Graphical Models

Exponential Families

Families of Distributions

- A Gaussian distribution vs. the set of all Gaussian distributions
- A multinomial distribution over K outcomes vs. the set of all multinomials over the same K outcomes
- A graphical model vs. the set of all graphical models with the same structure and CPD parameterization (but different parameters)

An Exponential Family

$$P_{\boldsymbol{\theta}}(\boldsymbol{x}) \quad = \quad \frac{1}{Z(\boldsymbol{\theta})} A(\boldsymbol{x}) \exp\left(\mathbf{t}(\boldsymbol{\theta})^{\top} \boldsymbol{\tau}(\boldsymbol{x})\right)$$

sufficient statistics function from Val(**X**) to $\mathbb{R}^K$

An Exponential Family

$$P_{\boldsymbol{\theta}}(\boldsymbol{x}) \quad = \quad \frac{1}{Z(\boldsymbol{\theta})} A(\boldsymbol{x}) \exp\left(\mathbf{t}(\boldsymbol{\theta})^{\top} \boldsymbol{\tau}(\boldsymbol{x})\right)$$

parameters in convex set $\Theta \subseteq \mathbb{R}^M$

An Exponential Family

$$P_{\boldsymbol{\theta}}(\boldsymbol{x}) \quad = \quad \frac{1}{Z(\boldsymbol{\theta})} A(\boldsymbol{x}) \exp\left(\mathbf{t}(\boldsymbol{\theta})^{\top} \boldsymbol{\tau}(\boldsymbol{x})\right)$$

natural parameter function from $\mathbb{R}^M$ to $\mathbb{R}^K$

parameters in convex set $\Theta \subseteq \mathbb{R}^M$

An Exponential Family

$$P_{\boldsymbol{\theta}}(\boldsymbol{x}) \quad = \quad \frac{1}{Z(\boldsymbol{\theta})} A(\boldsymbol{x}) \exp\left(\mathbf{t}(\boldsymbol{\theta})^{\top} \boldsymbol{\tau}(\boldsymbol{x})\right)$$

finite partition function

auxiliary measure

An Exponential Family

$$
\begin{aligned}
P_{\boldsymbol{\theta}}(\boldsymbol{x}) &= \frac{1}{Z(\boldsymbol{\theta})} A(\boldsymbol{x}) \exp\left(\mathbf{t}(\boldsymbol{\theta})^{\top} \boldsymbol{\tau}(\boldsymbol{x})\right) \\
Z(\boldsymbol{\theta}) &= \sum_{\boldsymbol{x} \in \mathrm{Val}(\boldsymbol{X})} A(\boldsymbol{x}) \exp\left(\mathbf{t}(\boldsymbol{\theta})^{\top} \boldsymbol{\tau}(\boldsymbol{x})\right)
\end{aligned}
$$

An Exponential Family

$$
\begin{aligned}
P_{\boldsymbol{\theta}}(\boldsymbol{x}) &= \frac{1}{Z(\boldsymbol{\theta})} A(\boldsymbol{x}) \exp\left(\mathbf{t}(\boldsymbol{\theta})^\top \boldsymbol{\tau}(\boldsymbol{x})\right) \\
Z(\boldsymbol{\theta}) &= \sum_{\boldsymbol{x} \in \mathrm{Val}(\boldsymbol{X})} A(\boldsymbol{x}) \exp\left(\mathbf{t}(\boldsymbol{\theta})^\top \boldsymbol{\tau}(\boldsymbol{x})\right) \\
\mathcal{P} &= \{P_{\boldsymbol{\theta}} \mid \boldsymbol{\theta} \in \boldsymbol{\Theta}\}
\end{aligned}
$$

parametric family

Example: Bernoulli

$$
\begin{aligned}
P_{\boldsymbol{\theta}}(\boldsymbol{x}) &= \frac{1}{Z(\boldsymbol{\theta})} A(\boldsymbol{x}) \exp\left(\mathbf{t}(\boldsymbol{\theta})^\top \boldsymbol{\tau}(\boldsymbol{x})\right) \\
Z(\boldsymbol{\theta}) &= \sum_{\boldsymbol{x} \in \mathrm{Val}(\boldsymbol{X})} A(\boldsymbol{x}) \exp\left(\mathbf{t}(\boldsymbol{\theta})^\top \boldsymbol{\tau}(\boldsymbol{x})\right) \\
\mathcal{P} &= \{P_{\boldsymbol{\theta}} \mid \boldsymbol{\theta} \in \boldsymbol{\Theta}\}
\end{aligned}
$$

- $\boldsymbol{\Theta} = [0, 1]$
- $\boldsymbol{\tau}(x) = \langle x == \text{heads}, x == \text{tails} \rangle$
- $\mathbf{t}(\theta) = \langle \ln \theta, \ln(1 - \theta) \rangle$
  - (note: image not convex!)
- $\exp(\mathbf{t}(\theta)^\top \boldsymbol{\tau}(x)) =$ either θ or $1-\theta$
- $Z(\theta) = 1$

