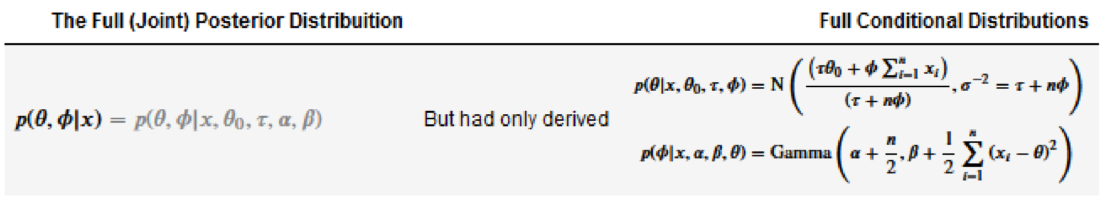
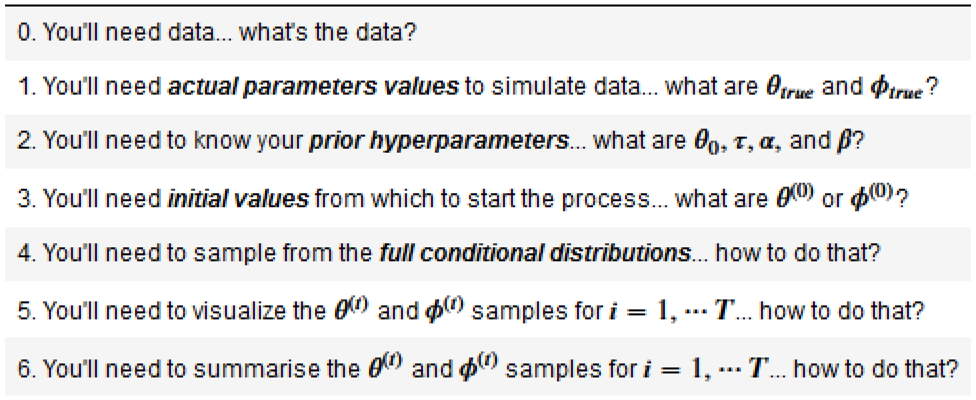
Class Activity 3 [25 minutes]: normal-gamma toy model

Last we left out intrepid heros, we desired samples from



The Full (Joint) Posterior Distribuition		Full Conditional Distributions
$p(\theta, \phi \mid x) = p(\theta, \phi \mid x, \theta_0, \tau, \alpha, \beta)$	But had only derived	$p(\theta \mid x, \theta_0, \tau, \phi) = \text{N}\left(\frac{\left(\tau\theta_0 + \phi \sum_{i=1}^n x_i\right)}{(\tau + n\phi)}, \sigma^{-2} = \tau + n\phi\right)$ $p(\phi \mid x, \alpha, \beta, \theta) = \text{Gamma}\left(\alpha + \frac{n}{2}, \beta + \frac{1}{2}\sum_{i=1}^n (x_i - \theta)^2\right)$

Alternatingly sample, back and fourth, between the two full conditionals, conditioning the sample draw for the current parameter on the last drawn value of the other parameter. . .

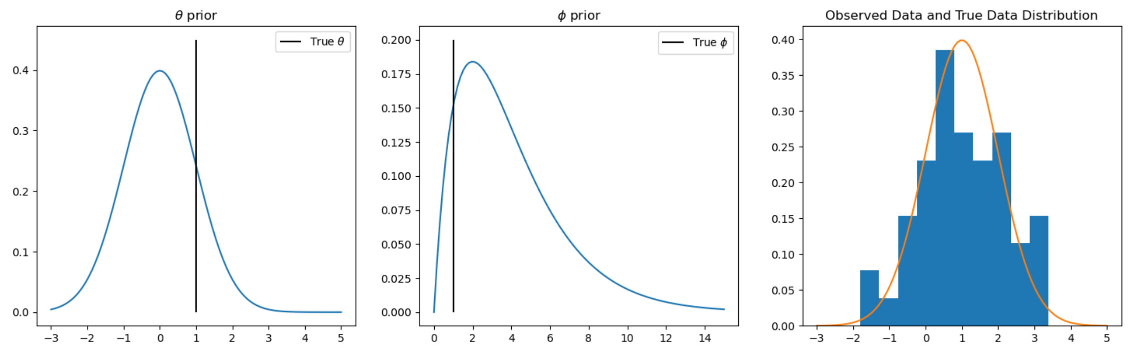


0. You'll need data... what's the data?
1. You'll need ***actual parameters values*** to simulate data... what are θ_{true} and ϕ_{true}?
2. You'll need to know your ***prior hyperparameters***... what are θ_0, τ, α, and β?
3. You'll need ***initial values*** from which to start the process... what are $\theta^{(0)}$ or $\phi^{(0)}$?
4. You'll need to sample from the ***full conditional distributions***... how to do that?
5. You'll need to visualize the $\theta^{(t)}$ and $\phi^{(t)}$ samples for $i = 1, \cdots T$... how to do that?
6. You'll need to summarise the $\theta^{(t)}$ and $\phi^{(t)}$ samples for $i = 1, \cdots T$... how to do that?

Class Activity 3: Solution [5 minutes]

[2]:
```python
import numpy as np; from scipy import stats; import matplotlib.pyplot as plt

theta_0,tau = 0,1; alpha,beta = 2,1/2 # Initialize Prior Hyperparameters: specify prior distributions
theta_prior = stats.norm(loc=theta_0, scale=tau) # https://en.wikipedia.org/wiki/Gamma_distribution
phi_prior = stats.gamma(a=alpha, scale=1/beta)   # Note: scale is 1/ beta (beta is rate parameter)

# In real world we probably wouldn't know for sure what distribution our data x is from:
# We wouldn't know the theta_true / phi_true, or even if the likelihood was normally distributed...
# and don't forget about the priors/hyperparameters above... these also require considerations...
theta_true,phi_true = 1,1; true_data_model = stats.norm(loc=theta_true,scale=phi_true)
n = 50; np.random.seed(seed=123); x = true_data_model.rvs(n);
```

