



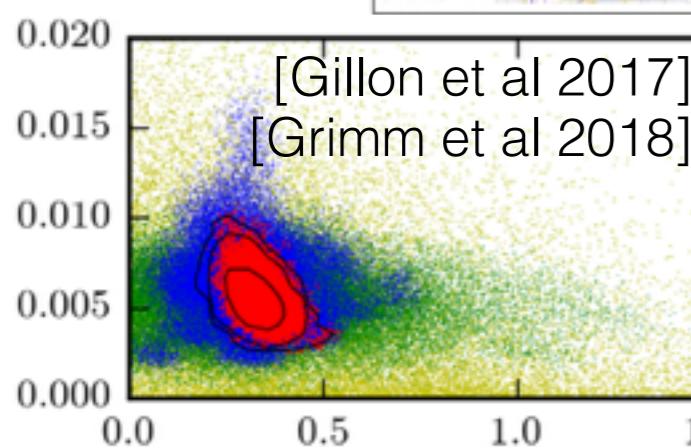
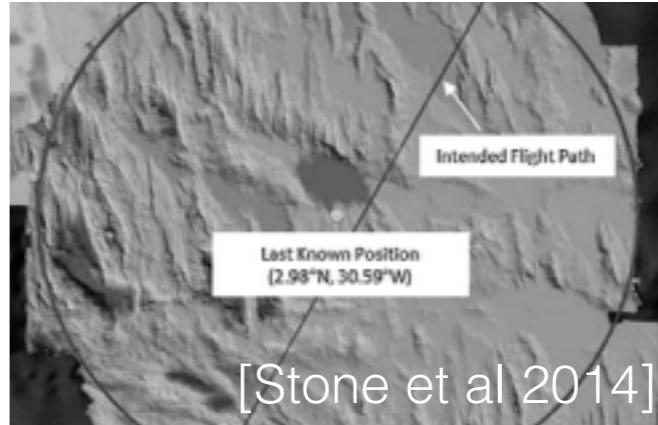
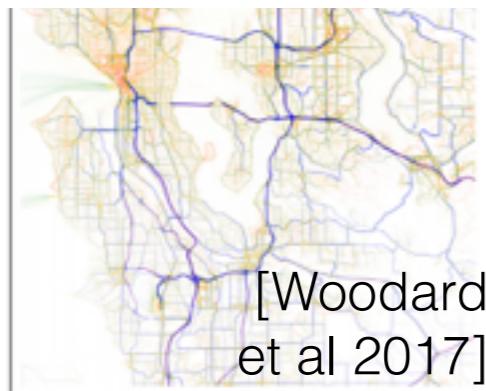
Automated Scalable Bayesian Inference via Data Summarization

Tamara Broderick
ITT Career Development
Assistant Professor,
MIT

With: Trevor Campbell, Jonathan Huggins

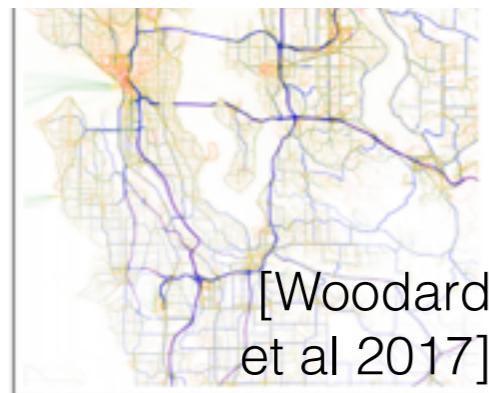
<http://www.tamarabroderick.com/tutorials.html>

Bayesian inference



- Desiderata:
 - Point estimates, coherent uncertainties
 - Interpretable, complex, modular; prior information

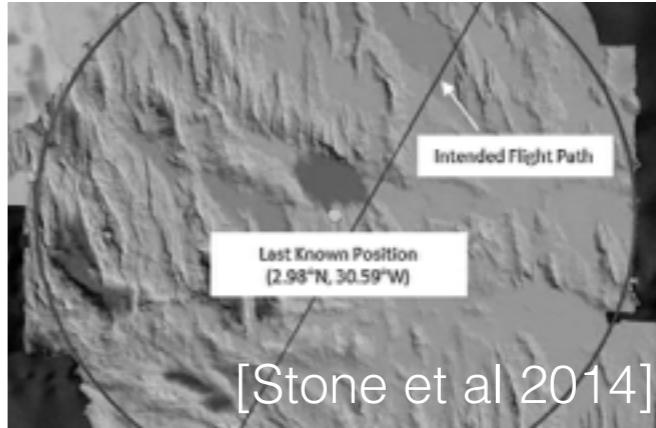
Bayesian inference



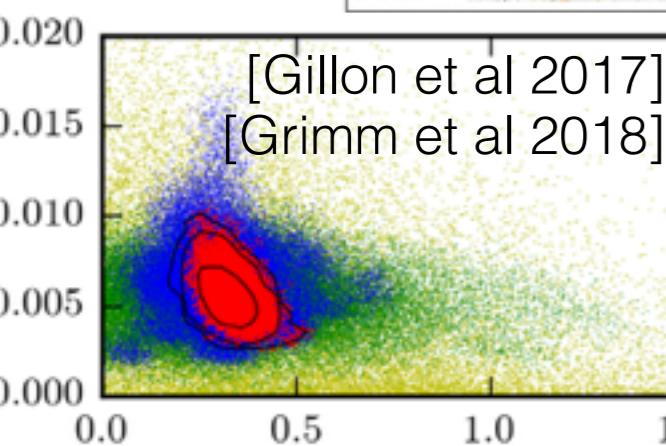
[Woodard
et al 2017]



[ESO/
L. Calçada/
M. Kornmesser
2017] [Abbott et al 2016a,b]



[Stone et al 2014]



[Gillon et al 2017]
[Grimm et al 2018]



[Meager 2018a,b]



