.08)
    pgm.add_edge("b", "c", head_length=0.08)

    return pgm
```

```
In [20]: %%capture
         pgm_question6("images/pgm/question6.png")
```

Out[20]:



Answer: No!

A can influence B via C.

$$P(A, B|C) = \frac{P(A, B, C)}{P(C)} = \frac{P(A)P(B)P(C|A, B)}{P(C)}$$

This does not factorize in general to $P(A|C)P(B|C)$.

Example: Battery, Fuel, and Gauge

Consider three binary random variables

- Battery B is either charged $(B = 1)$ or dead, $(B = 0)$
- Fuel tank F is either full $(F = 1)$ or empty, $(F = 0)$
- Fuel gauge G either indicates full $(G = 1)$ or empty, $(G = 0)$

Assume $(B \perp F)$ with priors

- $P(B = 1) = 0.9$
- $P(F = 1) = 0.9$

Example: Battery, Fuel, and Gauge

Given the state of the fuel tank and the battery, the fuel gauge reads full with probabilities:

- $p(G = 1 \mid B = 1, F = 1) = 0.8$
- $p(G = 1 \mid B = 1, F = 0) = 0.2$
- $p(G = 1 \mid B = 0, F = 1) = 0.2$
- $p(G = 1 \mid B = 0, F = 0) = 0.1$

Example: Battery, Fuel, and Gauge

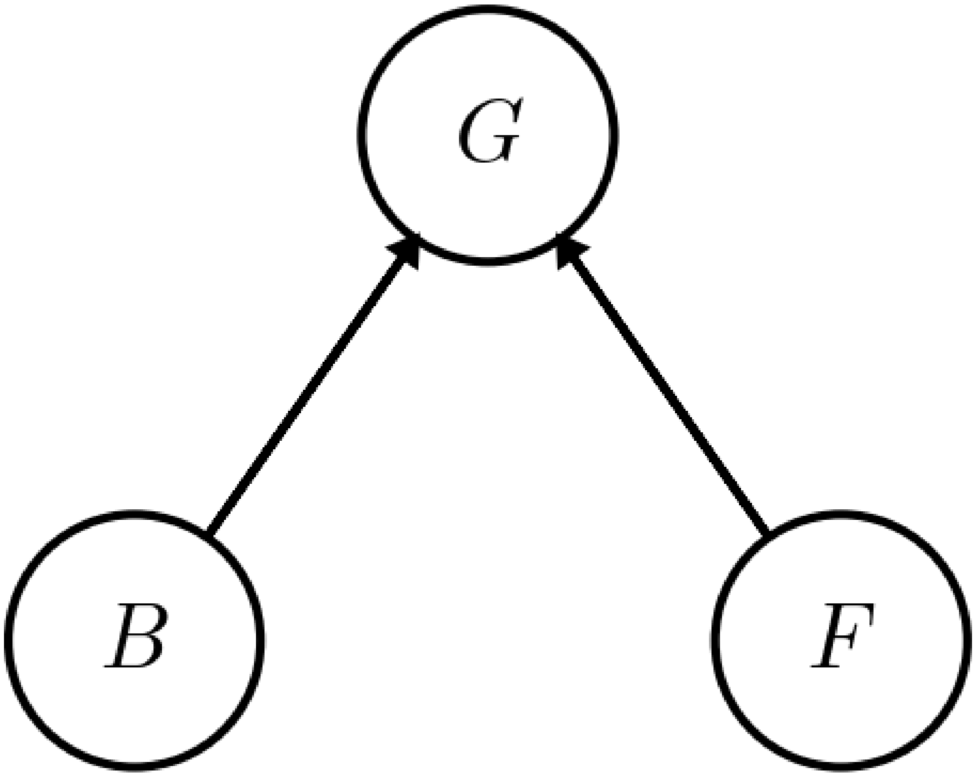
Without any observations, the probability of an empty fuel tank is

$$P(F = 0) = 1 - P(F = 1) = 0.1$$

In [21]:
```
@pgm_render
def pgm_bfg_1():
    pgm = daft.PGM([4, 4], origin=[0, 0])

    # Nodes
    pgm.add_node(daft.Node("G", r"$G$", 2, 3.5))
    pgm.add_node(daft.Node("B", r"$B$", 1.3, 2.5))
    pgm.add_node(daft.Node("F", r"$F$", 2.7, 2.5))

    # Add in the edges.
    pgm.add_edge("B", "G", head_length=0.08)
    pgm.add_edge("F", "G", head_length=0.08)

    return pgm;
```

In [22]:
```
%%capture
pgm_bfg_1("images/pgm/bfg-1.png")
```

Out[22]:



Example: Empty Gauge

Now, suppose the gauge reads $G = 0$. We have

$$P(G=0) = \sum_{B\in\{0,1\}} \sum_{F\in\{0,1\}} P(G=0 \mid B,F)P(B)P(F) = 0.315$$

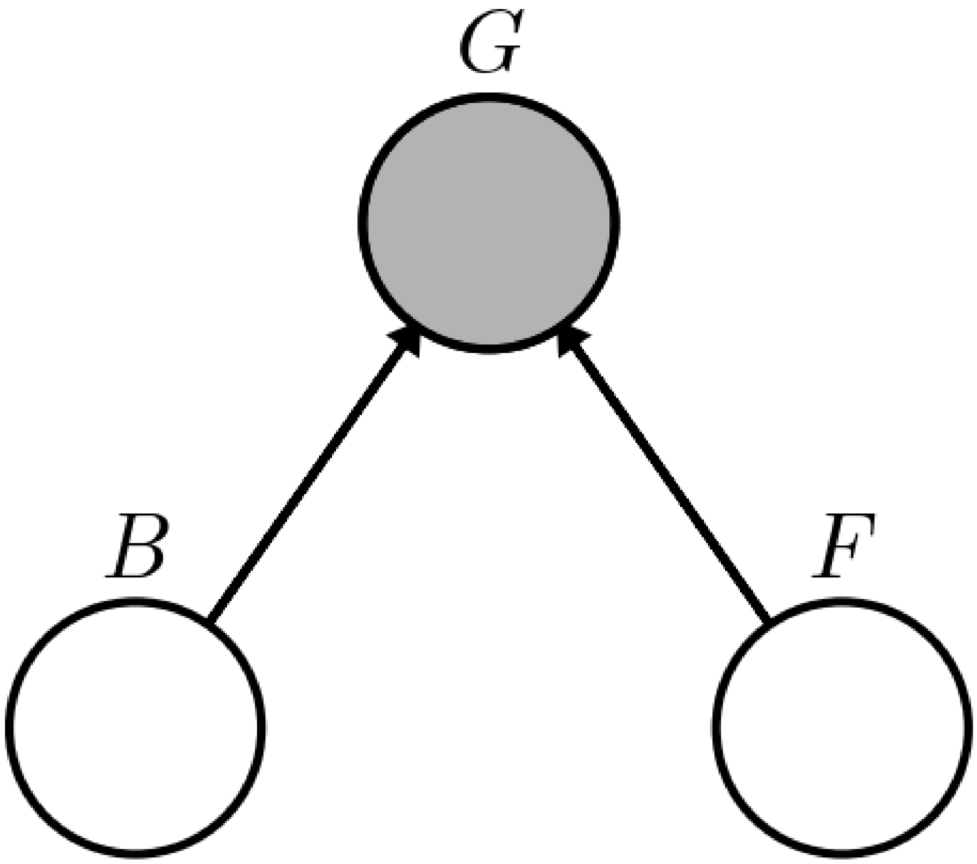
Verify this!

Example: Emtpy Gauge

In [23]:
```
@pgm_render
def pgm_bfg_2():
    pgm = daft.PGM([4, 4], origin=[0, 0])