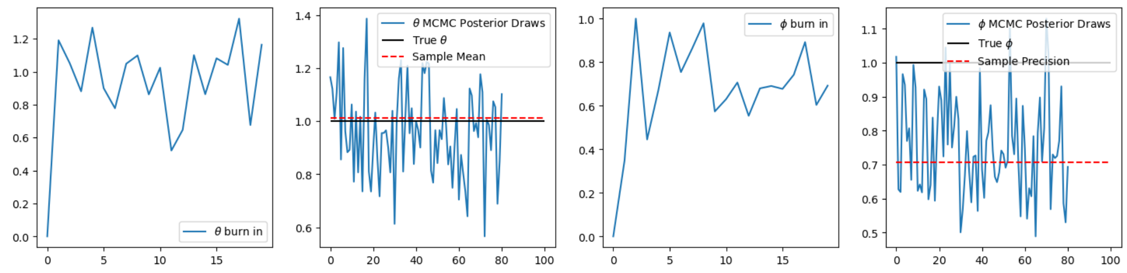
```
Rplus = np.linspace(0,15,100); Rpm = np.linspace(-3,5,100)
fig,ax = plt.subplots(1,3,figsize=(18,5)); ax[0].plot(Rpm, theta_prior.pdf(Rpm));
 ↪ ax[0].set_title('$\\theta$ prior'); ax[0].vlines(theta_true,0,.
 ↪45,'k',label='True $\\theta$'); ax[0].legend(); ax[1].plot(Rplus, phi_prior.
 ↪pdf(Rplus)); ax[1].vlines(phi_true,0,.2,'k',label='True $\\phi$'); ax[1].
 ↪legend(); ax[1].set_title('$\\phi$ prior'); ax[2].hist(x, density=True); ax[2].
 ↪plot(Rpm, true_data_model.pdf(Rpm)); ax[2].set_title('Observed Data and True␣
 ↪Data Distribution');
```



Class Activity 3: Solution [5 minutes]

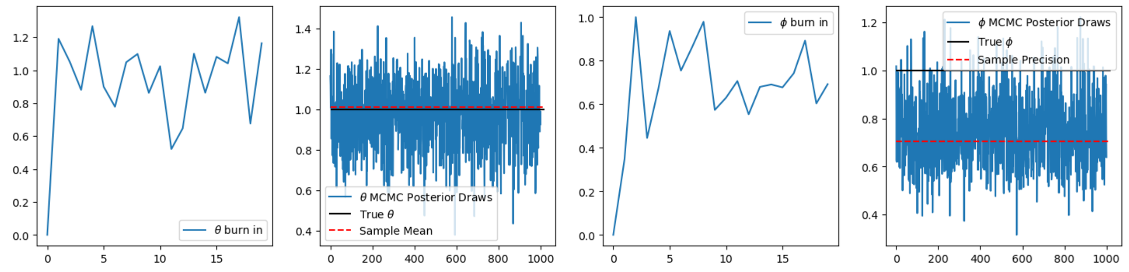
[5]:
```
# Solution from Leo Watson
iterations = 100 # Gibbs Samples
theta_gibbs_posterior_mcmc_draws,phi_gibbs_posterior_mcmc_draws = np.
 ↪zeros(iterations+1),np.zeros(iterations+1)
# initial_theta,initial_phi = 0,0 # Not really an initial phi as we'll do the␣
 ↪phi first per update
# Ideally we want our initial values near the "typical set" which along with␣
 ↪similar density values
# comprise the large majority of the probability of the distribution so the␣
 ↪convergence is faster
np.random.seed(123)
for i in range(1, iterations + 1):
    theta_old = theta_gibbs_posterior_mcmc_draws[i-1]

    phi_new = stats.gamma(a = alpha+n/2, scale = (1/(beta+1/2*((x-theta_old)**2).
 ↪sum()))).rvs()
    phi_gibbs_posterior_mcmc_draws[i] = phi_new

    theta_new = stats.norm(loc= (tau*theta_0+phi_new*sum(x))/(tau+n*phi_new),
                           scale= 1/np.sqrt(tau+n*phi_new)).rvs()
    theta_gibbs_posterior_mcmc_draws[i] = theta_new
```

```
burn = 20
fig,ax = plt.subplots(1,4, figsize=(18,4)); ax[0].
 ↪plot(theta_gibbs_posterior_mcmc_draws[:burn],label="$\\theta$ burn in"); ax[1].
 ↪plot(theta_gibbs_posterior_mcmc_draws[burn:],label="$\\theta$ MCMC Posterior␣
 ↪Draws"); ax[2].plot(phi_gibbs_posterior_mcmc_draws[:burn], label="$\\phi$ burn␣
 ↪in"); ax[3].plot(phi_gibbs_posterior_mcmc_draws[burn:], label="$\\phi$ MCMC␣
 ↪Posterior Draws"); ax[1].hlines(theta_true,0,iterations,'k',label='True␣
 ↪$\\theta$'); ax[3].hlines(phi_true,0,iterations,'k',label='True $\\phi$');␣
 ↪ax[1].hlines(x.mean(),0,iterations,'r',linestyle='dashed',label='Sample Mean');
 ↪ ax[1].legend(); ax[3].hlines(1/x.
 ↪var(),0,iterations,'r',linestyle='dashed',label='Sample Precision'); ax[3].
 ↪legend(); ax[0].legend(); ax[2].legend();
```



Class Activity 3: Solution [3 minutes]