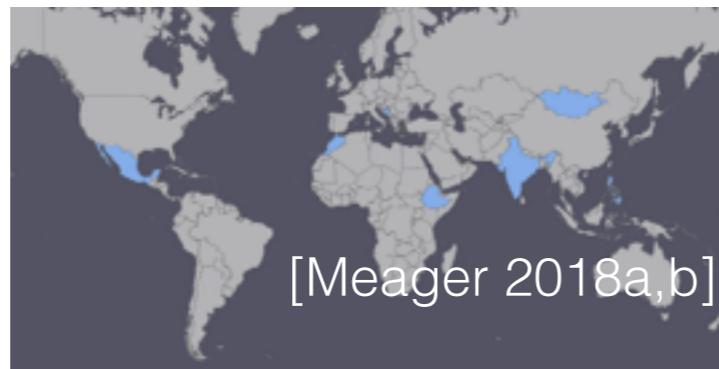
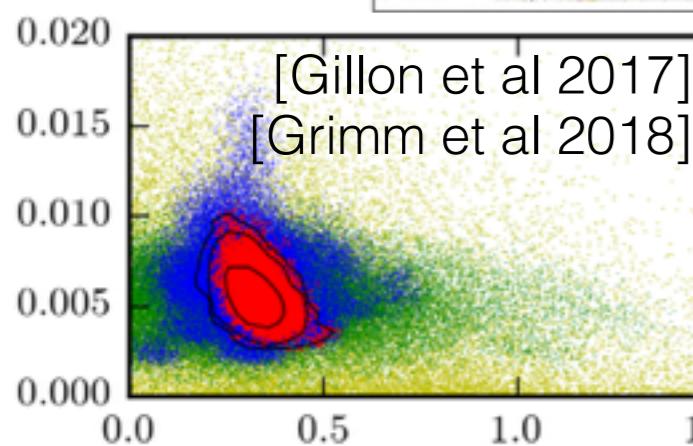
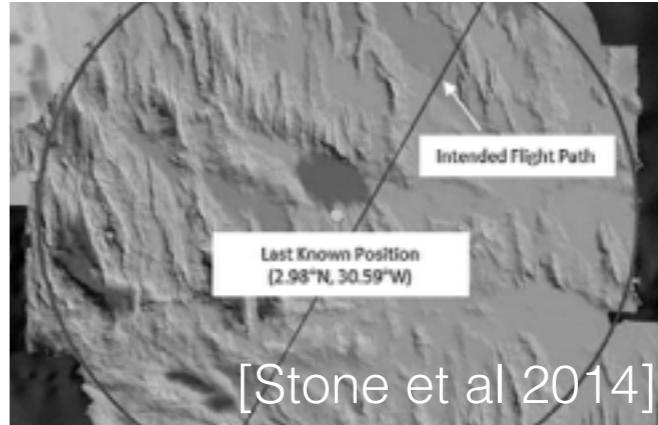
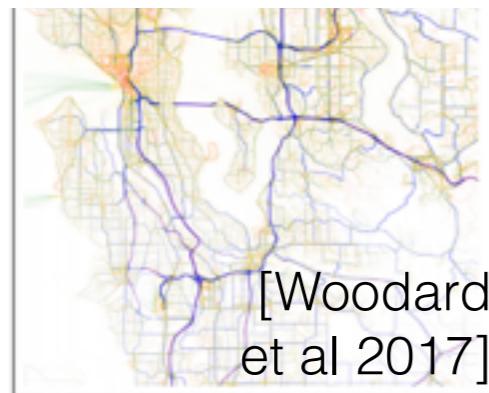
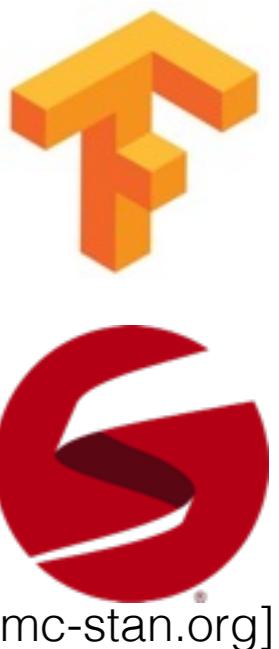
[Chati, Balakrishnan
2017]



[Kuikka et al 2014]
[Baltic Salmon Fund]

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 - Interpretable, complex, modular; prior information
- Challenge: existing methods can be slow, tedious, unreliable

Bayesian inference



- Desiderata:
 - Point estimates, coherent uncertainties
 - Interpretable, complex, modular; prior information
- Challenge: existing methods can be slow, tedious, unreliable
- Our proposal: use *efficient data summaries* for **scalable, automated** algorithms with **error bounds** for finite data

Roadmap

- Approximate Bayes review
- The “core” of the data set
- Uniform data subsampling isn’t enough
- Importance sampling for “coresets”
- Optimization for “coresets”
- Approximate sufficient statistics