Example: Gaussian

$$
\begin{aligned}
P_{\boldsymbol{\theta}}(\boldsymbol{x}) &= \frac{1}{Z(\boldsymbol{\theta})} A(\boldsymbol{x}) \exp\left(\mathbf{t}(\boldsymbol{\theta})^{\top} \boldsymbol{\tau}(\boldsymbol{x})\right) \\
Z(\boldsymbol{\theta}) &= \sum_{\boldsymbol{x} \in \mathrm{Val}(\boldsymbol{X})} A(\boldsymbol{x}) \exp\left(\mathbf{t}(\boldsymbol{\theta})^{\top} \boldsymbol{\tau}(\boldsymbol{x})\right) \\
\mathcal{P} &= \{P_{\boldsymbol{\theta}} \mid \boldsymbol{\theta} \in \boldsymbol{\Theta}\}
\end{aligned}
$$

- $\boldsymbol{\Theta} = \langle \mathbb{R}, \mathbb{R}^{+} \rangle$
- $\boldsymbol{\tau}(x) = \langle x, x^2 \rangle$
- $\mathbf{t}(\mu, \sigma^2) = \langle \mu / \sigma^2, -1 / 2\sigma^2 \rangle$

Many Others!

- Poisson, exponential, geometric, Gamma, …
- Sometimes more than one family can encode the same class of distributions.
  - Want $\boldsymbol{\Theta}$ to be convex and open
  - Want $P_{\boldsymbol{\theta}} = P_{\boldsymbol{\theta}'}$ to imply that $\boldsymbol{\theta} = \boldsymbol{\theta}'$ (nonredundant)
    - Equivalently, $\mathbf{t}$ is invertible over $\boldsymbol{\Theta}$.
- Counter examples?

When **t** is the Identity Function

- "Natural parameters" for the sufficient statistic function **τ**
- Should be familiar: **linear exponential family**

$$P_{\boldsymbol{\theta}}(\boldsymbol{x}) = \frac{1}{Z(\boldsymbol{\theta})} \exp\left(\boldsymbol{\theta}^\top \boldsymbol{\tau}(\boldsymbol{x})\right)$$

$$Z(\boldsymbol{\theta}) = \sum_{\boldsymbol{x} \in \mathrm{Val}(\boldsymbol{X})} \exp\left(\boldsymbol{\theta}^\top \boldsymbol{\tau}(\boldsymbol{x})\right)$$

Example: Natural Parameters for $\langle x, x^2 \rangle$

- $\boldsymbol{\eta} = \langle \mu / \sigma^2, -1 / 2\sigma^2 \rangle$

$$
\begin{aligned}
P_{\boldsymbol{\theta}}(\boldsymbol{x}) &= \frac{1}{Z(\boldsymbol{\theta})} \exp\left(\boldsymbol{\theta}^\top \boldsymbol{\tau}(\boldsymbol{x})\right) \\
Z(\boldsymbol{\theta}) &= \sum_{\boldsymbol{x} \in \mathrm{Val}(\boldsymbol{X})} \exp\left(\boldsymbol{\theta}^\top \boldsymbol{\tau}(\boldsymbol{x})\right) \\
&= \int_{-\infty}^{\infty} \exp\left(\eta_1 x + \eta_2 x^2\right) \, dx
\end{aligned}
$$

Example: Natural Parameters for $\langle x, x^2 \rangle$

- $\boldsymbol{\eta} = \langle \mu / \sigma^2, -1 / 2\sigma^2 \rangle$
- Z is only finite when η_2 is negative!

$$
\begin{aligned}
P_{\boldsymbol{\theta}}(\boldsymbol{x}) &= \frac{1}{Z(\boldsymbol{\theta})} \exp\left(\boldsymbol{\theta}^\top \boldsymbol{\tau}(\boldsymbol{x})\right) \\
Z(\boldsymbol{\theta}) &= \sum_{\boldsymbol{x} \in \mathrm{Val}(\boldsymbol{X})} \exp\left(\boldsymbol{\theta}^\top \boldsymbol{\tau}(\boldsymbol{x})\right) \\
&= \int_{-\infty}^{\infty} \exp\left(\eta_1 x + \eta_2 x^2\right) \, dx
\end{aligned}
$$

Linear Exponential Families

- Basically boils down to the sufficient statistic function $\boldsymbol{\tau}$
  - Natural parameter space $\boldsymbol{\Theta}$ is whatever it needs to be to make Z finite

Natural Parameter Space for the Bernoulli

$$
\begin{aligned}
P_{\boldsymbol{\theta}}(\boldsymbol{x}) &= \frac{1}{Z(\boldsymbol{\theta})} A(\boldsymbol{x}) \exp\left(\mathbf{t}(\boldsymbol{\theta})^\top \boldsymbol{\tau}(\boldsymbol{x})\right) \\
Z(\boldsymbol{\theta}) &= \sum_{\boldsymbol{x} \in \mathrm{Val}(\boldsymbol{X})} A(\boldsymbol{x}) \exp\left(\mathbf{t}(\boldsymbol{\theta})^\top \boldsymbol{\tau}(\boldsymbol{x})\right) \\
\mathcal{P} &= \{P_{\boldsymbol{\theta}} \mid \boldsymbol{\theta} \in \boldsymbol{\Theta}\}
\end{aligned}
$$

- $\boldsymbol{\tau}(x) = \langle x == \text{heads}, x == \text{tails} \rangle$
- $\boldsymbol{\Theta} = \mathbb{R}^2$
- $Z(\boldsymbol{\theta}) = \exp(\theta_1) + \exp(\theta_2)$

- Problem: overparameterization (add $c\mathbf{1}$ to $\boldsymbol{\theta}$)