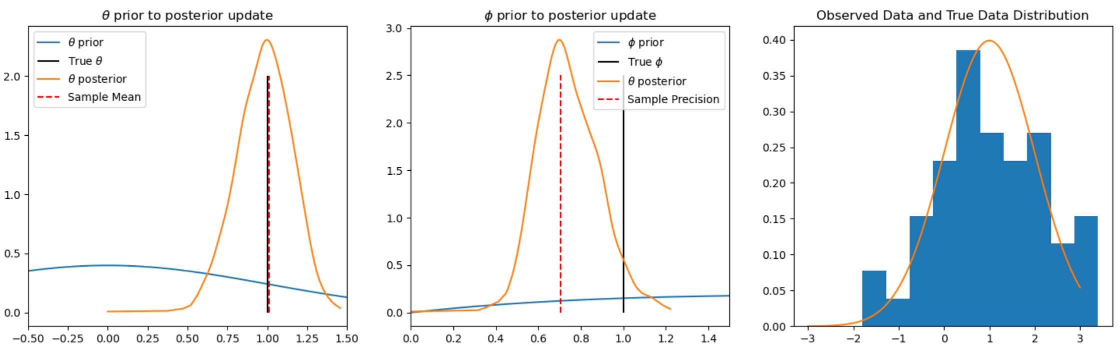
[6]:
```
# Solution from Leo Watson # DEPENDENCE GETS WASHED OUT AND PROBABLY STOPS␣
 ↪MATTERING IN THE LONG RUN
iterations = 1020 # Gibbs Samples
theta_gibbs_posterior_mcmc_draws,phi_gibbs_posterior_mcmc_draws = np.
 ↪zeros(iterations+1),np.zeros(iterations+1)
# initial_theta,initial_phi = 0,0 # Not really an initial phi as we'll do the␣
 ↪phi first per update
# Ideally we want our initial values near the "typical set" which along with␣
 ↪similar density values
# comprise the large majority of the probability of the distribution so the␣
 ↪convergence is faster
np.random.seed(123)
for i in range(1, iterations + 1):
    theta_old = theta_gibbs_posterior_mcmc_draws[i-1]

    phi_new = stats.gamma(a = alpha+n/2, scale = (1/(beta+1/
 ↪2*sum((x-theta_old)**2)))).rvs()
    phi_gibbs_posterior_mcmc_draws[i] = phi_new
    theta_new = stats.norm(loc= (tau*theta_0+phi_new*sum(x))/(tau+n*phi_new),
                           scale= 1/np.sqrt(tau+n*phi_new)).rvs()
    theta_gibbs_posterior_mcmc_draws[i] = theta_new

burn = 20
fig,ax = plt.subplots(1,4, figsize=(18,4)); ax[0].
 ↪plot(theta_gibbs_posterior_mcmc_draws[:burn],label="$\\theta$ burn in"); ax[1].
 ↪plot(theta_gibbs_posterior_mcmc_draws[burn:],label="$\\theta$ MCMC Posterior␣
 ↪Draws"); ax[2].plot(phi_gibbs_posterior_mcmc_draws[:burn], label="$\\phi$ burn␣
 ↪in"); ax[3].plot(phi_gibbs_posterior_mcmc_draws[burn:], label="$\\phi$ MCMC␣
 ↪Posterior Draws"); ax[1].hlines(theta_true,0,iterations,'k',label='True␣
 ↪$\\theta$'); ax[3].hlines(phi_true,0,iterations,'k',label='True $\\phi$');␣
 ↪ax[1].hlines(x.mean(),0,iterations,'r',linestyle='dashed',label='Sample Mean');
 ↪ ax[1].legend(); ax[3].hlines(1/x.
 ↪var(),0,iterations,'r',linestyle='dashed',label='Sample Precision'); ax[3].
 ↪legend(); ax[0].legend(); ax[2].legend();
```



Class Activity 3: Solution [4 minutes]

```
[8]: import numpy as np; from scipy import stats; import matplotlib.pyplot as plt
theta_0,tau = 0,1; alpha,beta = 2,1/2 # Initialize Prior Hyperparameters:␣
 ↪specify prior distributions
theta_prior = stats.norm(loc=theta_0, scale=tau) # https://en.wikipedia.org/wiki/
 ↪Gamma_distribution
phi_prior = stats.gamma(a=alpha, scale=1/beta)   # Note: scale is 1/ beta (beta␣
 ↪is rate parameter)
# In real world we probably wouldn't know for sure what distribution our data x␣
 ↪is from:
# We wouldn't know the theta_true / phi_true, or even if the likelihood was␣
 ↪normally distributed...
# and don't forget about the priors/hyperparameters above... these also require␣
 ↪considerations...
theta_true,phi_true = 1,1; true_data_model = stats.
 ↪norm(loc=theta_true,scale=phi_true)
n = 50; np.random.seed(seed=123); x = true_data_model.rvs(n);
```

```
Rplus = np.linspace(0,15,100); Rpm = np.linspace(-3,3,100)
fig,ax = plt.subplots(1,3,figsize=(18,5)); ax[0].plot(Rpm, theta_prior.pdf(Rpm),␣
 ↪label='$\\theta$ prior'); ax[0].set_title('$\\theta$ prior to posterior␣
 ↪update'); ax[0].vlines(theta_true,0,2,'k',label='True $\\theta$'); ax[1].
 ↪plot(Rplus, phi_prior.pdf(Rplus), label='$\\phi$ prior'); ax[1].
 ↪vlines(phi_true,0,2.5,'k',label='True $\\phi$'); ax[1].set_title('$\\phi$␣
 ↪prior to posterior update'); ax[2].hist(x, density=True); ax[2].plot(Rpm,␣
 ↪true_data_model.pdf(Rpm)); ax[2].set_title('Observed Data and True Data␣
 ↪Distribution');
from scipy.stats import gaussian_kde
theta_gibbs_posterior_mcmc_draws_sorted =␣
 ↪sorted(theta_gibbs_posterior_mcmc_draws);
ax[0].
 ↪plot(theta_gibbs_posterior_mcmc_draws_sorted,gaussian_kde(theta_gibbs_posterior_mcmc_draws_so
 ↪label='$\\theta$ posterior'); ax[0].vlines(x.
 ↪mean(),0,2,'r',linestyle='dashed',label='Sample Mean');
phi_gibbs_posterior_mcmc_draws_sorted = sorted(phi_gibbs_posterior_mcmc_draws);
ax[1].
 ↪plot(phi_gibbs_posterior_mcmc_draws_sorted,gaussian_kde(phi_gibbs_posterior_mcmc_draws_sorted
 ↪label='$\\theta$ posterior'); ax[1].vlines(1/x.var(),0,2.
 ↪5,'r',linestyle='dashed',label='Sample Precision'); ax[0].legend(); ax[1].
 ↪legend(); ax[0].set_xlim([-.5,1.5]); ax[1].set_xlim([0,1.5]);
```



Gibbs Sampling: History [8 minutes]