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Bayesian inference

Bayesian inference

$$p(\theta)$$

Bayesian inference

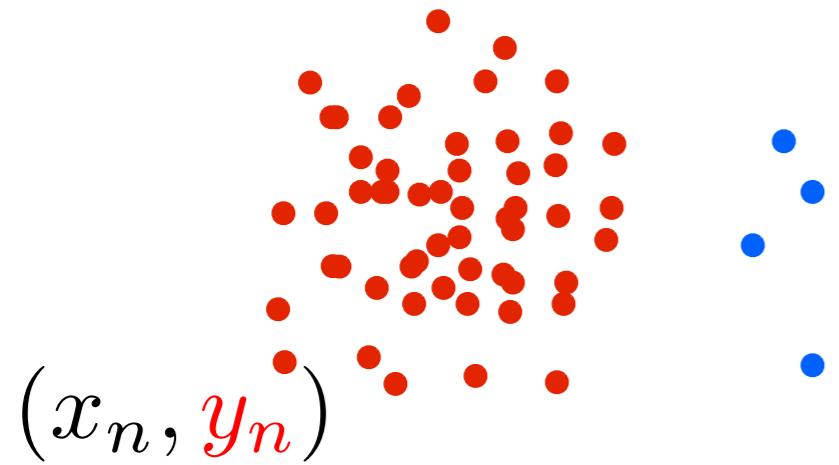
$$p(y|\theta)p(\theta)$$

Bayesian inference

$$p(\theta|y) \propto_{\theta} p(y|\theta)p(\theta)$$