Natural Parameter Space for the Bernoulli

$$
\begin{aligned}
P_{\boldsymbol{\theta}}(\boldsymbol{x}) &= \frac{1}{Z(\boldsymbol{\theta})} A(\boldsymbol{x}) \exp\left(\mathbf{t}(\boldsymbol{\theta})^\top \boldsymbol{\tau}(\boldsymbol{x})\right) \\
Z(\boldsymbol{\theta}) &= \sum_{\boldsymbol{x} \in \mathrm{Val}(\boldsymbol{X})} A(\boldsymbol{x}) \exp\left(\mathbf{t}(\boldsymbol{\theta})^\top \boldsymbol{\tau}(\boldsymbol{x})\right) \\
\mathcal{P} &= \{P_{\boldsymbol{\theta}} \mid \boldsymbol{\theta} \in \boldsymbol{\Theta}\}
\end{aligned}
$$

- **τ**(x) = ⟨x == heads~~, x == tails~~⟩
- **Θ** = $\mathbb{R}$
- Z(θ) = 1 + exp(θ)

Natural Parameter Space for the Multinomial

$$
\begin{aligned}
P_{\boldsymbol{\theta}}(\boldsymbol{x}) &= \frac{1}{Z(\boldsymbol{\theta})} A(\boldsymbol{x}) \exp\left(\mathbf{t}(\boldsymbol{\theta})^{\top} \boldsymbol{\tau}(\boldsymbol{x})\right) \\
Z(\boldsymbol{\theta}) &= \sum_{\boldsymbol{x} \in \mathrm{Val}(\boldsymbol{X})} A(\boldsymbol{x}) \exp\left(\mathbf{t}(\boldsymbol{\theta})^{\top} \boldsymbol{\tau}(\boldsymbol{x})\right) \\
\mathcal{P} &= \{P_{\boldsymbol{\theta}} \mid \boldsymbol{\theta} \in \boldsymbol{\Theta}\}
\end{aligned}
$$

- $\boldsymbol{\tau}(x) = \langle x == x_2, x == x_3, \ldots, x == x_K \rangle$
- $\boldsymbol{\Theta} = \mathbb{R}^{K-1}$
- What is **t**?

Log-Linear Models

$$
\begin{aligned}
P_{\boldsymbol{\theta}}(\boldsymbol{x}) &= \frac{1}{Z(\boldsymbol{\theta})} A(\boldsymbol{x}) \exp\left(\mathbf{t}(\boldsymbol{\theta})^{\top} \boldsymbol{\tau}(\boldsymbol{x})\right) \\
Z(\boldsymbol{\theta}) &= \sum_{\boldsymbol{x} \in \mathrm{Val}(\boldsymbol{X})} A(\boldsymbol{x}) \exp\left(\mathbf{t}(\boldsymbol{\theta})^{\top} \boldsymbol{\tau}(\boldsymbol{x})\right) \\
\mathcal{P} &= \{P_{\boldsymbol{\theta}} \mid \boldsymbol{\theta} \in \boldsymbol{\Theta}\}
\end{aligned}
$$

- $\tau(\mathbf{x}) = \langle f_1(\mathbf{d}_1), \ldots, f_K(\mathbf{d}_K) \rangle$
- By extension, discrete Markov networks are exponential families.

Putting together exponential families …

Products

- It's easy to show that a product of exponential factor families' *unnormalized* probabilities gives … another exponential family.
- Same thing for linear exponential factor families!
- Markov net as a Gibbs distribution

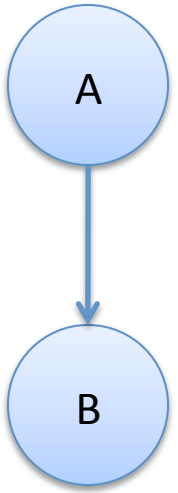
$$1/Z(\theta) \prod_{c \in cliques} \psi(c) = 1/Z(\theta) \prod_{c \in cliques} \exp(\eta^T f(c)) = 1/Z(\theta) \exp(\eta^T \sum_{c \in cliques} f(c))$$

Bayesian Networks

- A Bayesian network with exponential CPDs is an exponential family.
  - Multinomials
  - Linear Gaussians
- However: local normalization is important here!

Bayesian Network as an Exponential Family

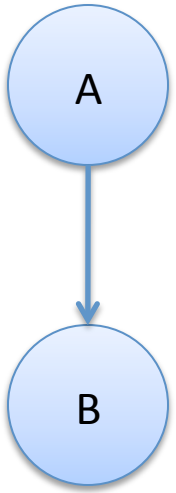
- $\mathbf{t}_{P(A)} = \langle \ln P(A = 0), \ln P(A = 1) \rangle$
- $\mathbf{t}_{P(B \mid A)} = \langle \ln P(B = 0 \mid A = 0),$
  $\ln P(B = 1 \mid A = 0),$
  $\ln P(B = 0 \mid A = 1),$
  $\ln P(B = 1 \mid A = 1) \rangle$



- 6 parameters, but only 3 degrees of freedom.