    # Nodes
    pgm.add_node(daft.Node("G", r"$G$", 2, 3.5, offset=(0, 20), observed=True))
    pgm.add_node(daft.Node("B", r"$B$", 1.3, 2.5, offset=(0, 20)))
    pgm.add_node(daft.Node("F", r"$F$", 2.7, 2.5, offset=(0, 20)))

    # Add in the edges.
    pgm.add_edge("B", "G", head_length=0.08)
    pgm.add_edge("F", "G", head_length=0.08)

    return pgm;
```

```
In [24]: %%capture
         pgm_bfg_2("images/pgm/bfg-2.png");
```

Out[24]:



Example: Empty Gauge

Now, we also have

$$p(G=0 \mid F=0) = \sum_{B\in\{0,1\}} p(G=0 \mid B, F=0)p(B) = 0.81$$

Applying Bayes' Rule,

$$\begin{aligned} p(F=0 \mid G=0) &= \frac{p(G=0 \mid F=0)p(F=0)}{p(G=0)} \\ &\approx 0.257 > p(F=0) = 0.10 \end{aligned}$$

Observing an empty gauge makes it more likely that the tank is empty!

Example: Emtpy Gauge, Dead Battery

Now, suppose we *also* observe a dead battery $B = 0$. Then,

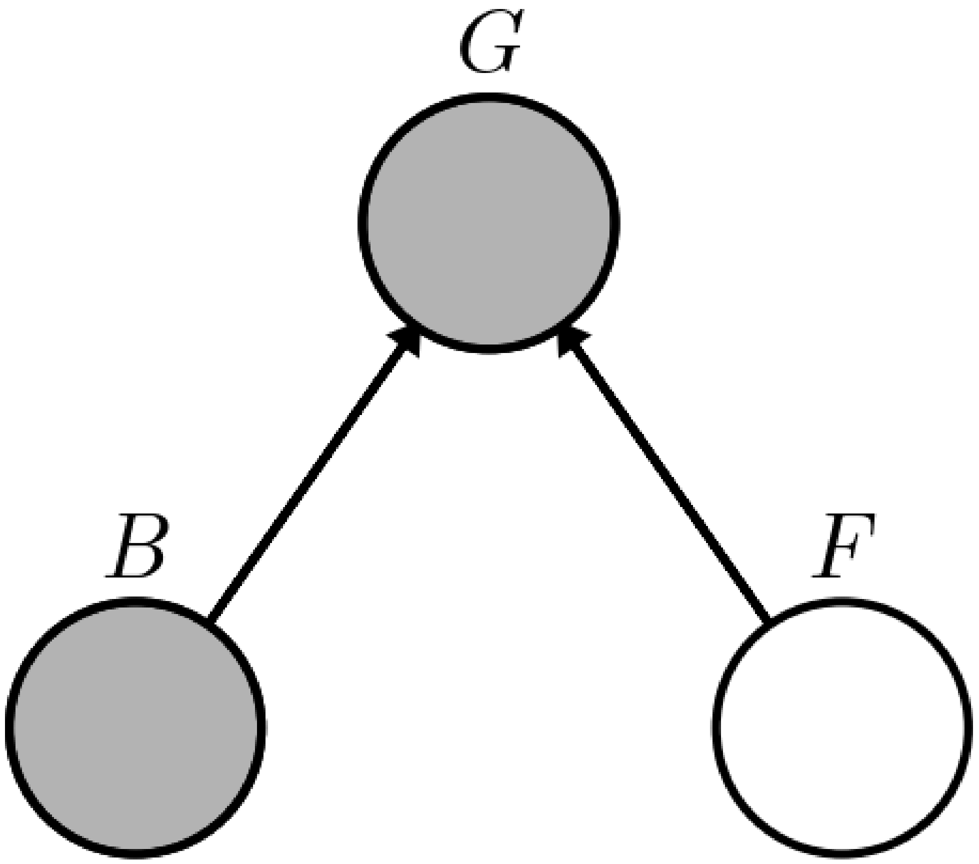
$$\begin{aligned} p(F = 0 \mid G = 0, B = 0) &= \frac{p(G = 0 \mid B = 0, F = 0) p(F = 0)}{\sum_{F \in \{0,1\}} p(G = 0 \mid B = 0, F) p(F)} \\ &\approx 0.111 \end{aligned}$$

Example: Emtpy Gauge, Dead Battery

In [25]:
```
@pgm_render
def pgm_bfg_3():
    pgm = daft.PGM([4, 4], origin=[0, 0])

    # Nodes
    pgm.add_node(daft.Node("G", r"$G$", 2, 3.5, offset=(0, 20),
observed=True))
    pgm.add_node(daft.Node("B", r"$B$", 1.3, 2.5, offset=(0, 2
0), observed=True))
    pgm.add_node(daft.Node("F", r"$F$", 2.7, 2.5, offset=(0, 2
0)))