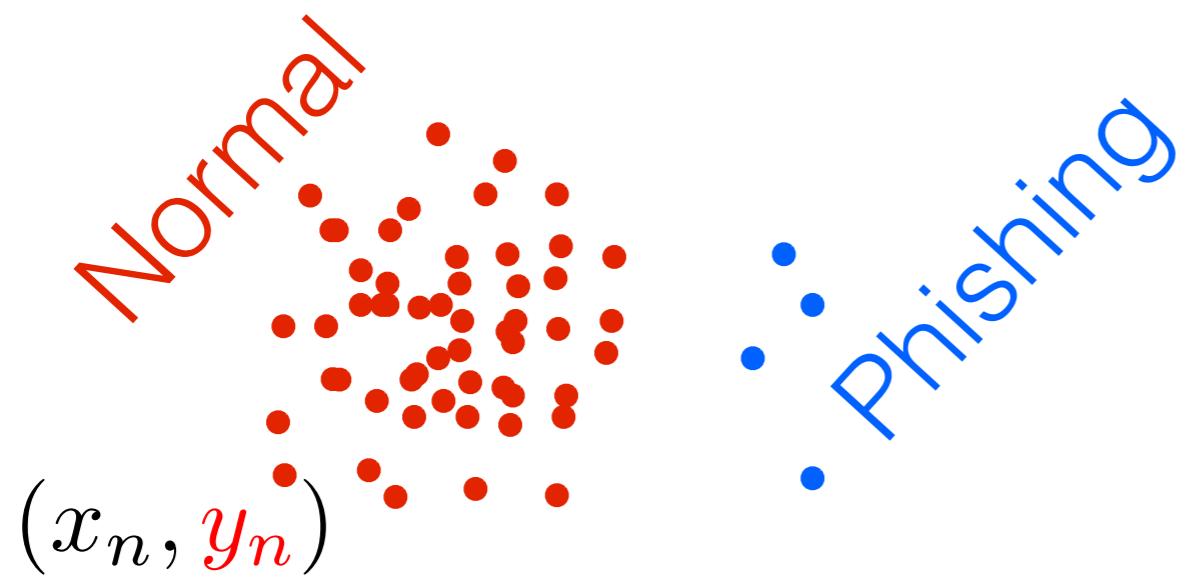
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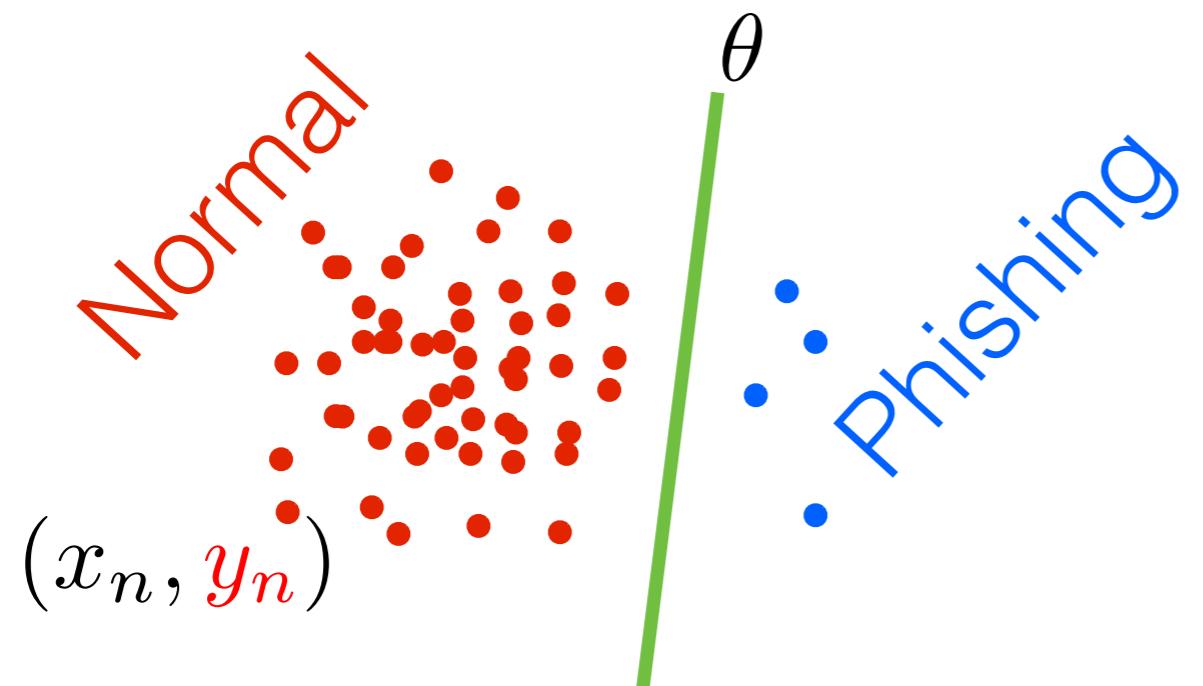
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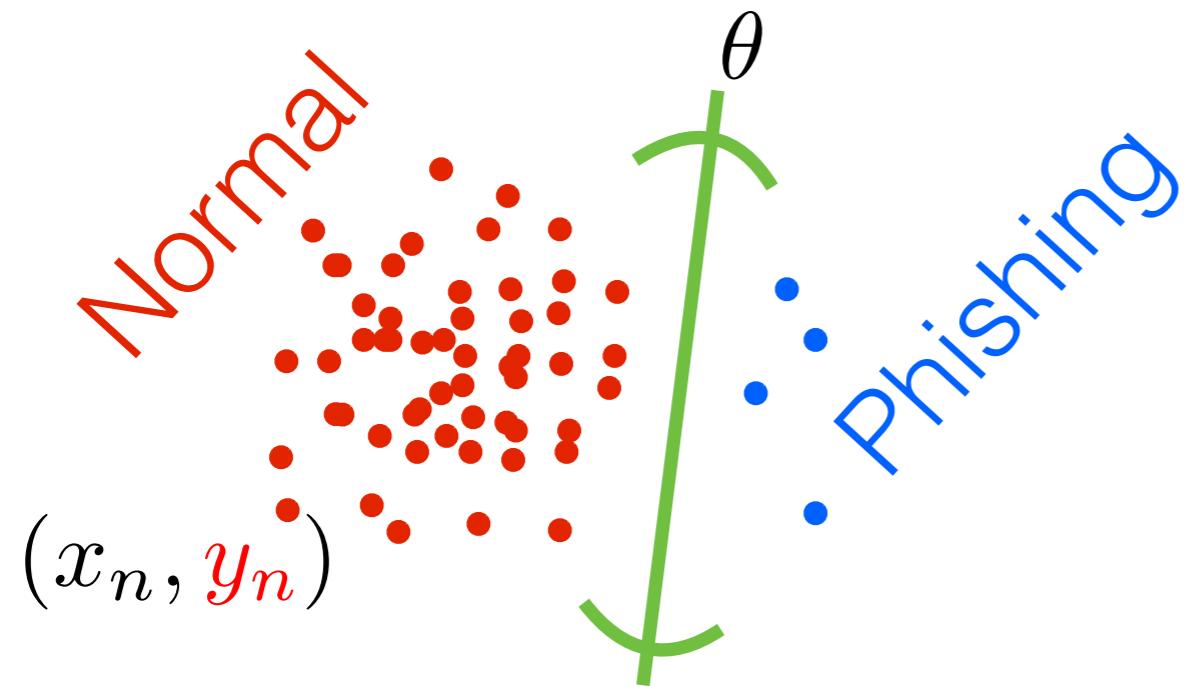