Bayesian Network as an Exponential Family

- $\mathbf{t}_{P(A)} = \langle \ln P(A = 1) / \ln P(A = 0) \rangle$
- $\mathbf{t}_{P(B \mid A)} = \langle \ln P(B = 1 \mid A = 0) / \ln P(B = 0 \mid A = 0),$
  $\ln P(B = 1 \mid A = 1) / \ln P(B = 0 \mid A = 1) \rangle$
- Consider $P_{\boldsymbol{\theta}}(A = 1, B = 1)$ and $P_{\boldsymbol{\theta}}(A = 0, B = 0)$ … what is $Z(\boldsymbol{\theta})$?

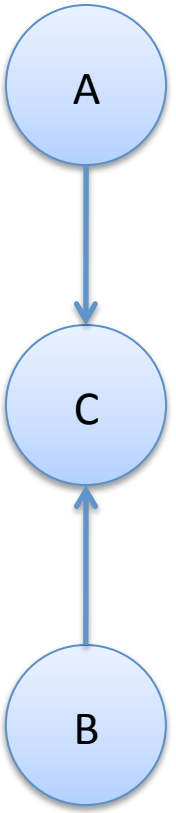


Understanding the Failure

- The global normalizer $Z(\boldsymbol{\theta})$ cannot do the work of local normalization within each conditional probability distribution.
- Need to make sure each CPD is normalized.

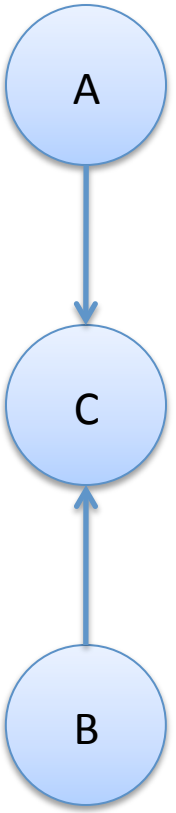
Another Example

- Allowing for general CPDs, need the sufficient statistics to modify any of these without modifying the others:
  - P(A = 0, B = 0, C = 0)
  - P(A = 0, B = 1, C = 0)
  - P(A = 1, B = 0, C = 0)
  - P(A = 1, B = 1, C = 0)



Another Example

- The τ coordinates for these four outcomes must be linearly independent.
  - Without loss of generality, use indicator functions for those four outcomes for $\boldsymbol{\tau}$.
- Resulting linear family is a Markov network over the clique {A, B, C}.
- Marginal independence between A and B may not hold!



Are Bayesian Networks *Linear* Exponential Families?

- Not in general; any network with immoralities does not induce a *linear* exponential family.

Some Consequences of Using an Exponential Family

- Entropy
- KL Divergence
- Projections

Entropy

- Number of bits or nats needed on average to encode an outcome.

$$H(P(\boldsymbol{X})) \quad = \quad - \sum_{\boldsymbol{x} \in \mathrm{Val}(\boldsymbol{X})} P(\boldsymbol{X} = \boldsymbol{x}) \ln P(\boldsymbol{X} = \boldsymbol{x})$$

- For an exponential family:

$$H(P_{\boldsymbol{\theta}}(\boldsymbol{X})) \quad = \quad \ln Z(\boldsymbol{\theta}) - \mathbf{t}(\boldsymbol{\theta})^{\top} \mathbb{E}_{P_{\boldsymbol{\theta}}}[\boldsymbol{\tau}(\boldsymbol{X})]$$

Entropy of a Markov Network

$$H(P(\boldsymbol{X})) \quad = \quad \ln Z + \sum_k \mathbb{E}_P[-\log_2 \phi_k(\boldsymbol{D}_k)]$$

- (Are these quantities easy to compute?)

Entropy of a Bayesian Network

$$H(P(\boldsymbol{X})) \quad = \quad \sum_i H(P(X_i \mid \text{Parents}(X_i))$$

- (Are these quantities easy to compute?)

Entropy of a Bayesian Network

$$H(P(\boldsymbol{X})) \leq \sum_i \max_{\boldsymbol{u} \in \mathrm{Val}(\mathrm{Parents}(X_i))} H(P(X_i \mid \mathrm{Parents}(X_i) = \boldsymbol{u})$$

$$H(P(\boldsymbol{X})) \geq \sum_i \min_{\boldsymbol{u} \in \mathrm{Val}(\mathrm{Parents}(X_i))} H(P(X_i \mid \mathrm{Parents}(X_i) = \boldsymbol{u})$$

- Bounds.

KL Divergence (Relative Entropy)

$$D(P\|Q) \quad = \quad \sum_{\boldsymbol{x}\in \mathrm{Val}(\boldsymbol{X})} P(\boldsymbol{X}=\boldsymbol{x}) \log \frac{P(\boldsymbol{X}=\boldsymbol{x})}{Q(\boldsymbol{X}=\boldsymbol{x})}$$

- A measurement of "distance" between two distributions.
  - Not symmetric.
- For exponential family P and any Q:

$$D(Q\|P_{\boldsymbol{\theta}}) \quad = \quad -H(Q(\boldsymbol{X})) - \mathbf{t}(\boldsymbol{\theta})^{\top}\mathbb{E}_Q[\boldsymbol{\tau}(\boldsymbol{X})] + \ln Z(\boldsymbol{\theta})$$