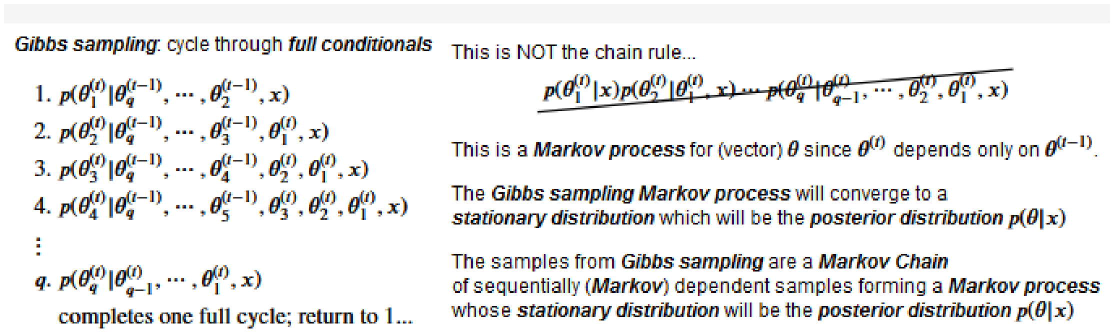
- There is a log-linear model known as the Boltzmann distribution… > The ***Boltzmann distribution*** is also called the ***Gibbs distribution*** after the statistical physicist whose research frequently utilized and explored it
- In 1984 the ***Geman brothers*** figured out an algorithm to sample from the Boltzmann distribution that had analogy to a statistical physics processes analyzed by Gibbs, *so they named their* ***sampler*** after ***Gibbs***…
- In 1990 [my first advisor from 2005-2007] Alan Gelfand introduced a generalized ***Gibbs sampling*** algorithm to the statistical community as a powerful tool for generalized ***Bayesian***

posterior analysis...

Gibbs sampling initially dominated Bayesian posterior analysis; but, the cyclical "one dimension at a time" nature of ***Gibbs sampling*** suffers from a prohibitive "curse of dimensionality" limiting its application to low dimentional parameter spaces. ***Hamiltonian Monte Carlo*** (***HMC***) generally avoids this for ***continuous*** distributions, so ***Gibbs sampling*** is now only used in ***discrete contexts*** (often in conjuction with ***Metropolis-Hastings***) where ***HMC*** can't be used.

Gibbs Sampling: Algorithm [10 minutes]

The Gibbs Sampler is a simple algorithm... cyclically sampling through *Full Conditional Distributions* produces samples from the corresponding *Full (Joint) Posterior Distribution*just as you've done above for the class activity...



Gibbs sampling: cycle through ***full conditionals***

1. $p(\theta_1^{(t)} | \theta_q^{(t-1)}, \cdots, \theta_2^{(t-1)}, x)$
2. $p(\theta_2^{(t)} | \theta_q^{(t-1)}, \cdots, \theta_3^{(t-1)}, \theta_1^{(t)}, x)$
3. $p(\theta_3^{(t)} | \theta_q^{(t-1)}, \cdots, \theta_4^{(t-1)}, \theta_2^{(t)}, \theta_1^{(t)}, x)$
4. $p(\theta_4^{(t)} | \theta_q^{(t-1)}, \cdots, \theta_5^{(t-1)}, \theta_3^{(t)}, \theta_2^{(t)}, \theta_1^{(t)}, x)$

$\vdots$

q. $p(\theta_q^{(t)} | \theta_{q-1}^{(t)}, \cdots, \theta_1^{(t)}, x)$

completes one full cycle; return to 1...

This is NOT the chain rule...

$$\cancel{p(\theta_1^{(t)}|x)p(\theta_2^{(t)}|\theta_1^{(t)}, x) \cdots p(\theta_q^{(t)}|\theta_{q-1}^{(t)}, \cdots, \theta_2^{(t)}, \theta_1^{(t)}, x)}$$

This is a ***Markov process*** for (vector) $\boldsymbol{\theta}$ since $\boldsymbol{\theta}^{(t)}$ depends only on $\boldsymbol{\theta}^{(t-1)}$.

The ***Gibbs sampling Markov process*** will converge to a ***stationary distribution*** which will be the ***posterior distribution*** $p(\boldsymbol{\theta}|\mathbf{x})$

The samples from ***Gibbs sampling*** are a ***Markov Chain*** of sequentially (***Markov***) dependent samples forming a ***Markov process*** whose ***stationary distribution*** will be the ***posterior distribution*** $p(\boldsymbol{\theta}|\mathbf{x})$

Markov Chain Monte Carlo (MCMC): Idea [4 minutes]

Bayesain posterior analysis is based on **Markov Chain Monte Carlo** - ***Markov Chain***: sequentially dependent samples (from a stationary/posterior distribution) - ***Monte Carlo (Integration)***: since **expectation** $\equiv$ **integration** so **integration** $\equiv$ **estimation**

This is because Bayesian posterior inference takes two forms:

- $\bar{x} = \frac{1}{T}\sum_{t=1}^{N} x_i \approx E[X] = \int xf(x)dx$

Markov Chain Monte Carlo (MCMC): Idea [6 minutes]

Bayesain posterior analysis is based on **Markov Chain Monte Carlo** - ***Markov Chain***: sequentially dependent samples (from a stationary/posterior distribution) - ***Monte Carlo (Integration)***: since **expectation** $\equiv$ **integration** so **integration** $\equiv$ **estimation**

This is because Bayesian posterior inference takes two forms:

- $E[\theta|x] = \int \theta p(\theta|x) d\theta \quad$ is estimated with $\quad \bar{\theta} = \frac{1}{T}\sum_{t=1}^{T} \theta^{(t)} \quad$ for $\quad \theta^{(t)} \sim p(\theta|x)$

  - Estimation is an "average" of possible parameter values "weighted" by their uncertainty which is encoded in our posterior belief about the parameters… "fairly" takes into account all possibilities
  - Whereas "best choice" MLE or $\theta^{\text{MAP}} = \max_\theta p(\theta|x)$ is sensitive to sample overfitting…
    MLE or θ^{MAP} just the best for the sample at hand but doesn't take into account uncertainty…

Markov Chain Monte Carlo (MCMC): Idea [2 minutes]

Bayesain posterior analysis is based on **Markov Chain Monte Carlo** - ***Markov Chain***: sequentially dependent samples (from a stationary/posterior distribution) - ***Monte Carlo (Integration)***: since **expectation** $\equiv$ **integration** so **integration** $\equiv$ **estimation**

This is because Bayesian posterior inference takes two forms:

- $\Pr(\theta \leq a) = \int_{-\infty}^{a} p(\theta|x)d\theta$ is estimated with $\hat{p}_{\theta \leq a} = \frac{1}{T}\sum_{t=1}^{T} 1_{[\infty,a]}(\theta^{(t)})$ for $\theta^{(t)} \sim p(\theta|x)$
  - Estimation is an "average" of possible parameter values "weighted" by their uncertainty which is encoded in our posterior belief about the parameters… "fairly" takes into account all possibilities
  - Whereas "best choice" MLE or $\theta^{\text{MAP}} = \max_\theta p(\theta|x)$ is sensitive to sample overfitting…it's just the best for the sample at hand but doesn't take into account uncertainty…

Markov Chain Monte Carlo (MCMC): Idea [6 minutes]

Bayesain posterior analysis is based on **Markov Chain Monte Carlo** - ***Markov Chain***: sequentially dependent samples (from a stationary/posterior distribution) - ***Monte Carlo (Integration)***: since **expectation** $\equiv$ **integration** so **integration** $\equiv$ **estimation**

This is because Bayesian posterior inference takes two forms:

- $\underset{\text{e.g., } \alpha = 0.05}{(1-\alpha)} \approx \int_a^b p(\theta|x)d\theta$ for $\underset{\text{where } \theta_{(k)} \text{ is the } k^{th} \text{ rank ordered posterior sample}}{a = \theta_{(\lfloor T\times\frac{\alpha}{2}\rfloor)} \text{ and } b = \theta_{(\lceil T\times(1-\frac{\alpha}{2})\rceil)}}$ and $\theta^{(t)} \sim p(\theta|x)$
  - Interval estimation is the range of possible parameter values we believe might be plausible based on our posterior uncertainty beliefs… given as the probability statement $\Pr_{\theta|x}(a \leq \theta \leq b) = 1 - \alpha$
  - This is a $100 \times (1-\alpha)\%$ ***Bayesian credible interval*** conveying posterior belief about parameter θ
    Bayesian posterior inference remains based upon ***integration*** rather than ***maximization***

Markov Chain Monte Carlo (MCMC): Idea [2 minutes]

Bayesain posterior analysis is based on **Markov Chain Monte Carlo** - ***Markov Chain***: sequentially dependent samples (from a stationary/posterior distribution) - ***Monte Carlo (Integration)***: since **expectation** $\equiv$ **integration** so **integration** $\equiv$ **estimation**

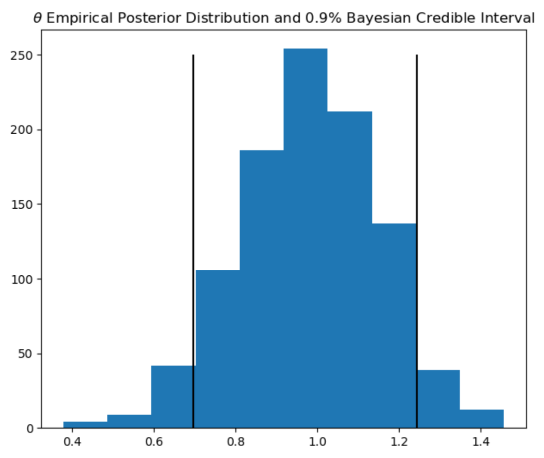
This is because Bayesian posterior inference takes two forms:

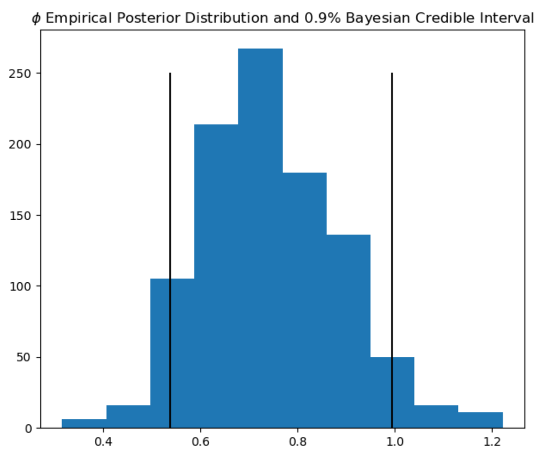
1. Estimating the ***posterior mean*** (expected value integration problem)via ***Markov Chain Monte Carlo Integration***
2. Solving the interval bounds of a (probability calculation) integration problemgiving a "plausible paramter range" probability statements via ***Markov Chain Monte Carlo Integration***

Gibbs sampling is not a ***chain rule*** decomposition of ***full (joint) posterior distributions*** $p(\theta|x)$ but nonetheless creates (sequentially [***Markov***] dependent) ***Markov chain*** samples from ***full (joint) posterior distribution*** $p(\theta|x)$.While sequentially dependent, they are still samples from $p(\theta|x)$ providing posterior MCMC integration inference

MCMC Bayesian Inference: Credible Intervals [10 minutes]

[39]:
```
# MCMC estimate posterior means / re-emphsize credible intervals from initial␣
↪problem
burn_in = 20; BayesianCredibleInterval_probability = 0.90
left_probability = (1-BayesianCredibleInterval_probability)/2
right_probability = left_probability + BayesianCredibleInterval_probability
fig,ax = plt.subplots(1,2,figsize=(16,6))
param=['$\\theta$','$\\phi$']
for i,posterior_samples in enumerate([theta_gibbs_posterior_mcmc_draws,␣
↪phi_gibbs_posterior_mcmc_draws]):
    BayesianCredibleInterval = np.quantile(posterior_samples[burn_in:
↪],[left_probability, right_probability])
    ax[i].hist(posterior_samples[20:]); ax[i].set_title(param[i]+" Empirical␣
↪Posterior Distribution and "+str(BayesianCredibleInterval_probability)+"%␣
↪Bayesian Credible Interval")
    ax[i].vlines(BayesianCredibleInterval,ymin=0,ymax=250,color ='k')
```





PyMC: Probabilistic Programming [10 minutes]

- ***Hamiltonian Monte Carlo*** (***HMC***) and ***Metropolis-Hastings*** (***M-H***)were mentioned when introducing ***Gibbs sampling***...
- Without yet knowing what these are, we can use them with PyMC

[38]:
```
theta_0,tau = 0,1; alpha,beta = 2,1/2 # Initialize Prior Hyperparameters:␣
↪specify prior distributions

import pymc as pm#; from scipy import stats; x = stats.norm().rvs(10)
normal_gamma_toy_model = pm.Model()
with normal_gamma_toy_model:
    theta = pm.Normal("theta", mu=0, sigma=1)
    phi = pm.Gamma("phi", alpha=1, beta=1)
    x_obs = pm.Normal("likelihood", mu=theta, sigma=1/phi**0.5, observed=x)
```

which specifies...