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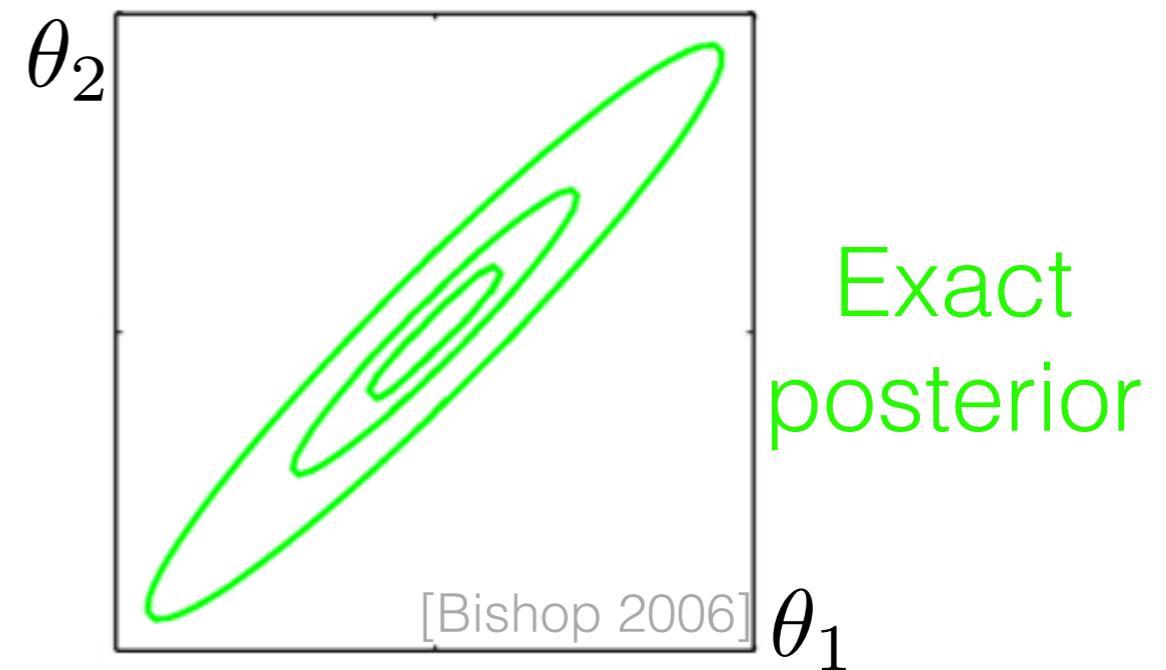
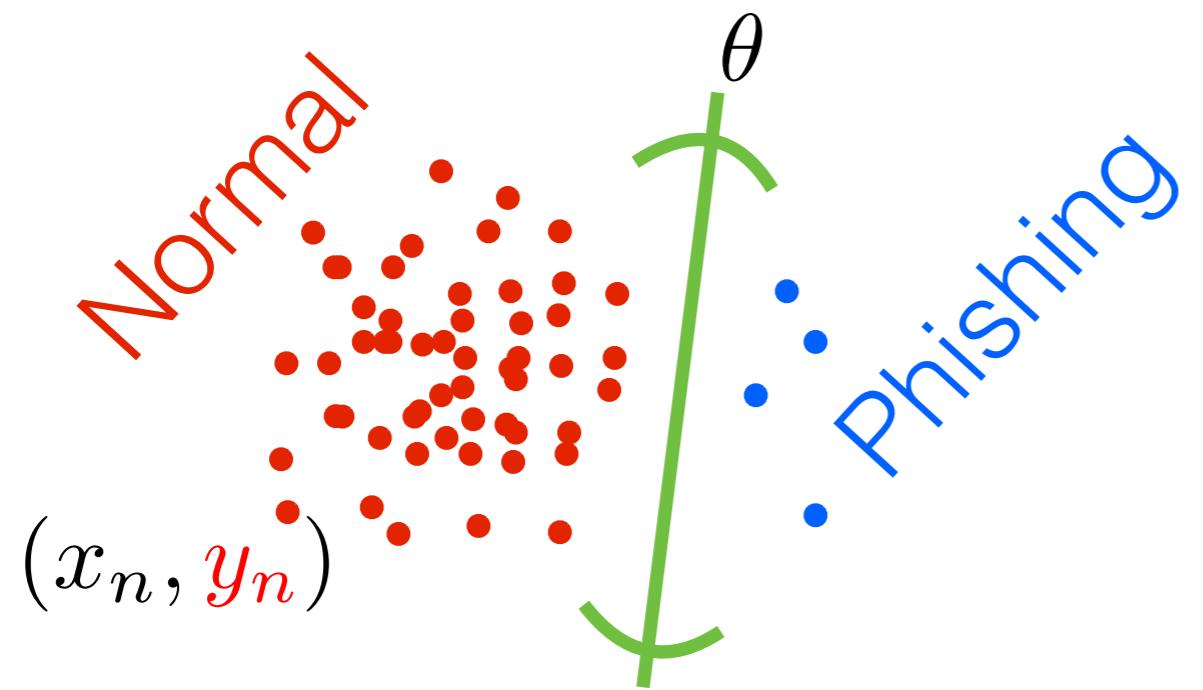
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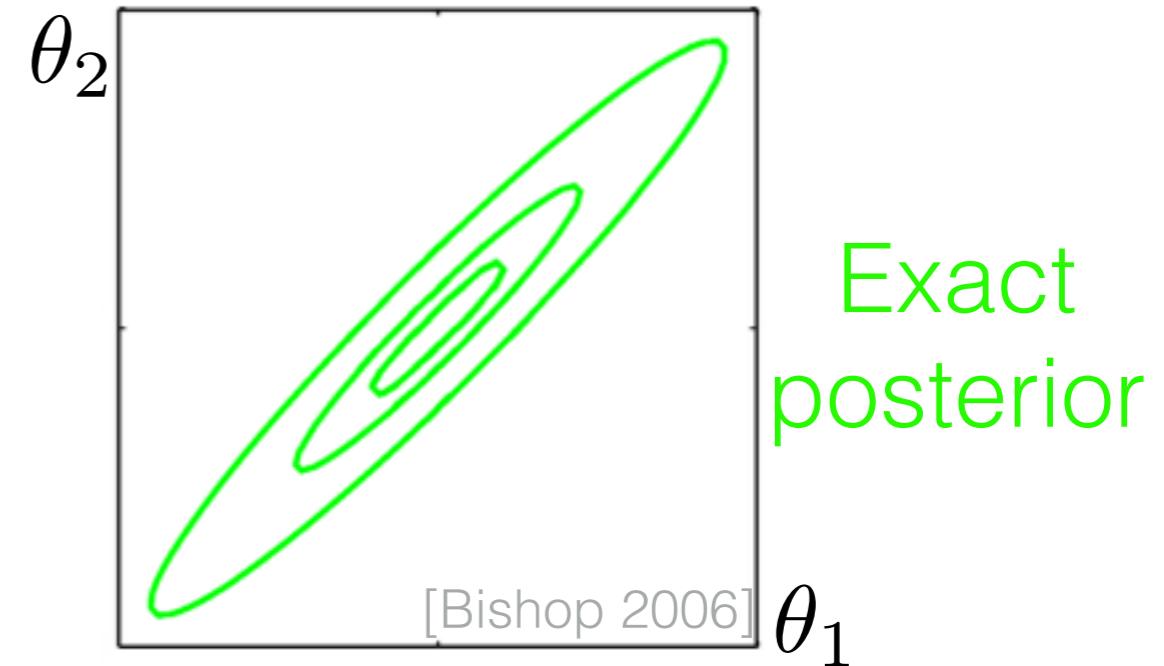
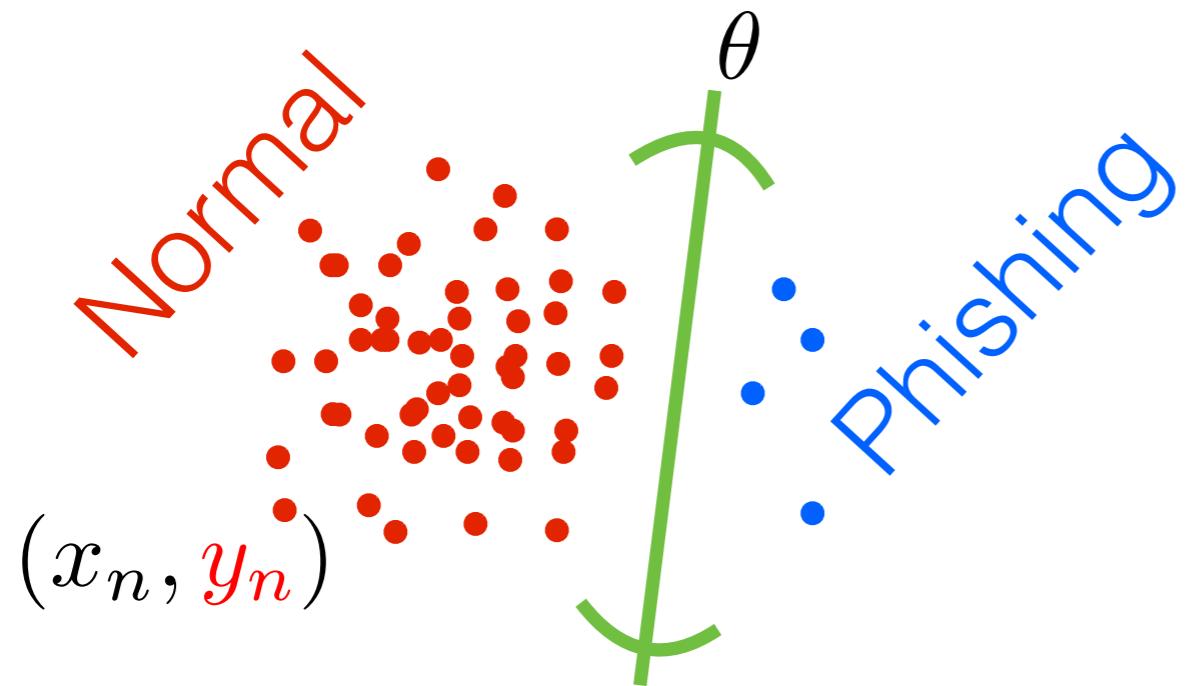