    # Add in the edges.
    pgm.add_edge("B", "G", head_length=0.08)
    pgm.add_edge("F", "G", head_length=0.08)

    return pgm;
```

In [26]:
```
%%capture
pgm_bfg_3("images/pgm/bfg-3.png")
```

Out[26]:



Example: Empty Gauge, Dead Battery

This is the **explaining away** phenomenon.

- The probability of an empty tank has decreased from 0.257 to 0.111 after observing the dead battery!
- A dead battery *explans* why the guage indicates an empty tank, reducing the probability that the tank is *really* empty.

Conditioning on a common child makes its parents dependent.

Break time

- Will extend deadline for project proposals by a few days.

Bayesian Networks: d-Separation

We say a trail $X \leftrightharpoons Z \leftrightharpoons Y$ is **active** when influence can flow from X to Y via Z.

- **Causal Trail:** $X \rightarrow Z \rightarrow Y$ is active iff Z is hidden.
- **Evidential Trail:** $X \leftarrow Z \leftarrow Y$ is active iff Z is hidden.
- **Common Cause:** $X \leftarrow Z \rightarrow Y$ is active iff Z is hidden.
- **Common Effect:** $X \rightarrow Z \leftarrow Y$ is active iff Z or a descendant of Z is observed.

Bayesian Networks: d-Separation

A longer trail $X_1 \leftrightharpoons X_2 \leftrightharpoons \cdots \leftrightharpoons X_n$ is **active** if influence can flow from X_1 to X_n along the trail.

- Requires that every $X_{k-1} \leftrightharpoons X_k \leftrightharpoons X_{k+1}$ is active.

In general, $X_1 \leftrightharpoons X_2 \leftrightharpoons \cdots \leftrightharpoons X_n$ is **active** given observed variables Y if

- Whenever we have a v-structure $X_{k-1} \rightarrow X_k \leftarrow X_{k+1}$ then X_k or one of its descendants is in Y.
- No other node along the trail is in Y.

Bayesian Networks: d-Separation

Some graphs may have more than one trail between two given nodes.

- One node may inflence another if there exists an active trail between them.

Let $\mathbf{X}$, $\mathbf{Y}$, and $\mathbf{Z}$ be sets of nodes in $\mathcal{G}$. We say $\mathbf{X}$ and $\mathbf{Y}$ are **d-separated** given $\mathbf{Z}$, denoted $\text{d-sep}_{\mathcal{G}}(\mathbf{X};\mathbf{Y} \mid \mathbf{Z})$ if there is no active trail between any nodes $X \in \mathbf{X}$ and $Y \in \mathbf{Y}$ given $\mathbf{Z}$.

Bayesian Networks: d-Separation