$$\begin{aligned} p(\theta,\phi|x) \propto p(\theta,\phi,x) &= \overset{N(\theta,\phi)}{p(x|\theta)}\ \overset{N(\theta_0,\tau)}{p(\theta)}\ \overset{\text{Gamma}(\alpha,\beta)}{p(\phi)} \qquad (\theta \perp\!\!\!\perp \phi) \leftarrow \text{priors} \\ &= \left[\prod_{i=1}^{n}\sqrt{\frac{\phi}{2\pi}}e^{-\frac{\phi(x_i-\theta)^2}{2}}\right]\sqrt{\frac{\tau}{2\pi}}e^{-\frac{\tau(\theta-\theta_0)^2}{2}}\frac{\beta^\alpha}{\Gamma(\alpha)}\phi^{\alpha-1}e^{-\beta\phi} \end{aligned}$$

PyMC: Posterior Sampling [5 minutes]

- ***Hamiltonian Monte Carlo*** (***HMC***) and ***Metropolis-Hastings*** (***M-H***) with PyMC
  - ***Gibbs sampling*** is not even an option for ***continuous variables*** in PyMC...

```
[61]: with normal_gamma_toy_model:
          idata_HMC = pm.sample() # default is the NUTS implementation of HMC
```

```
Auto-assigning NUTS sampler...
Initializing NUTS using jitter+adapt_diag...
Multiprocess sampling (4 chains in 4 jobs)
NUTS: [theta, phi]
```

```
100.00% [8000/8000 00:00<00:00 Sampling 4 chains, 0 divergences]
```

```
Sampling 4 chains for 1_000 tune and 1_000 draw iterations (4_000 + 4_000 draws total) took 0 seconds.
```

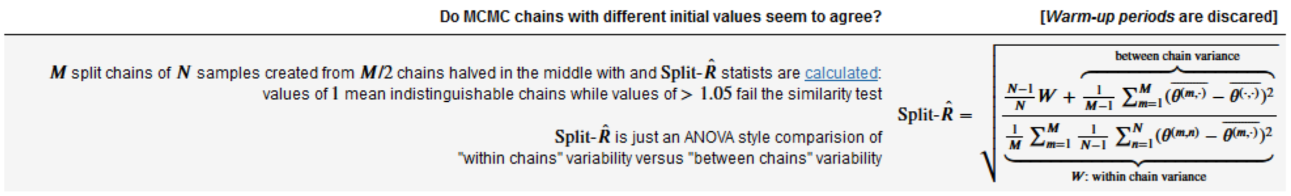
```
[42]: with normal_gamma_toy_model:
          MH = pm.Metropolis([theta, phi], S=np.array([0.1]), tune=False,␣
       ↪tune_interval=0)
          idata_MH = pm.sample(step=MH) # force MH
```

```
Multiprocess sampling (4 chains in 4 jobs)
CompoundStep
>Metropolis: [theta]
>Metropolis: [phi]
```

```
100.00% [8000/8000 00:00<00:00 Sampling 4 chains, 0 divergences]
```

```
Sampling 4 chains for 0 tune and 2_000 draw iterations (0 + 8_000 draws total) took 0 seconds.
The rhat statistic is larger than 1.01 for some parameters. This indicates problems during sampling. See https://arxiv.org
/abs/1903.08008 for details
The effective sample size per chain is smaller than 100 for some parameters.  A higher number is needed for reliable rhat
and ess computation. See https://arxiv.org/abs/1903.08008 for details
```

PyMC: Traceplot "Convergence" Checks [10 minutes]



Do MCMC chains with different initial values seem to agree? **[*Warm-up periods* are discared]**

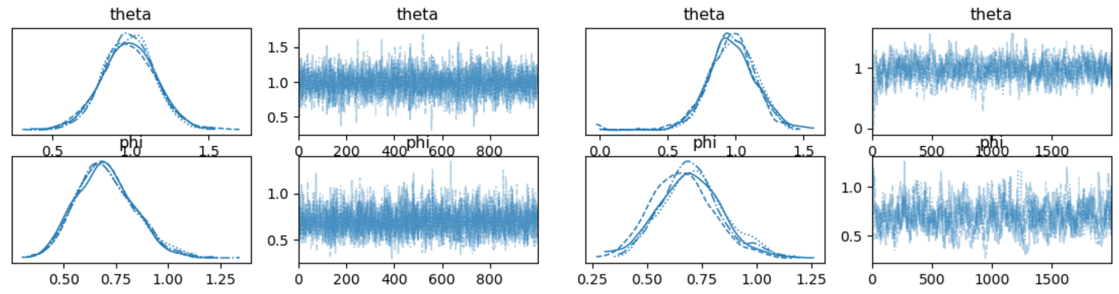
M split chains of ***N*** samples created from ***M*/2** chains halved in the middle with and **Split-$\hat{R}$** statists are calculated: values of **1** mean indistinguishable chains while values of **> 1.05** fail the similarity test

Split-$\hat{R}$ is just an ANOVA style comparision of "within chains" variability versus "between chains" variability

$$\text{Split-}\hat{R} = \sqrt{\frac{\frac{N-1}{N}W + \overbrace{\frac{1}{M-1}\sum_{m=1}^{M}(\overline{\theta^{(m,\cdot)}} - \overline{\theta^{(\cdot,\cdot)}})^2}^{\text{between chain variance}}}{\underbrace{\frac{1}{M}\sum_{m=1}^{M}\frac{1}{N-1}\sum_{n=1}^{N}(\theta^{(m,n)} - \overline{\theta^{(m,\cdot)}})^2}_{W\text{: within chain variance}}}}$$