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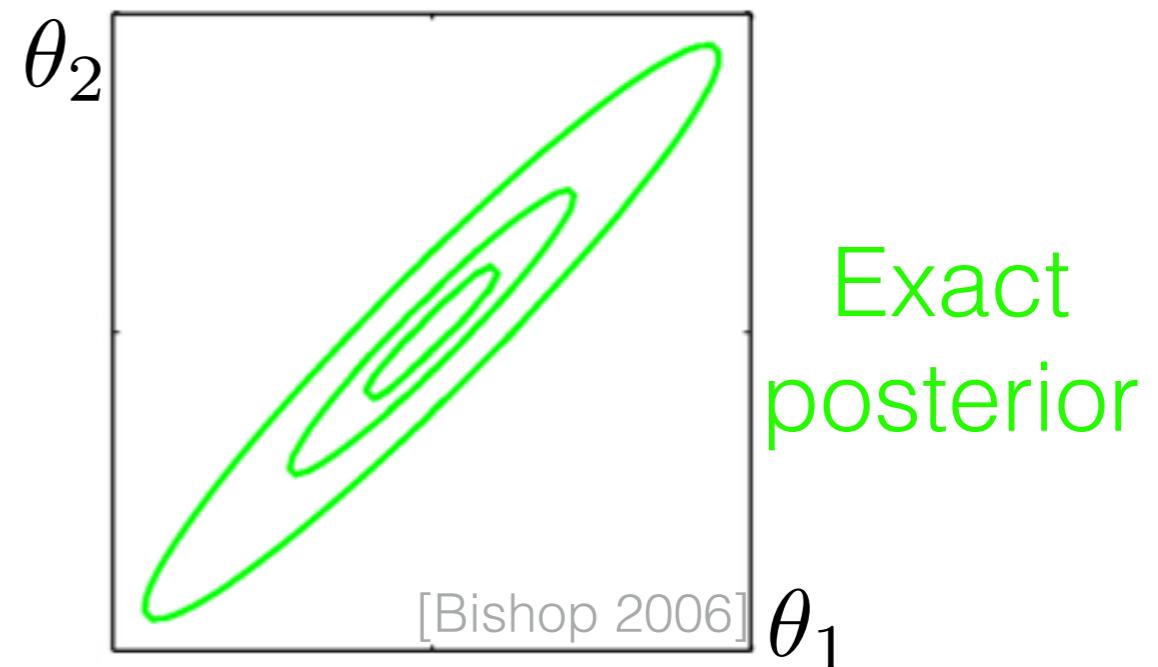
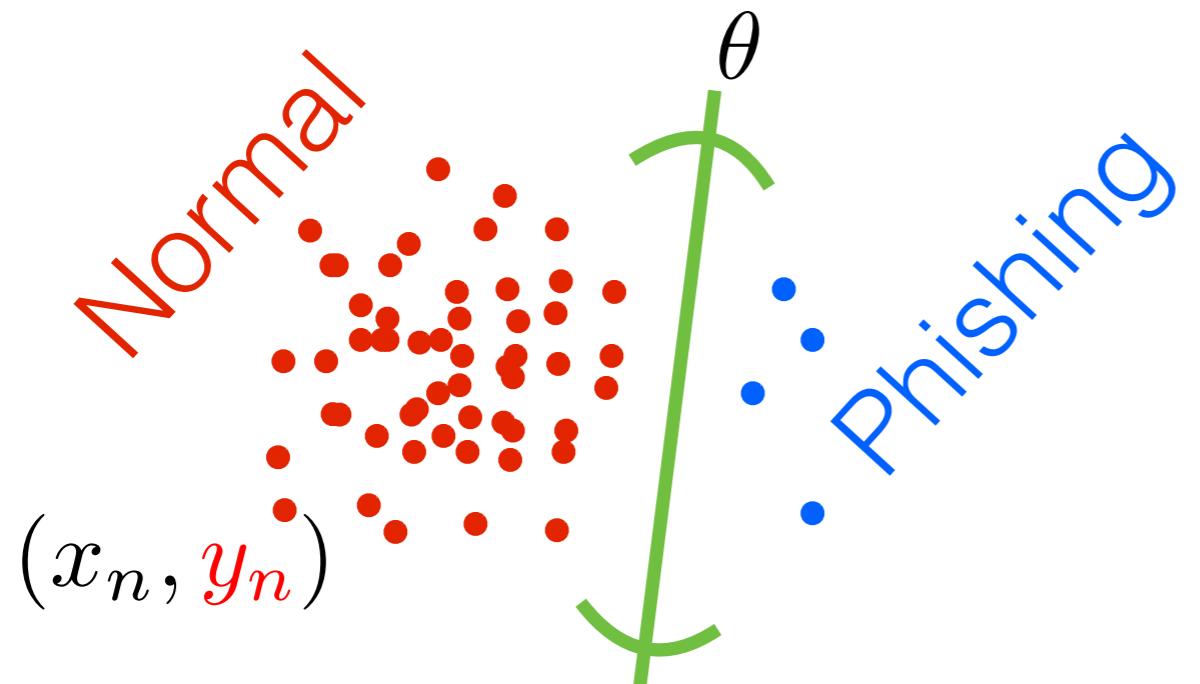
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- MCMC: Eventually accurate but can be slow [Bardenet, Doucet, Holmes 2017]