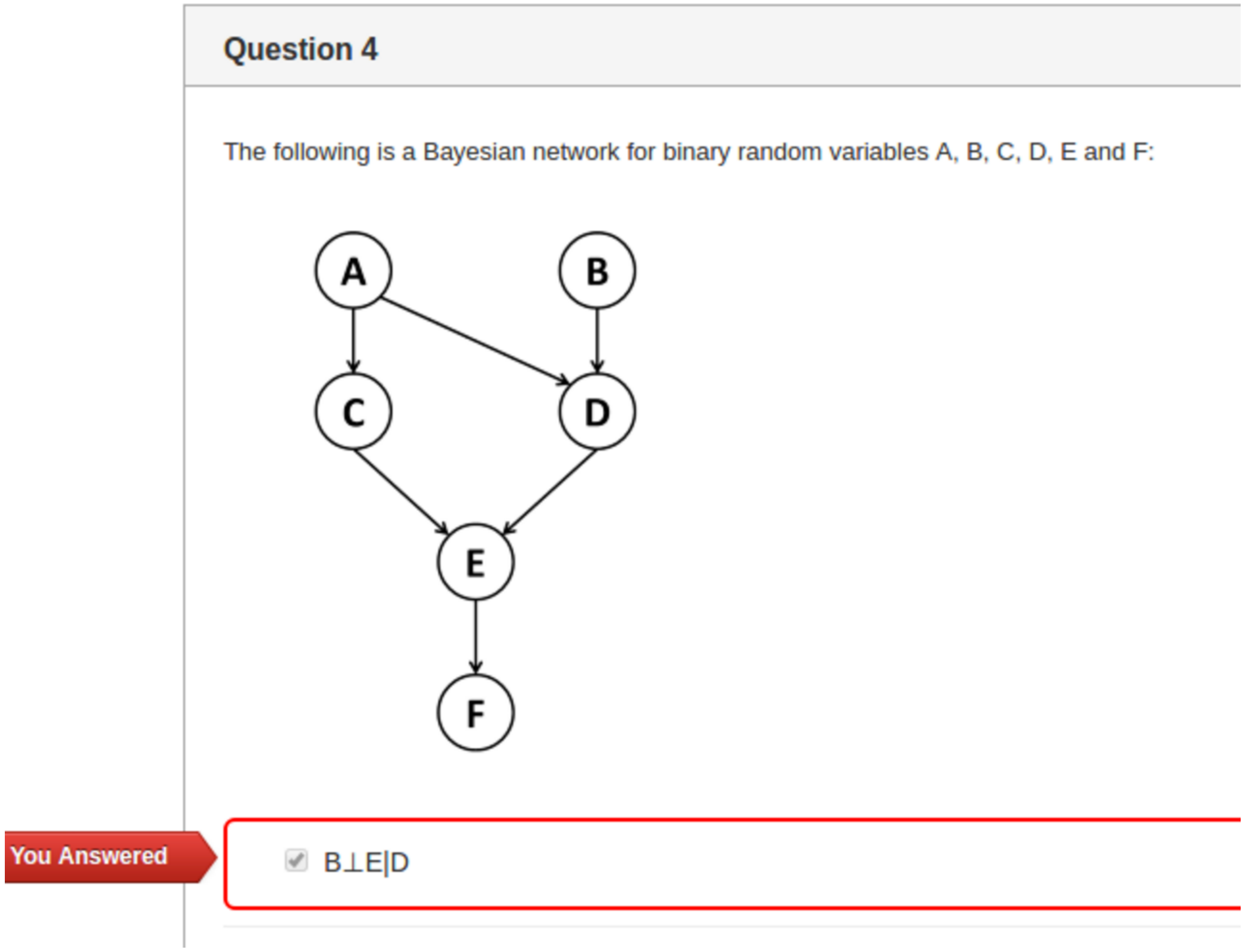
Theorem: (Koller & Friedman 3.5) For almost all distributions P that factorize over $\mathcal{G}$, we have

$$\text{d-sep}_{\mathcal{G}}(X;Y \mid Z) \iff (X \perp Y \mid Z)$$

That is, except on a set of measure zero in the space of distributions, the concept of d-separation in $\mathcal{G}$ exactly captures the concept of conditional independence.

- To check if variables are independent, check for d-separation.

Challenging quiz question:



Question 4

The following is a Bayesian network for binary random variables A, B, C, D, E and F:

$$\begin{tikzcd}
A \arrow[d] \arrow[drr] & & B \arrow[d] \\
C \arrow[dr] & & D \arrow[dl] \\
& E \arrow[d] & \\
& F &
\end{tikzcd}$$

✓ B⊥E|D

- Notice that there is an active path from B to E:

$$B \rightarrow \boxed{D} \leftarrow A \rightarrow C \rightarrow E$$

Clustering & K-Means

> Uses material from **[PRML]** §9.1

Clustering: Introduction

Goal: Partition data $\mathcal{X} = \{x_1, \dots, x_n\} \subset \mathbb{R}^d$ into K disjoint **clusters**.

- Points within a cluster should be more similar to each other than to points in other clusters.