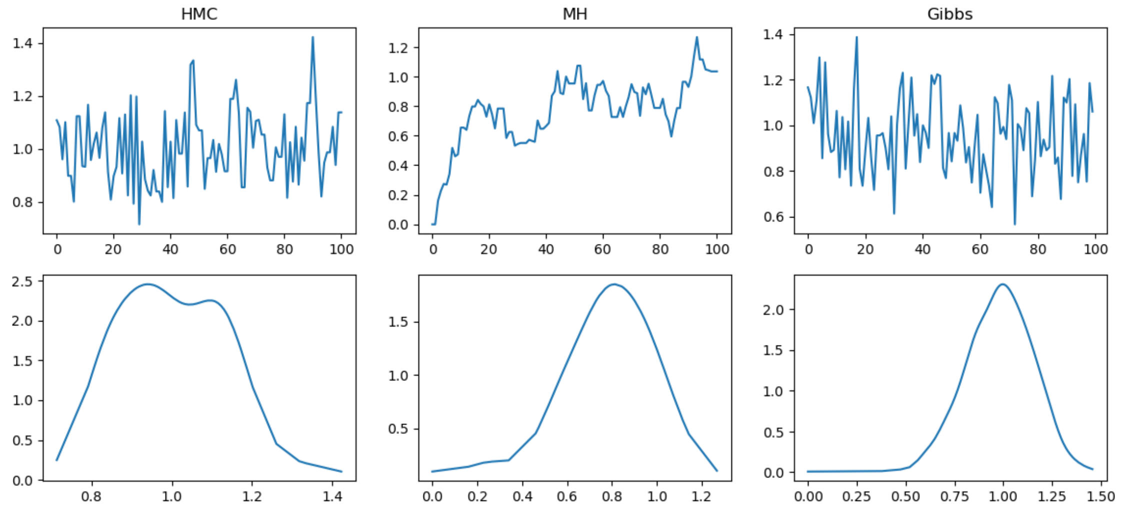
```
[43]: import arviz as az; import matplotlib.pyplot as plt; fig,ax = plt.subplots(2,4,␣
       ↪figsize=(14,3))
      az.plot_trace(idata_HMC, axes=ax[:2,:2]); az.plot_trace(idata_MH, axes=ax[:2,2:])
      print("HMC Split-Rhats", {k: np.round(v.values,4) for k,v in az.rhat(idata_HMC).
       ↪items()}, end=' | '); print('MH Split-Rhats',{k: np.round(v.values,4) for k,v␣
       ↪in az.rhat(idata_MH).items()})
```

```
HMC Split-Rhats {'theta': 1.0026, 'phi': 1.0007} | MH Split-Rhats {'theta':
1.0129, 'phi': 1.0277}
```



MCMC: A Closer Look [10 minutes]

```
[58]: from scipy.stats import gaussian_kde; import matplotlib.pyplot as plt; fig,ax =␣
       ↪plt.subplots(2,3, figsize=(14,6))
      n_mcmc_samples = 100
      mcmc_chain = idata_HMC.posterior["theta"].sel(chain=0, draw=slice(0,␣
       ↪n_mcmc_samples)).values; mcmc_chain_sorted = sorted(mcmc_chain)
      ax[0,0].plot(mcmc_chain); ax[1,0].
       ↪plot(mcmc_chain_sorted,gaussian_kde(mcmc_chain_sorted)(mcmc_chain_sorted));␣
       ↪ax[0,0].set_title("HMC");
      mcmc_chain = idata_MH.posterior["theta"].sel(chain=0, draw=slice(0,␣
       ↪n_mcmc_samples)).values; mcmc_chain_sorted = sorted(mcmc_chain)
      ax[0,1].plot(mcmc_chain); ax[1,1].
       ↪plot(mcmc_chain_sorted,gaussian_kde(mcmc_chain_sorted)(mcmc_chain_sorted));␣
       ↪ax[0,1].set_title("MH");
      ax[0,2].plot(theta_gibbs_posterior_mcmc_draws[burn:(burn+n_mcmc_samples)]);␣
       ↪ax[0,2].set_title("Gibbs");
      theta_gibbs_posterior_mcmc_draws_sorted =␣
       ↪sorted(theta_gibbs_posterior_mcmc_draws);
      ax[1,2].
       ↪plot(theta_gibbs_posterior_mcmc_draws_sorted,gaussian_kde(theta_gibbs_posterior_mcmc_draws_sc
       ↪
```