Bayesian inference

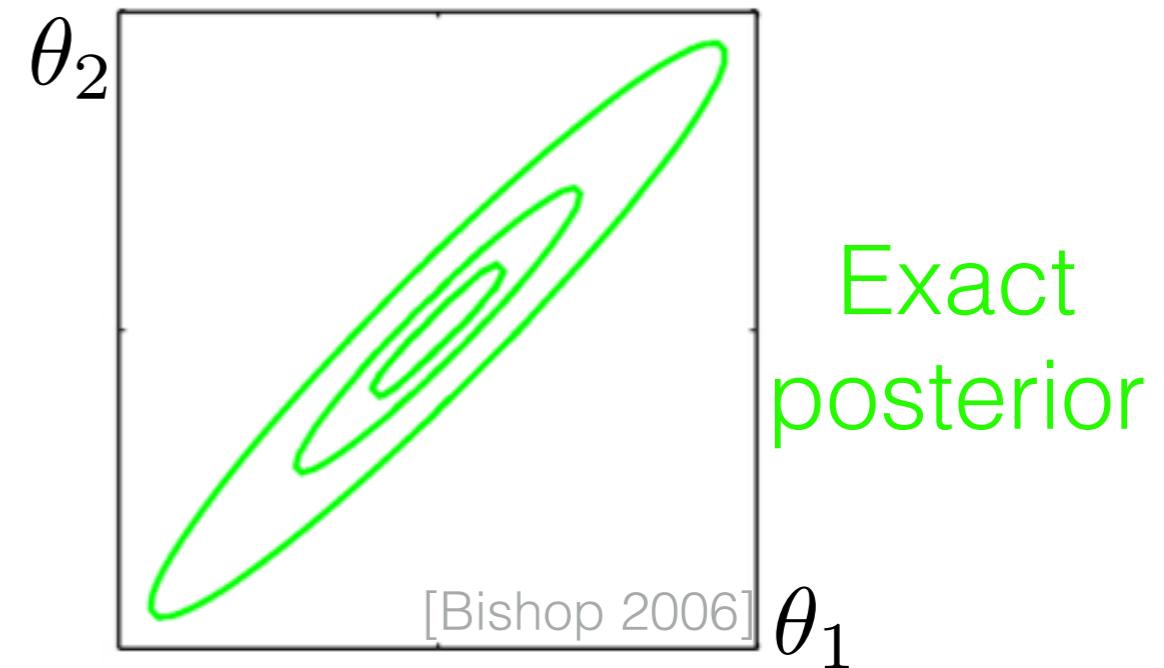
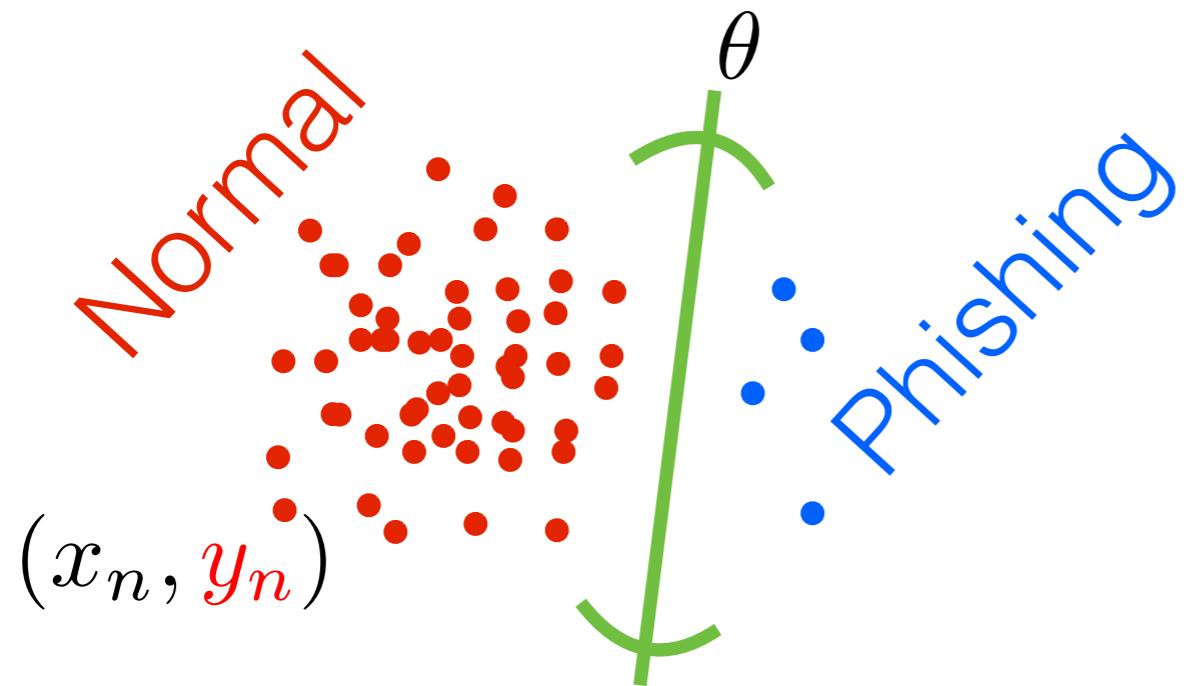
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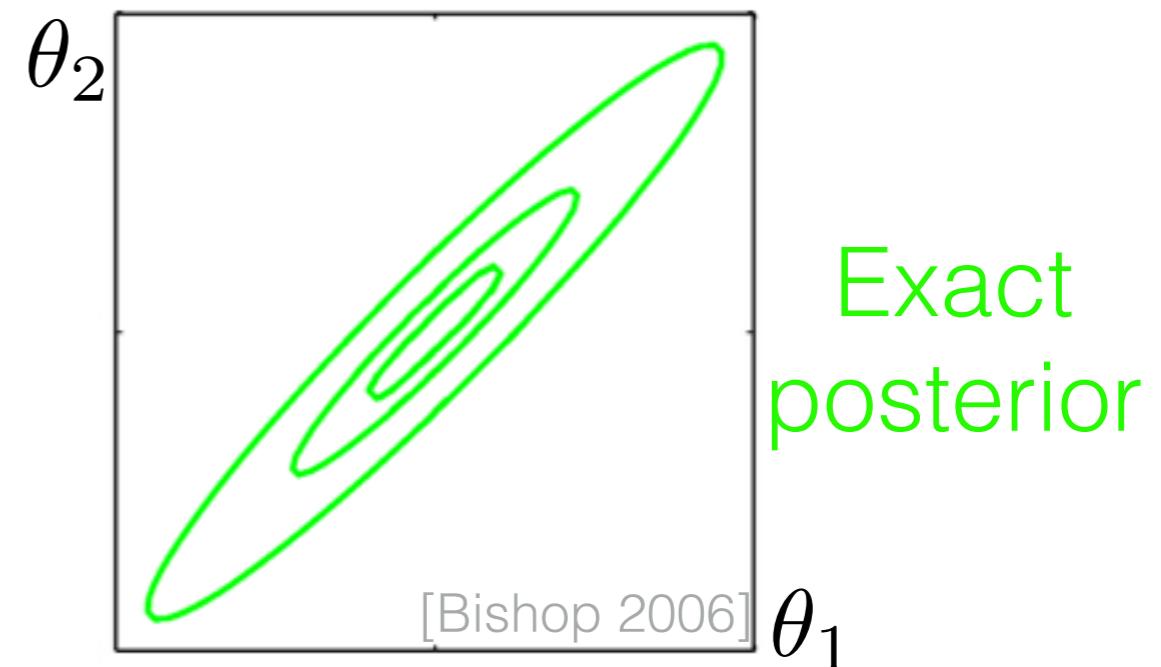
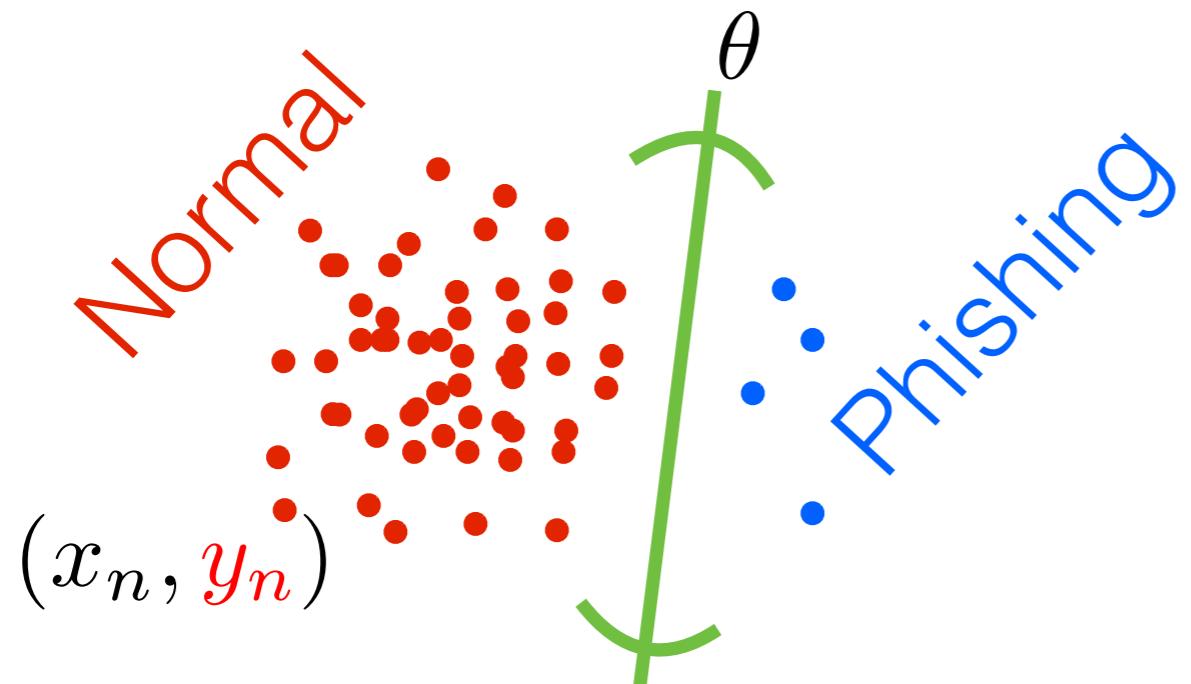
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 - Fast