- Estimate **cluster centers** $\mu_k \in \mathbb{R}^d$ for $k = 1, \dots, K$
- Estimate **cluster assignments** $z_j \in \{1, \dots, K\}$ for each point x_j

Usually, we fix K beforehand! Use model selection to overcome this limitation.

K-Means Clustering

The **K-Means** algorithm takes a simple, non-probabilistic approach.

- First, pick random cluster centers μ_k.

Then, repeat until convergence:

E-Step: Assign x_j to the nearest cluster center μ_k,

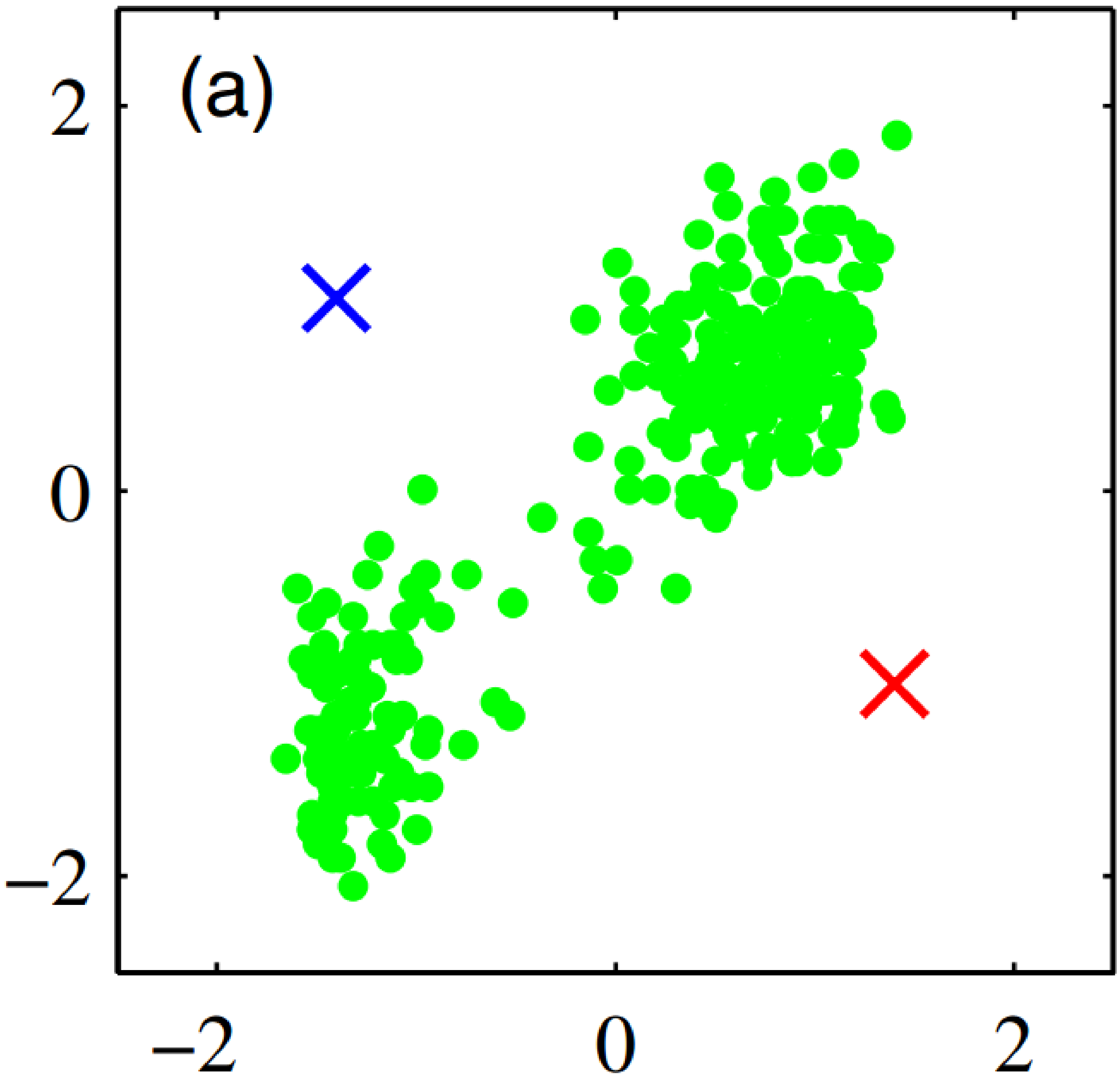
$$z_j = \arg\min_k ||x_j - \mu_k||^2$$

M-Step: Re-estimate cluster centers by averaging over assignments:

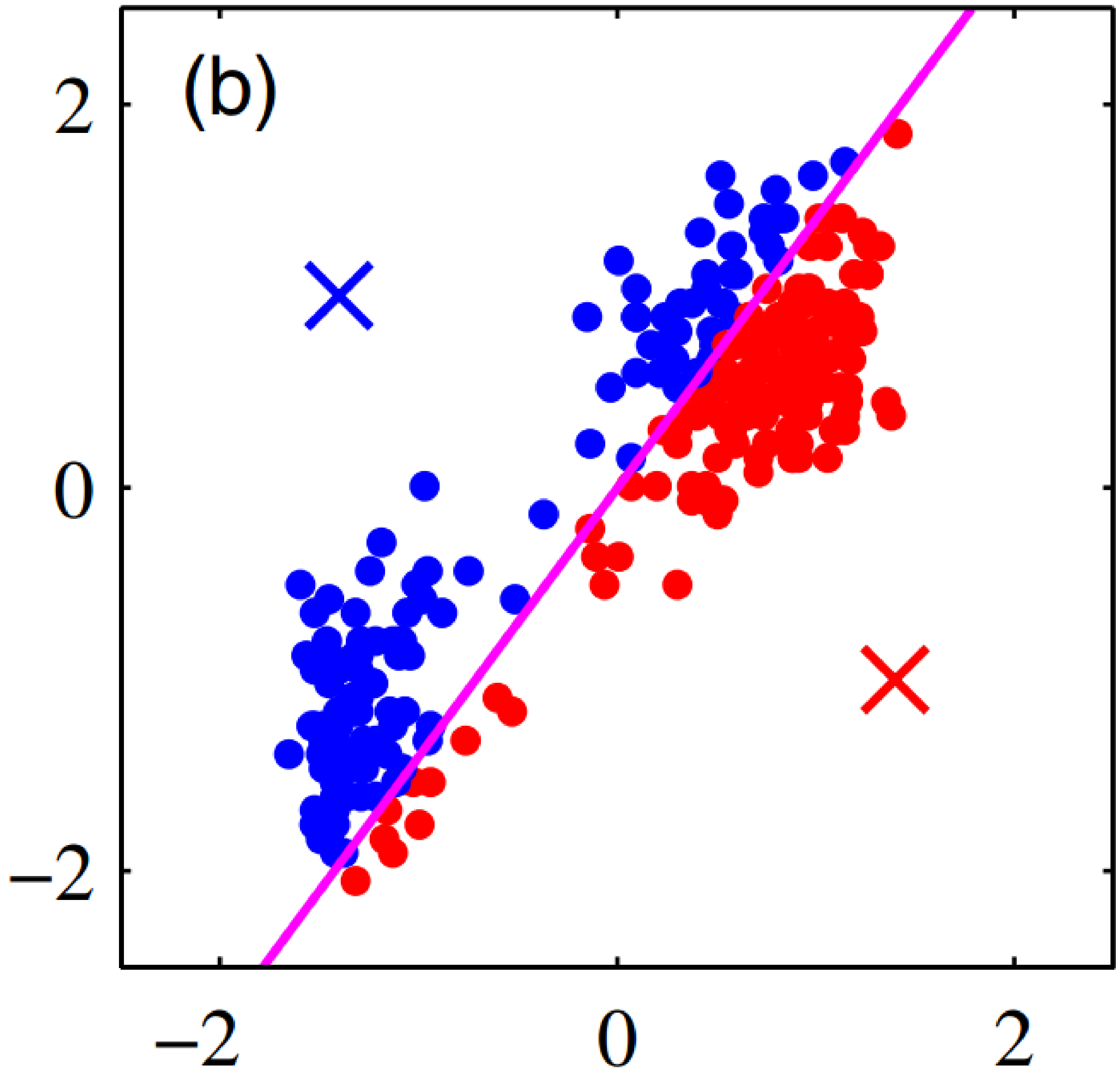
$$\mu_k = \frac{1}{\#\{j \mid z_j = k\}} \sum_{j=1}^{N} x_j \mathbb{I}(z_j = k)$$

K-Means Clustering: Initialization

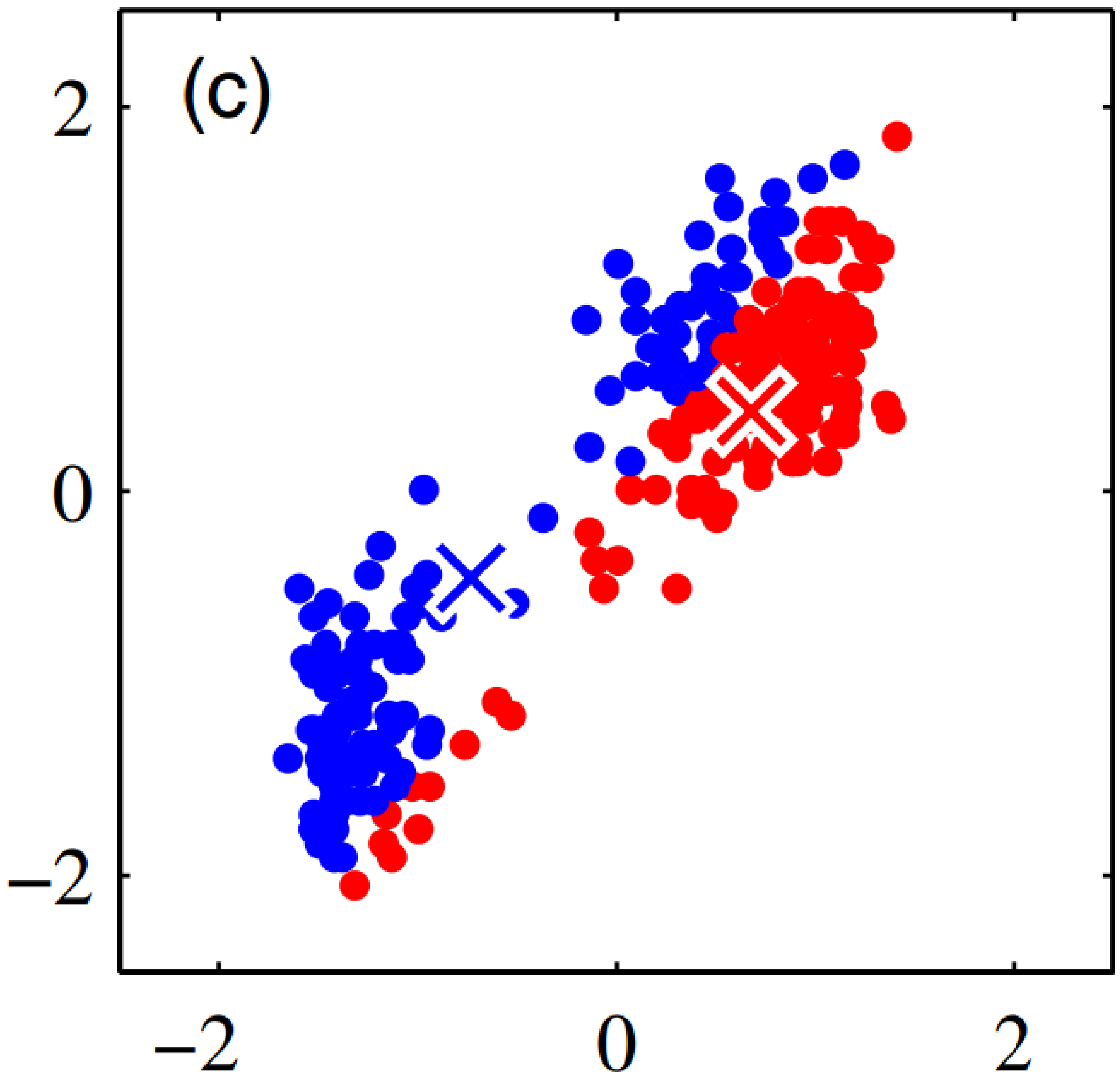
> Images taken from Bishop, **[PRML]**



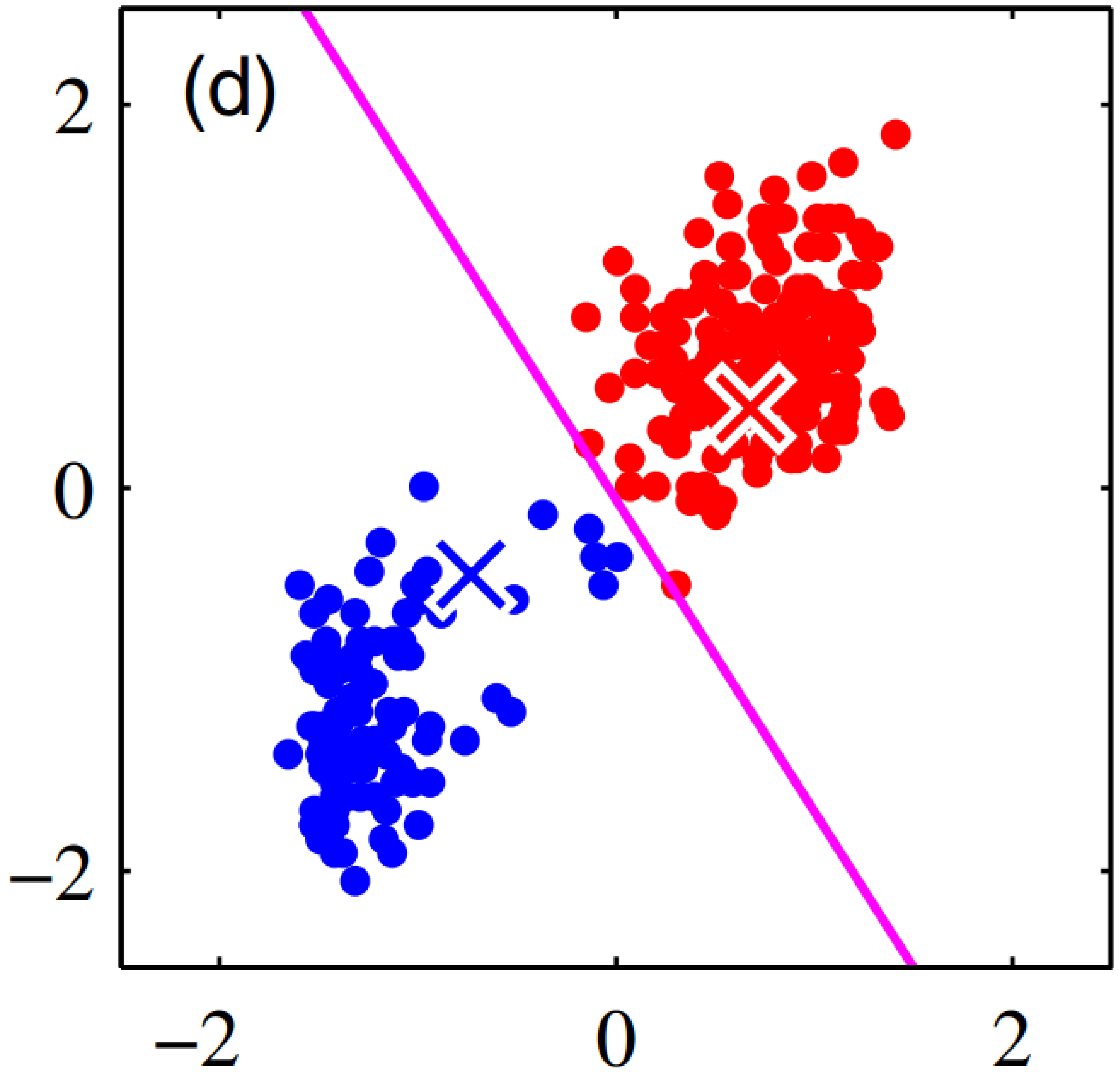
K-Means Clustering: E-Step



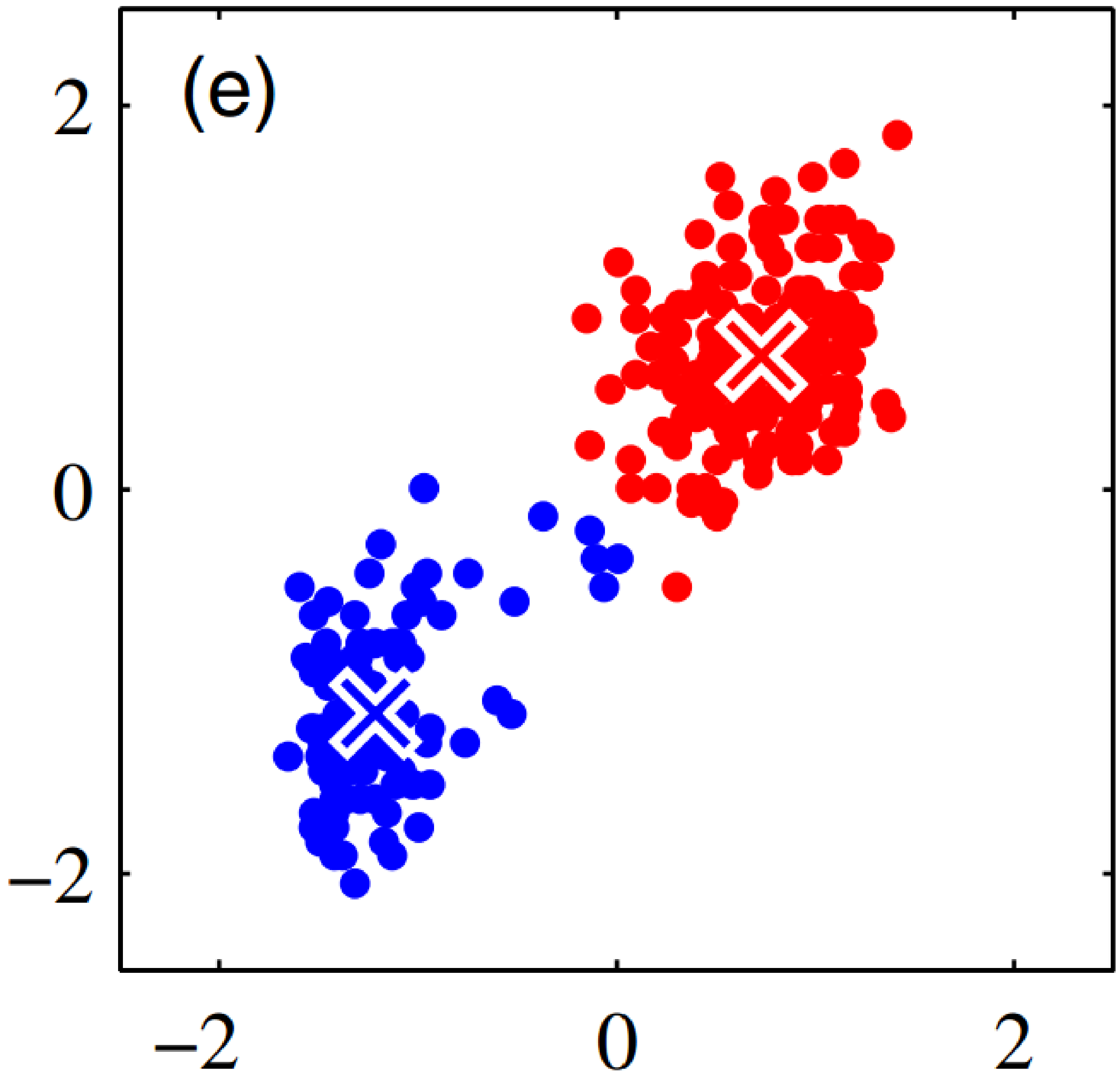
K-Means Clustering: M-Step



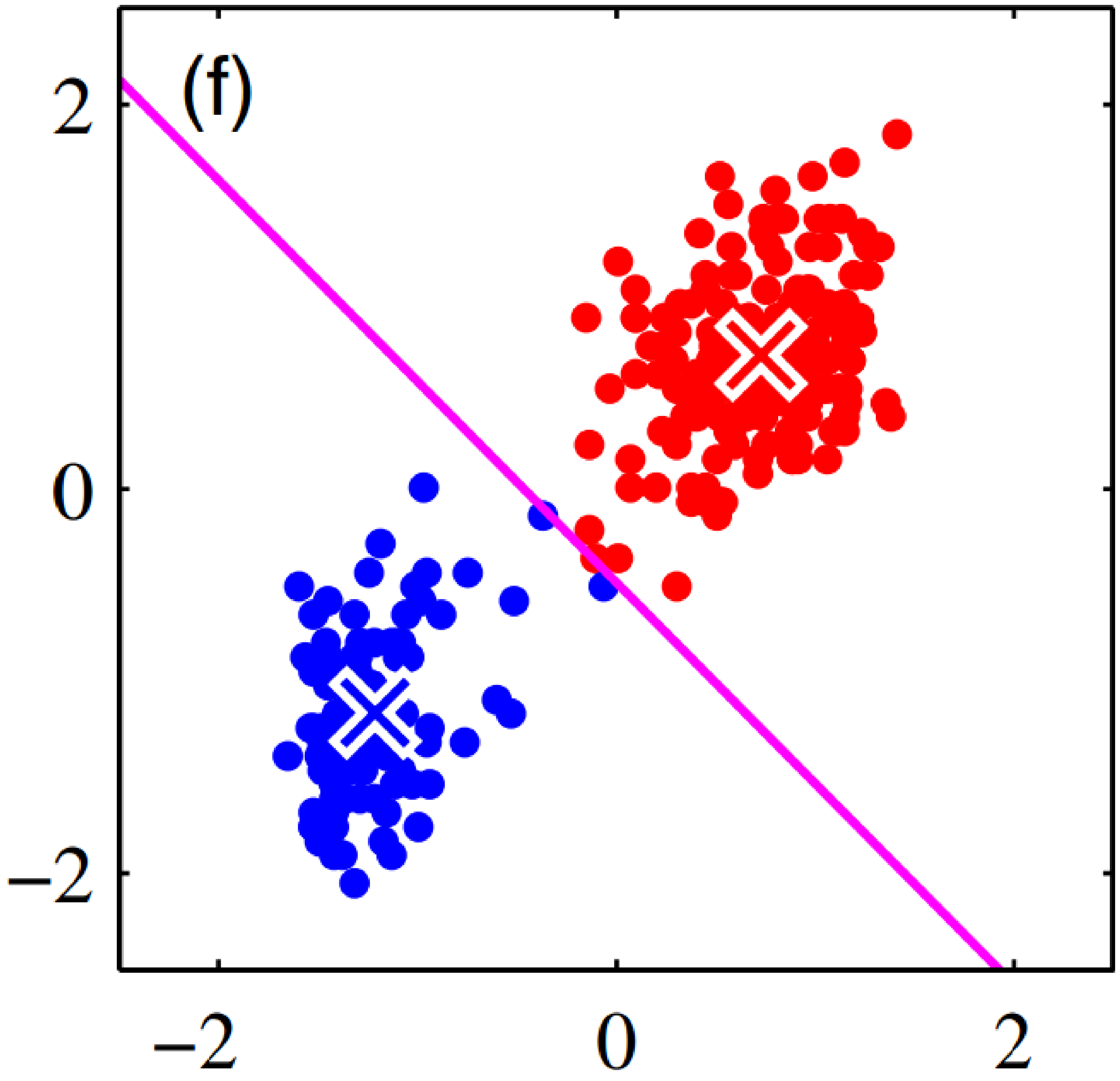
K-Means Clustering: E-Step



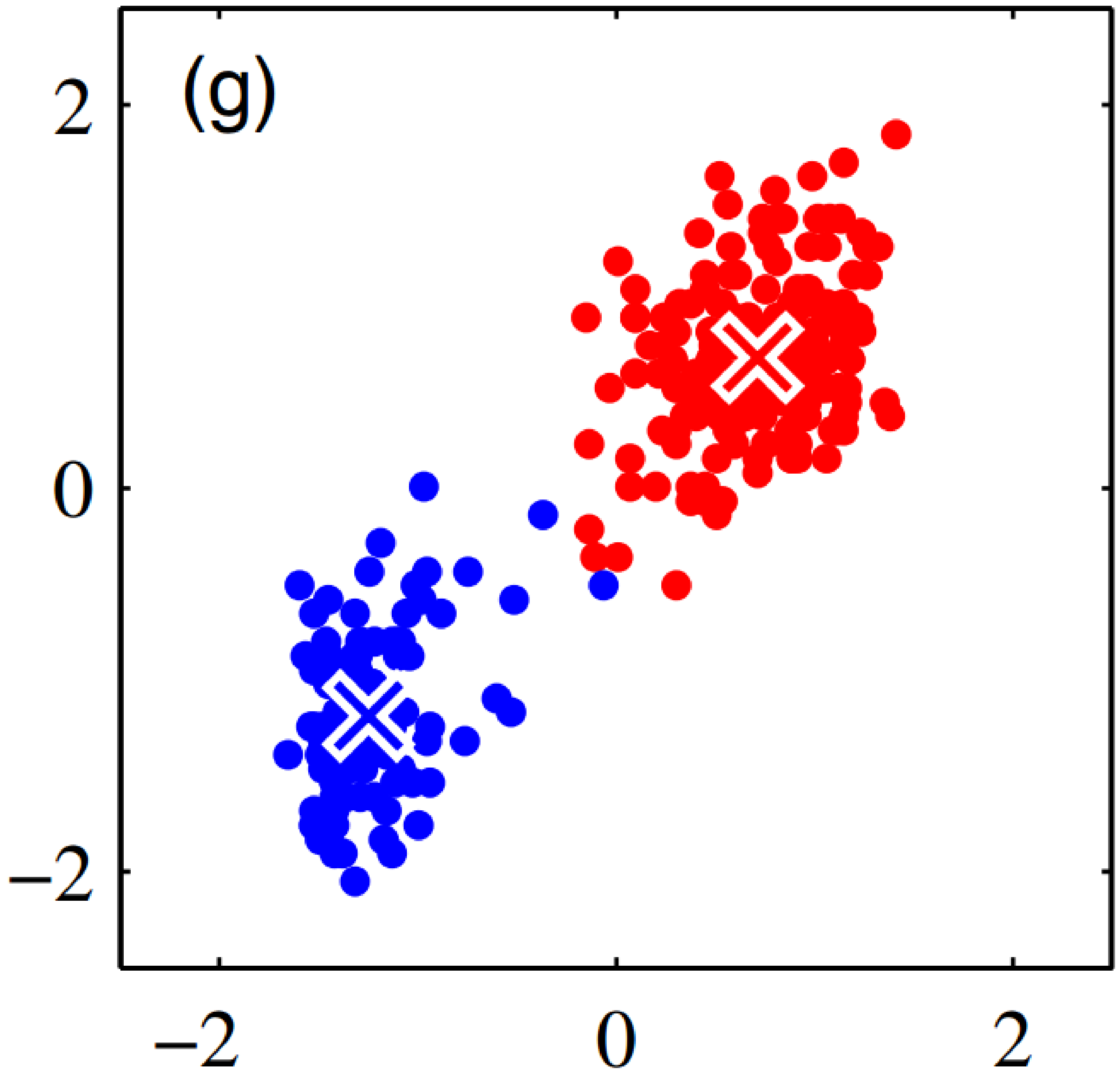
K-Means Clustering: M-Step



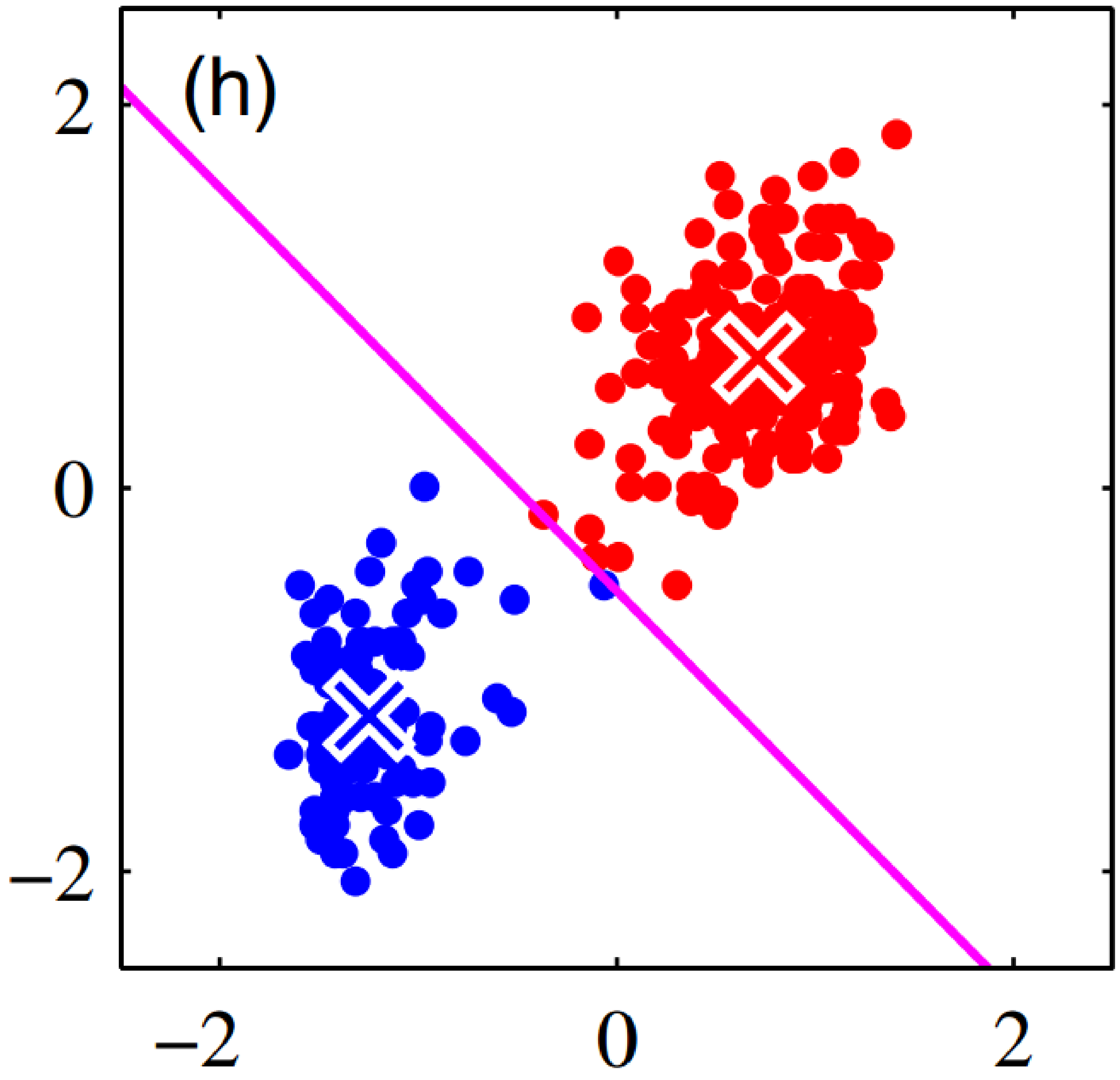