KL Divergence

- Two distributions in the same exponential family:

$$D(P_{\boldsymbol{\theta}_1} \| P_{\boldsymbol{\theta}_2}) = (\mathbf{t}(\boldsymbol{\theta}_1) - \mathbf{t}(\boldsymbol{\theta}_2))^\top \mathbb{E}_{P_{\boldsymbol{\theta}_1}}[\boldsymbol{\tau}(\boldsymbol{X})] - \ln \frac{Z(\boldsymbol{\theta}_1)}{Z(\boldsymbol{\theta}_2)}$$

Projections

- Given a distribution P and an exponential family $\mathcal{Q}$, find the distribution from $\mathcal{Q}$ that is closest to P.
  - I-projection (information projection):

$$\arg\min_{Q \in \mathcal{Q}} D(Q \| P)$$

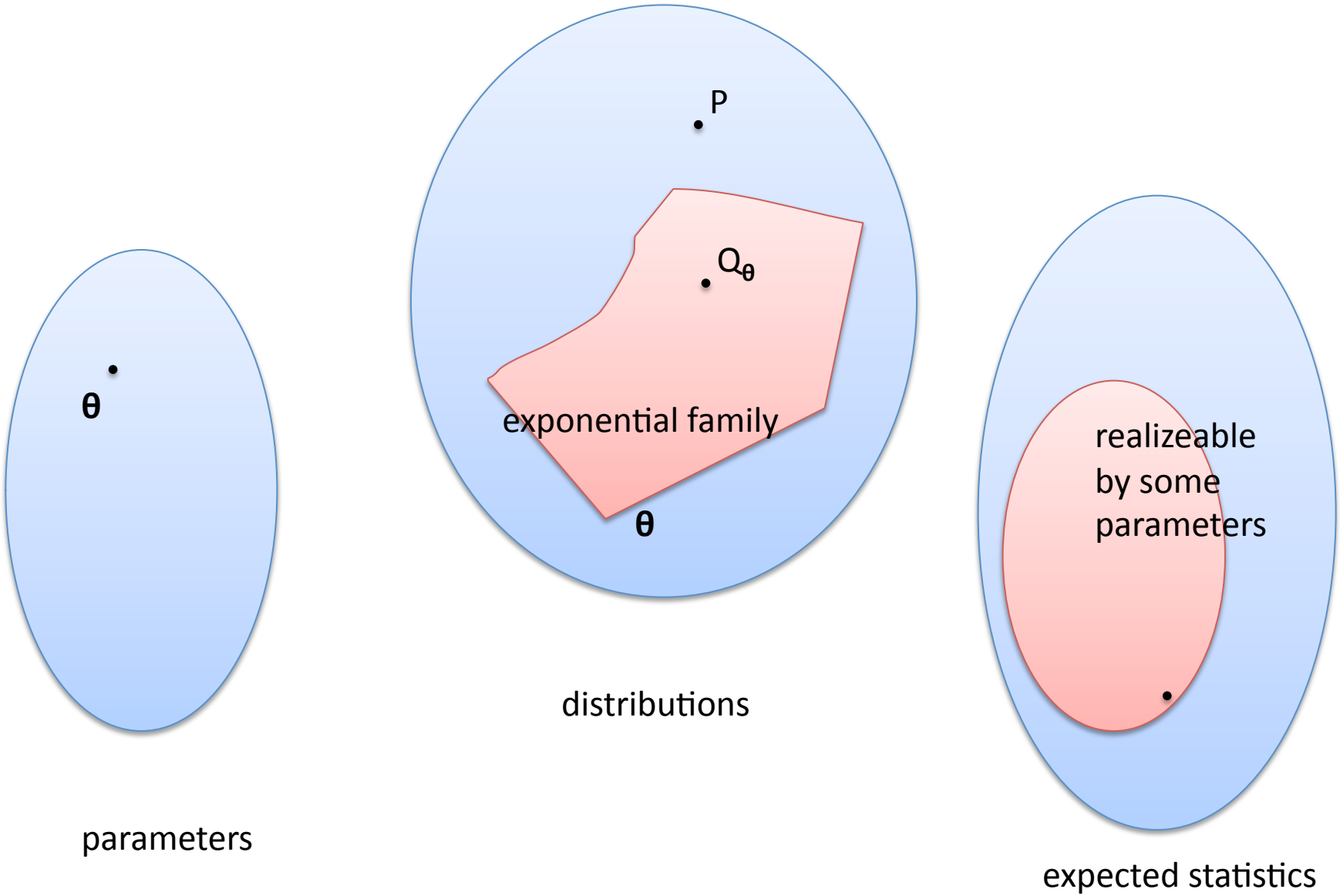
  - M-projection (moment projection):

$$\arg\min_{Q \in \mathcal{Q}} D(P \| Q)$$

M-Projection

- Example: let $\mathcal{Q}$ be the graph with no edges.
  - M-projection is the product of marginals from P.