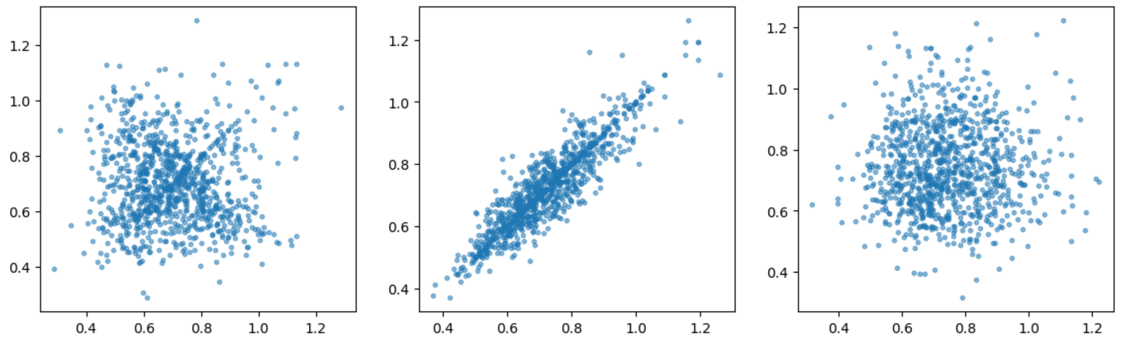


MCMC: Autocorrelation (10 minutes)

```
[62]: import numpy as np; import matplotlib.pyplot as plt; fig,ax = plt.subplots(1,3,␣
       ↪figsize=(14,4))
      max_mcmc_samples = 1000
      mcmc_chain = idata_HMC.posterior["phi"].sel(chain=0, draw=slice(0,␣
       ↪max_mcmc_samples-2)).values; mcmc_chain_one_step_ahead = idata_HMC.
       ↪posterior["phi"].sel(chain=0, draw=slice(1, max_mcmc_samples-1)).values; ax[0].
       ↪plot(mcmc_chain, mcmc_chain_one_step_ahead, '.', alpha=0.5)
      print("Autocorrelation for HMC (MCMC) chain", np.
       ↪corrcoef(mcmc_chain,mcmc_chain_one_step_ahead)[0,1], "                 ...is␣
       ↪negative autocorrelation good?")
      mcmc_chain = idata_MH.posterior["phi"].sel(chain=0, draw=slice(0,␣
       ↪max_mcmc_samples-2)).values; mcmc_chain_one_step_ahead = idata_MH.
       ↪posterior["phi"].sel(chain=0, draw=slice(1, max_mcmc_samples-1)).values; ax[1].
       ↪plot(mcmc_chain, mcmc_chain_one_step_ahead, '.', alpha=0.5);
      print("Autocorrelation for MH (MCMC) chain", np.
       ↪corrcoef(mcmc_chain,mcmc_chain_one_step_ahead)[0,1], "                   ...is␣
       ↪large positive autocorrelation good?")
      ax[2].plot(phi_gibbs_posterior_mcmc_draws[burn:
       ↪-1],phi_gibbs_posterior_mcmc_draws[(burn+1):], '.', alpha=0.5);
      print("Autocorrelation for Gibbs Sampling (MCMC) chain", np.
       ↪corrcoef(phi_gibbs_posterior_mcmc_draws[burn:
       ↪-1],phi_gibbs_posterior_mcmc_draws[(burn+1):])[0,1], "  ...is no␣
       ↪autocorrelation the best?")
```

```
Autocorrelation for HMC (MCMC) chain -0.0140628109479451                 ...is
negative autocorrelation good?
Autocorrelation for MH (MCMC) chain 0.9084368880554985                   ...is
```

```
large positive autocorrelation good?
Autocorrelation for Gibbs Sampling (MCMC) chain 0.021150850107231244   ...is no
autocorrelation the best?
```



MCMC: Effective Sample Size [10 minutes]

PyMC labels $n_{\text{eff}} = \frac{n}{\sum_{t=-\infty}^{\infty} \rho_t} = \frac{n}{1+2\sum_{t=1}^{\infty} \rho_t}$ for order t autocorrelations ρ_t in the MCMC chains

`ess_bulk` while `ess_tail` is the same but after converting to binary sequences estimating 5% tail quantiles.

[69]:
```
import arviz as az; print("number of MCMC samples:", idata_HMC.posterior['phi'].
 ↪values.flatten().shape[-1])
az.summary(idata_HMC, round_to=2) # https://python.arviz.org/en/stable/api/
 ↪generated/arviz.ess.html
```

```
number of MCMC samples: 4000
```

[69]:
```
        mean    sd  hdi_3%  hdi_97%  mcse_mean  mcse_sd  ess_bulk  ess_tail  \
theta   0.98  0.17    0.66     1.31        0.0      0.0   3880.51   2568.12
phi     0.70  0.14    0.45     0.96        0.0      0.0   3959.53   2736.66

        r_hat
theta     1.0
phi       1.0
```

[68]:
```
print("number of MCMC samples:", idata_MH.posterior['phi'].values.flatten().
 ↪shape[-1])
az.summary(idata_MH, round_to=2)
```

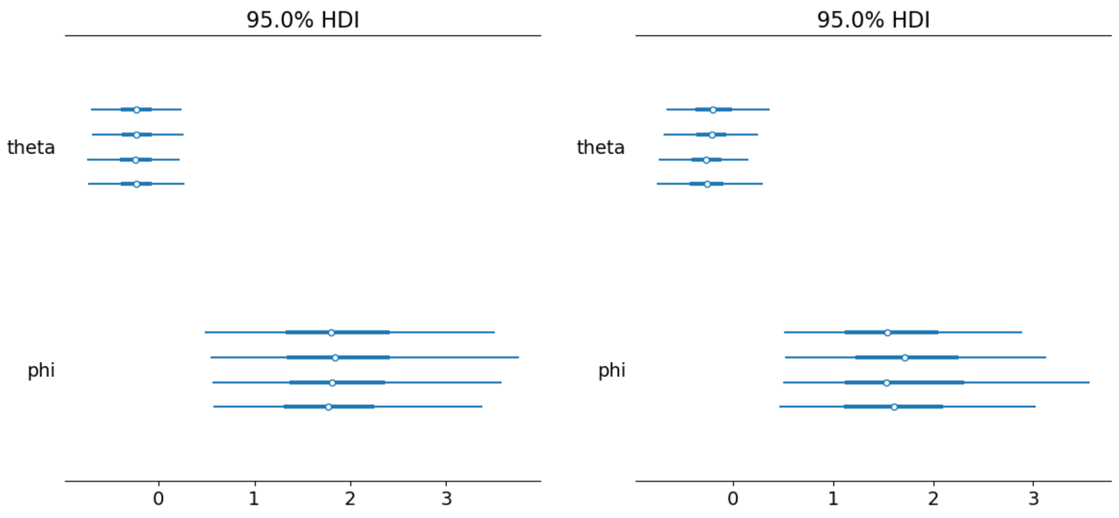
```
number of MCMC samples: 8000
```

[68]:
```
        mean    sd  hdi_3%  hdi_97%  mcse_mean  mcse_sd  ess_bulk  ess_tail  \
theta   0.97  0.18    0.65     1.30       0.01     0.01    390.50    561.12
phi     0.69  0.14    0.42     0.97       0.01     0.01    188.56    317.92
```

```
       r_hat
theta   1.01
phi     1.03
```

MCMC Bayesian Inference: Credible Intervals [5 minutes]

[258]:
```
import arviz as az; import matplotlib.pyplot as plt; fig,ax = plt.subplots(1,2,␣
↪figsize=(14,6))
az.plot_forest(idata_HMC, var_names=["theta","phi"], combined=False, hdi_prob=0.
↪95, ax=ax[0]);
az.plot_forest(idata_MH, var_names=["theta","phi"], combined=False, hdi_prob=0.
↪95, ax=ax[1]);
```



Homework #3 – *you'll need to do this on google colab*

0. Find data set on kaggle.
1. Provide posterior inference for a column of data with a `PyMC` ***normal-gamma specification***.
2. Find a different column of data for which a ***normal-gamma specification*** isn't justified.
3. Create a different `PyMC` specification that IS appropriate for this new data column:
   - here are your `PyMC` choices for continuous distributions
   - here are your `PyMC` choices for discrete distributions

. . . just make sure you've chosen a reasonable likelihood for your non-normal data and that the support of your priors makes sense for the values the parameters of your likelihood can take on. . .

4. Provide posterior inference for the parameters of your new specification given the column of non-normal data using `PyMC` and provide an analysis of the MCMC chains.