K-Means Clustering: E-Step



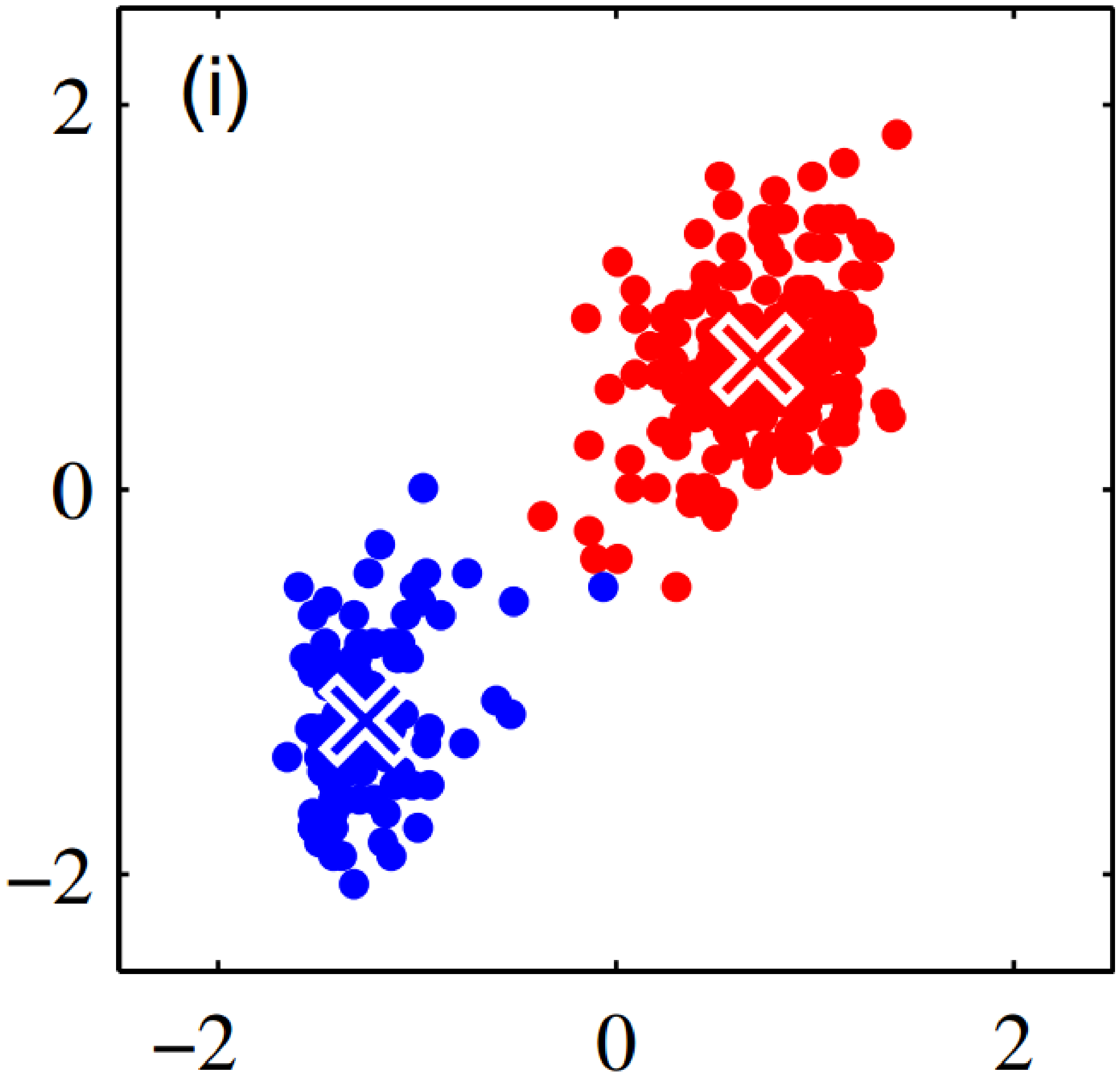
K-Means Clustering: M-Step



K-Means Clustering: E-Step



K-Means Clustering: M-Step



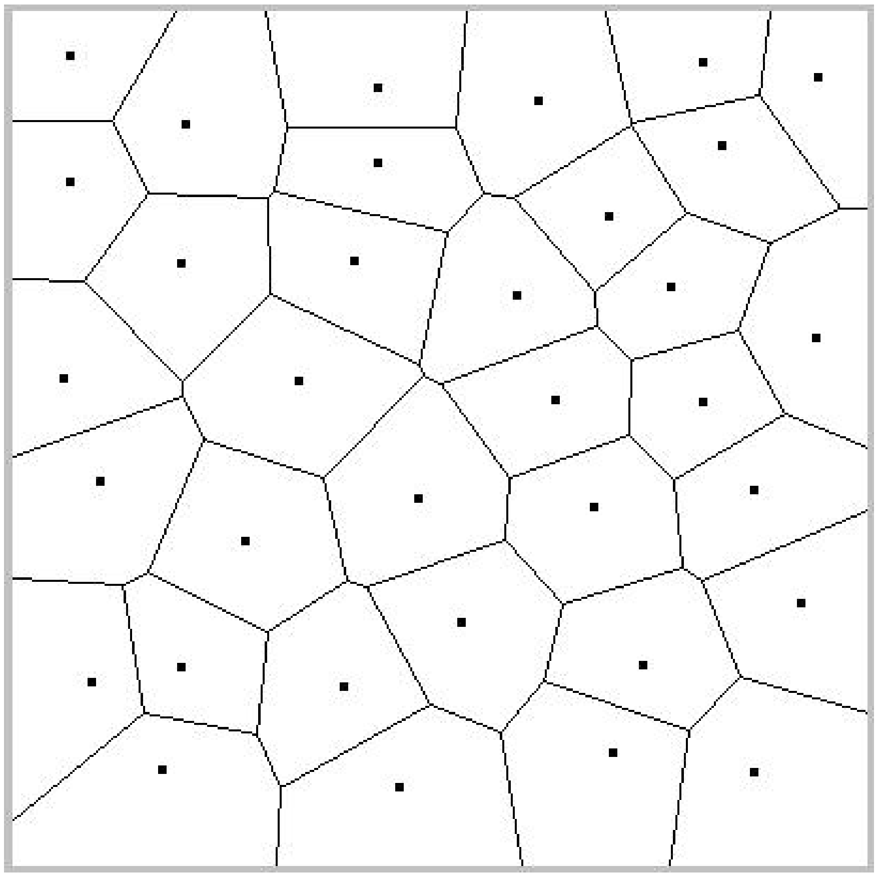
K-Means: Cluster Geometry

Clusters are convex *nearest-neighbor* regions or **Vornoi Cells**.

- Piecewise-linear boundaries

K-means will fail to identify non-convex clusters.

- However, **kernelized K-means** is possible!



K-Means Clustering: Analysis

Exercise: Show that the K-Means algorithm finds a local minimum of the **distortion measure**, given by

$$J(\mu_1, \ldots, \mu_k; z_1, \ldots, z_N) = \sum_{j=1}^{N} \sum_{k=1}^{K} \mathbb{I}(z_j = k) ||x_j - \mu_k||^2$$

K-Means: Variants

K-Means is simple and easy to extend:

- **K-Means++:** Intelligently pick initial cluster centers
- **K-Means--:** Handle outliers
- **Nonparametric K-Means:** Automatically select number of clusters
- **Kernelized K-Means:** Non-convex clusters

Next lecture, we will cover **probabilistic clustering** through the use of mixture models.

Variant: K-Means++ (http://ilpubs.stanford.edu:8090/778/1/2006-13.pdf)

Instead of initializing cluster centers randomly,