- General result: if there is a $\boldsymbol{\theta}$ such that the expected sufficient statistics $\boldsymbol{E}_{Q_\theta}[\tau(\mathbf{X})]$ match $\boldsymbol{E}_P[\tau(\mathbf{X})]$, then $Q_{\boldsymbol{\theta}}$ is the M-projection of P.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parameters
P
Q_θ
exponential family
θ
distributions
realizeable
by some
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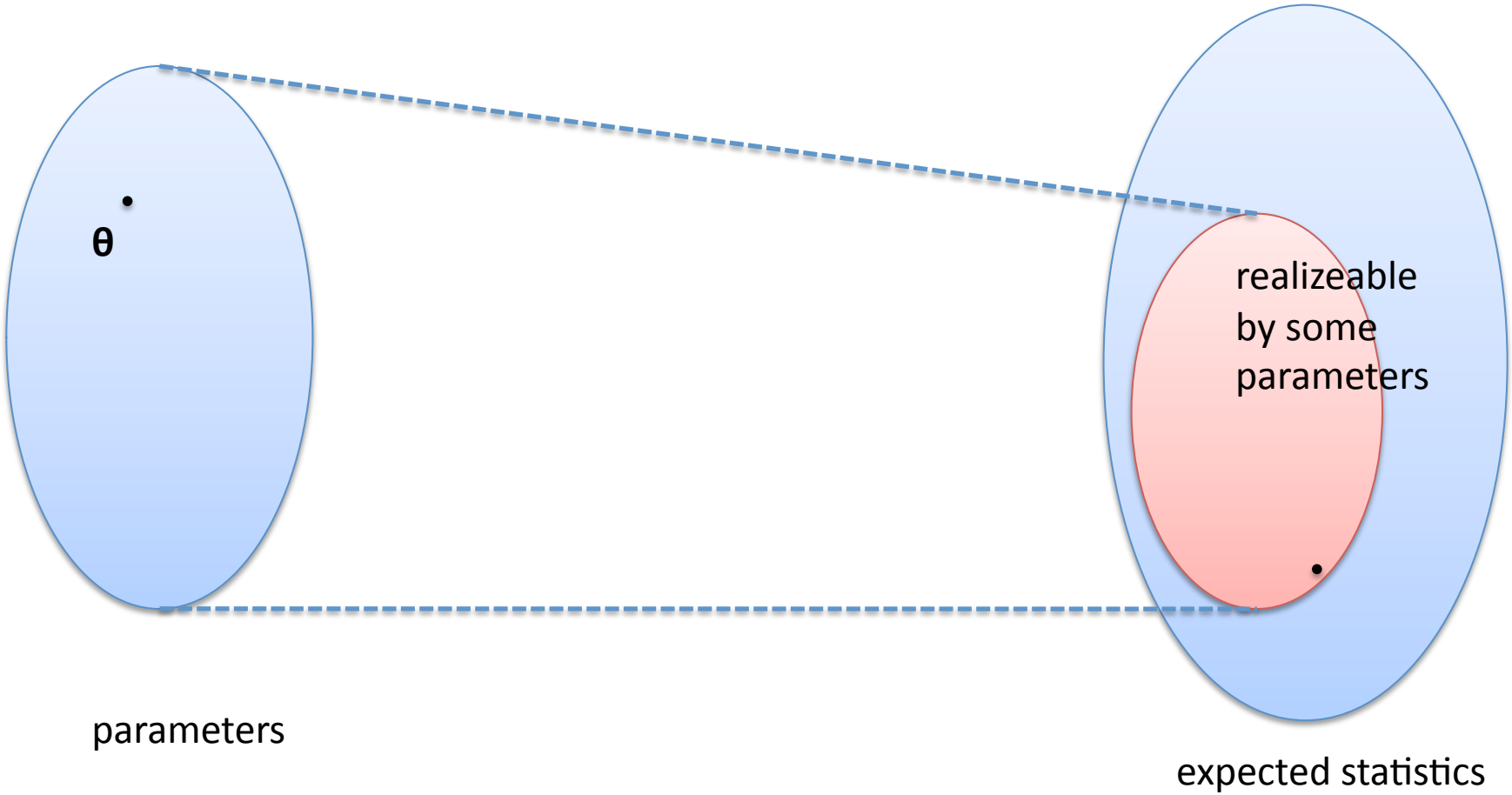