```
1. Choose the first cluster center to be a random datapoint.
2. Repeat until $K$ cluster centers have been selected:
    A. For each datapoint $x_j$, compute distance $D(x_j)$ to nearest cluster.
    B. Choose data point $x_j$ at random to be the new cluster center, with probability
       proportional to $D(x_j)^2$.
3. Run K-means as usual.
```

Variant: K-Means-- (http://pmg.it.usyd.edu.au/outliers.pdf)

Vanilla K-Means is sensitive to outliers. Instead, assume there are ℓ outliers, then

```
1. Choose initial cluster centers as usual.
2. For $k = 1, 2, \ldots$:
    A. For each datapoint $x_j$, compute distance $D(x_j)$ to nearest cluster.
    B. Set $L_k$ to be the $\ell$ datapoints farthest from any cluster.
    C. Perform the E and M steps as usual on $X \setminus L_k$.
3. Return most recent outlier estimate $L_k$ in addition to usual cluster data.
```

Variant: Nonparametric K-Means (http://www.cs.berkeley.edu/~jordan/papers/kulis-jordan-icml12.pdf)

Automatically add new clusters via a **maximum cluster radius** λ.

```
1. Init $K = 1$ and set $\mu_1$ to be the mean over datapoints.
2. Repeat until convergence:
    A. For each point $x_j$,
        a. Compute distance $D(x_j)$ to nearest cluster.
        b. If $D(x_j) > \lambda$, increment $K$ and create a new cluster centered at $x_j$.
        c. Otherwise, assign $x_j$ to a cluster as usual.
    B. Re-estimate cluster centers as usual.
```