expected statistics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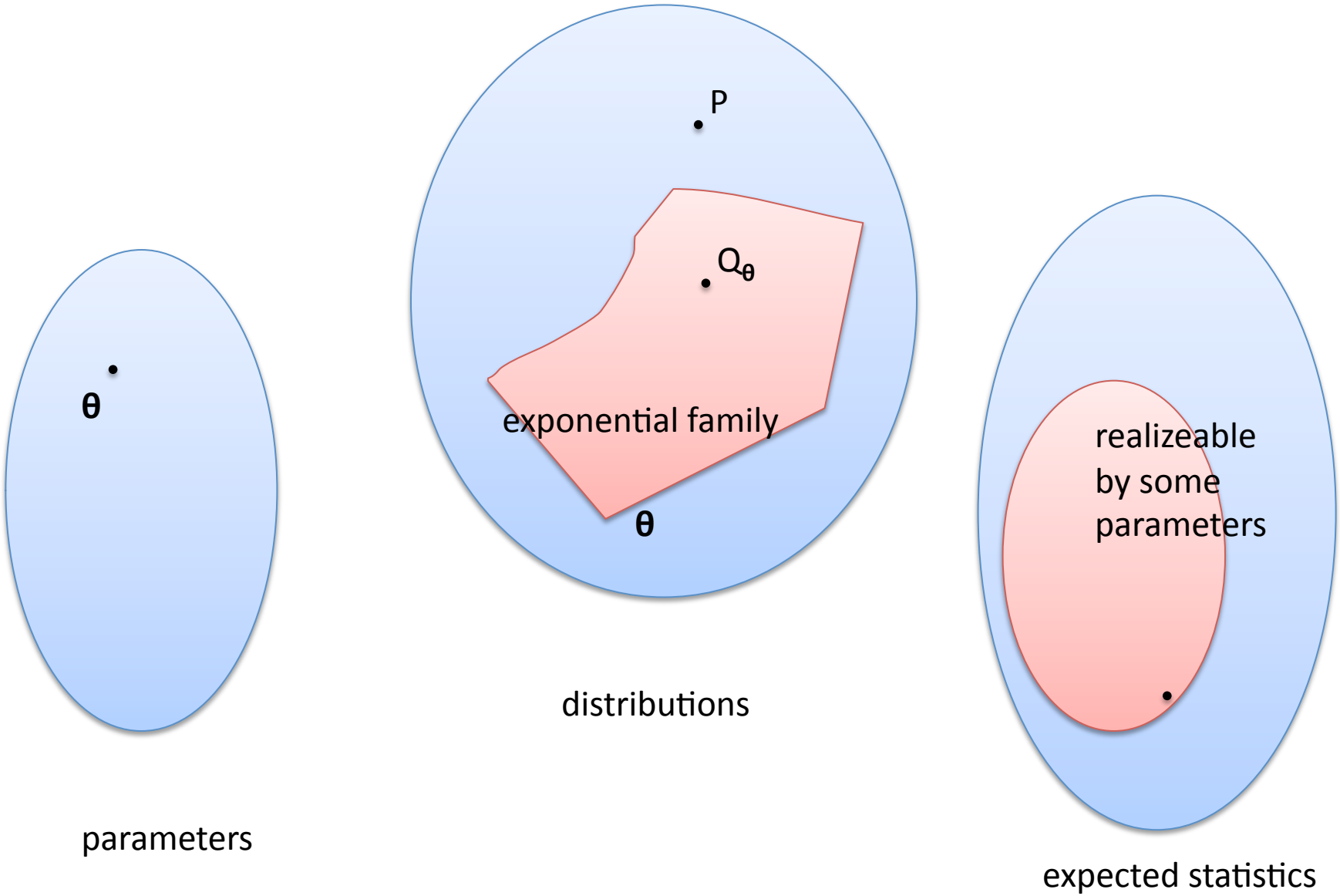
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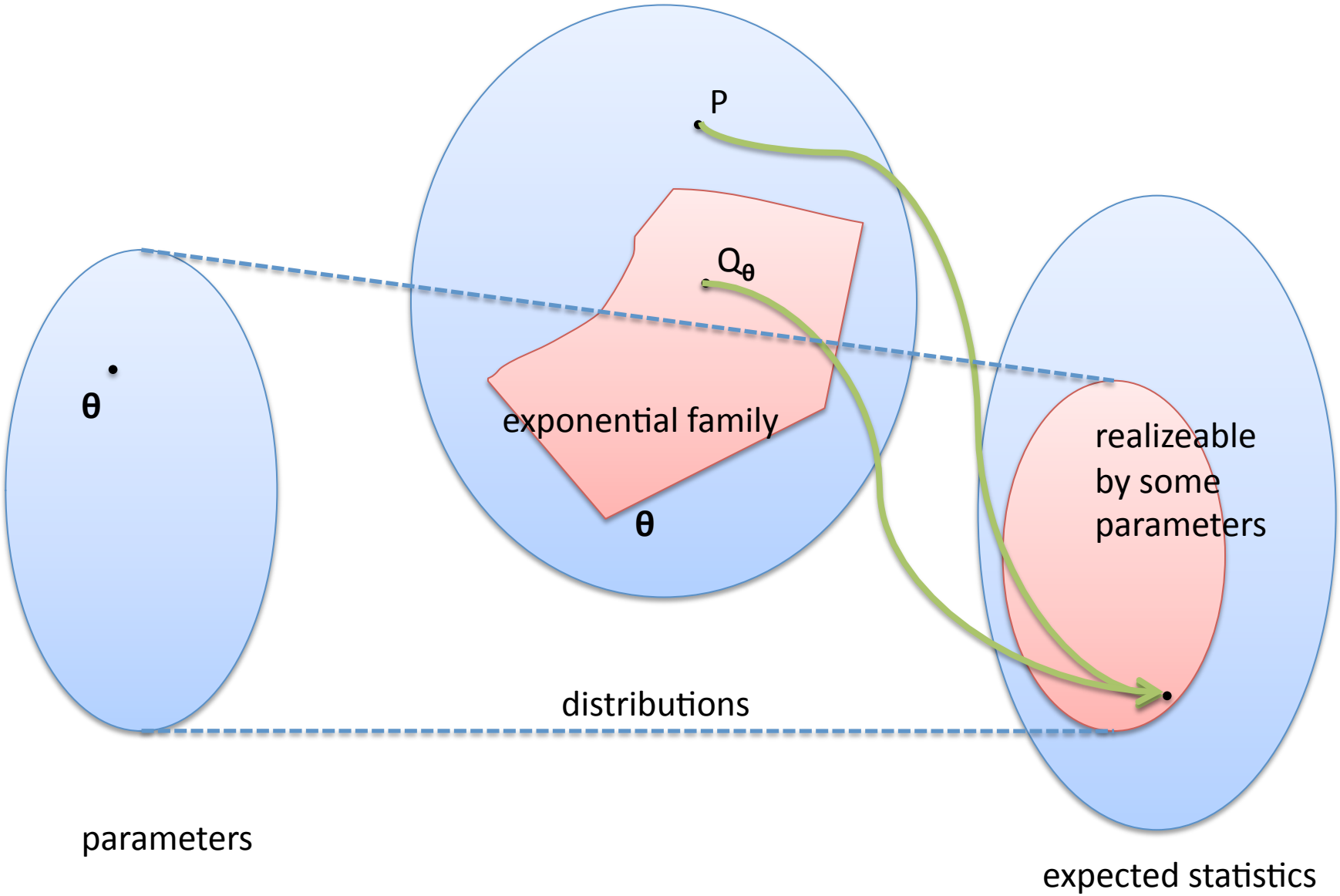
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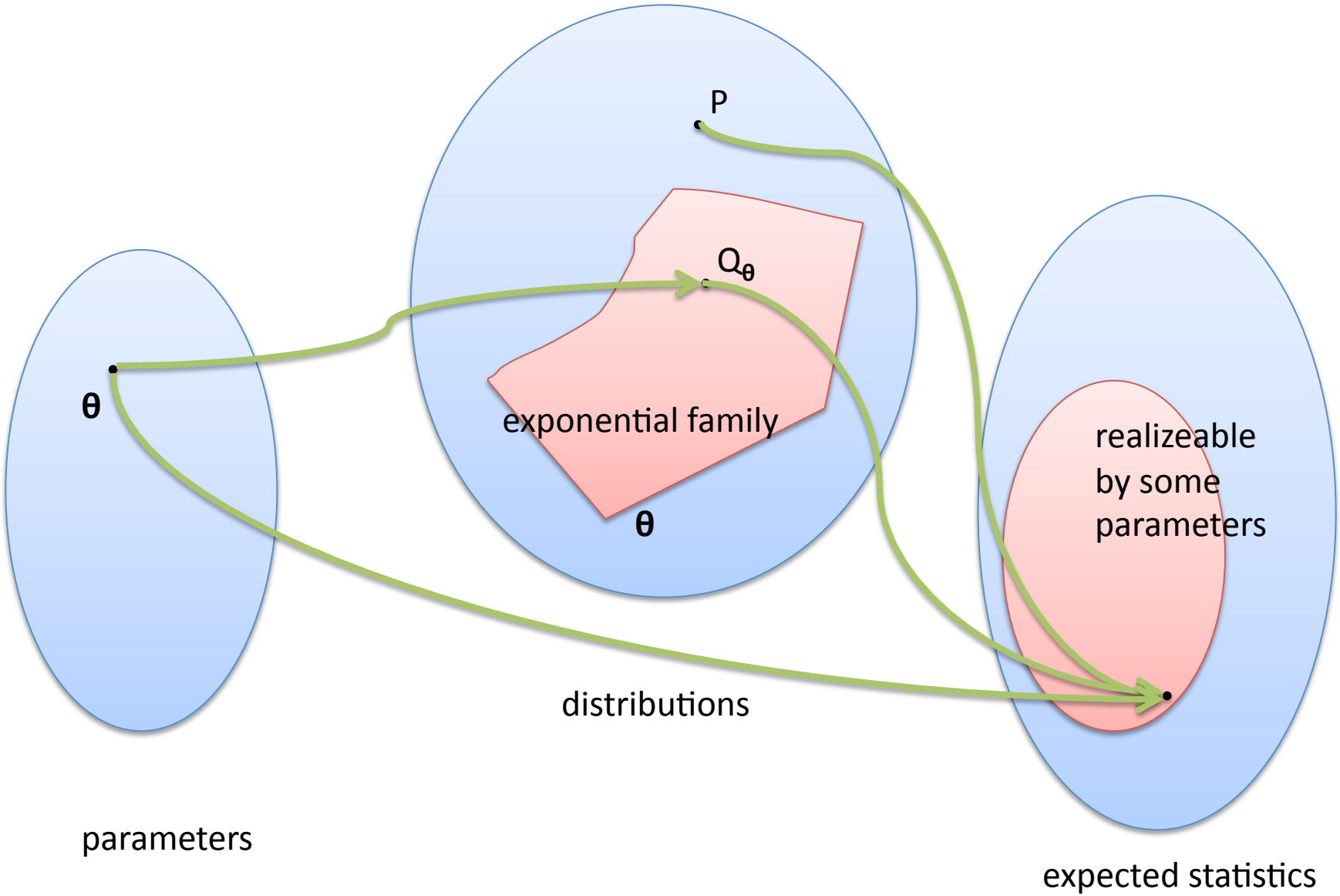
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expected statistics

Projections

- I-Projection is a bit harder:

$$D(Q_{\boldsymbol{\theta}} \| P) \quad = \quad -H(Q_{\boldsymbol{\theta}}(\boldsymbol{X})) - \mathbb{E}_{Q_{\boldsymbol{\theta}}}[\ln P(\boldsymbol{X})]$$

- The exponential form of Q isn't very helpful about the second term. If P has some structure, this could help.

Why Projections?

- M-projection is a foundation for learning.
- I-projection is used when answering difficult probabilistic queries.

- Note: I am not yet talking about algorithms for solving either!

What You Now Know

- What is an exponential family?
- What is a linear exponential family?
- How these relate to Bayesian and Markov networks.
- Information theoretic quantities.