Bayesian inference

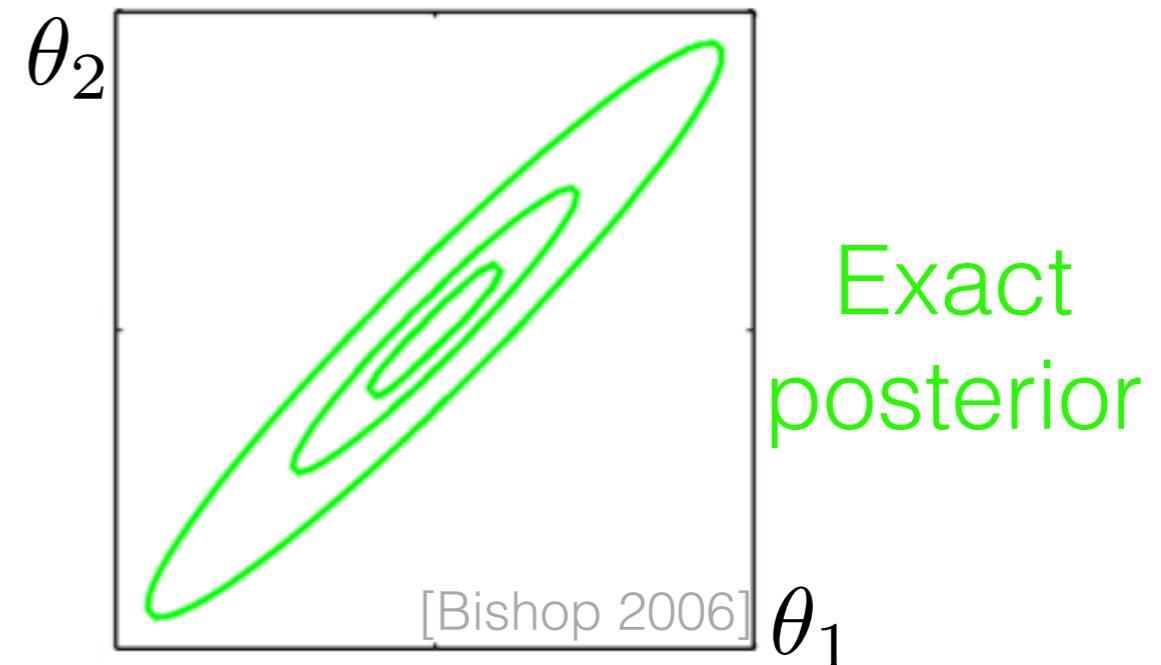
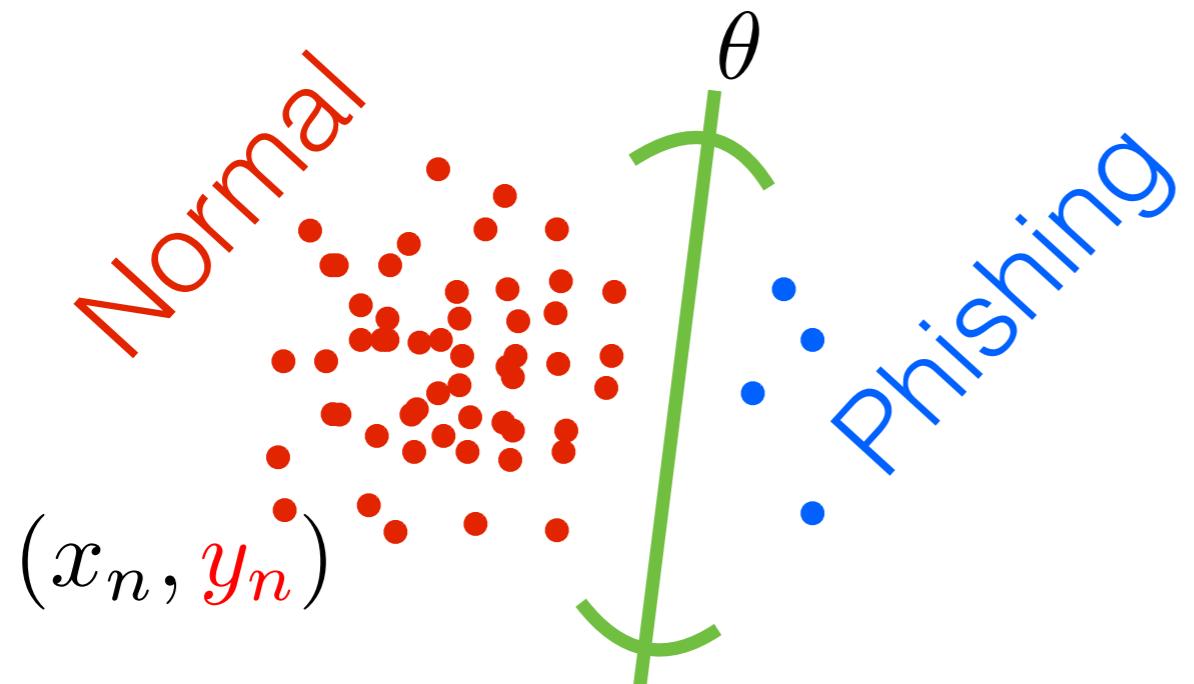
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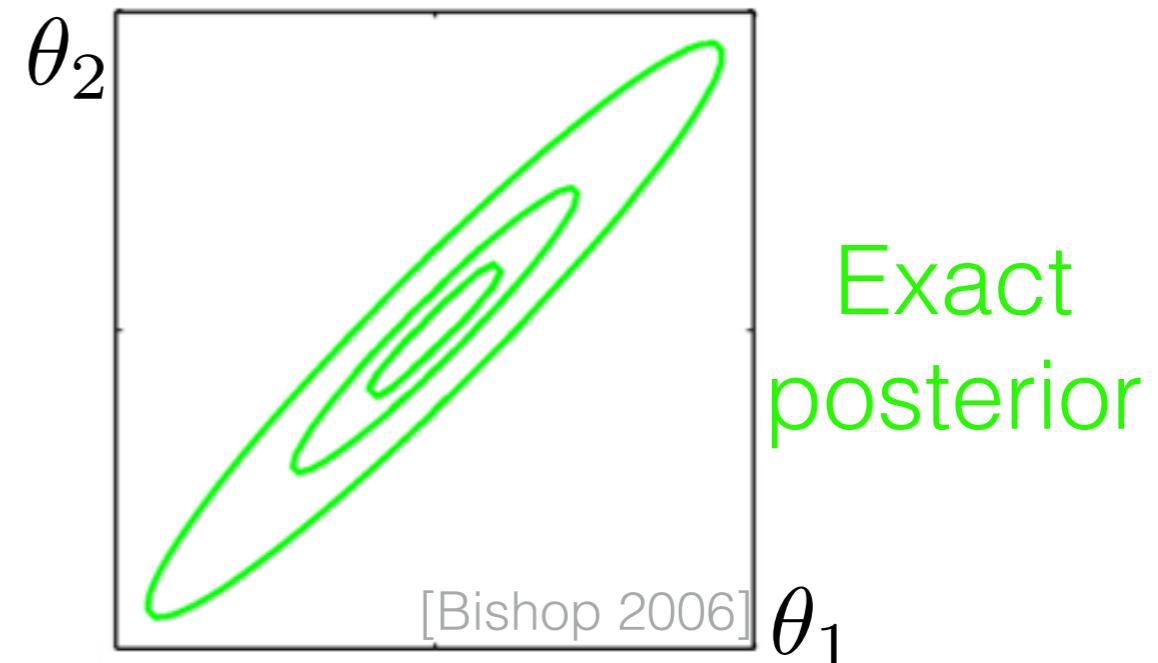
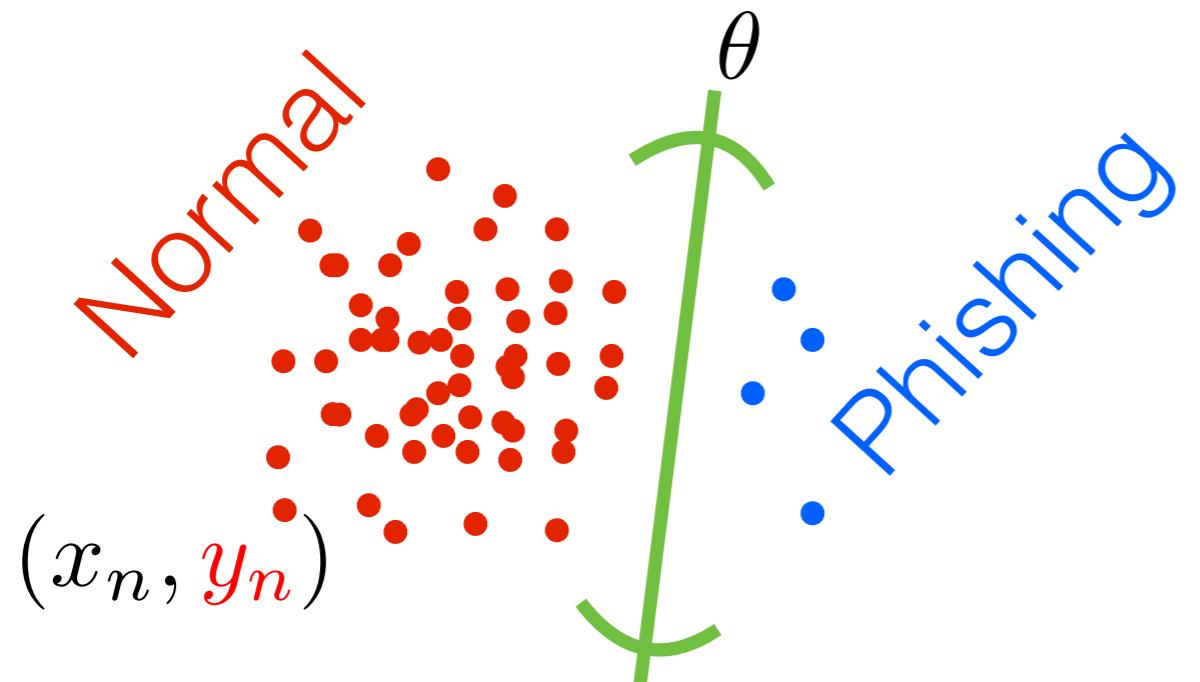
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(3.6M Wikipedia, 32 cores, ~hour)

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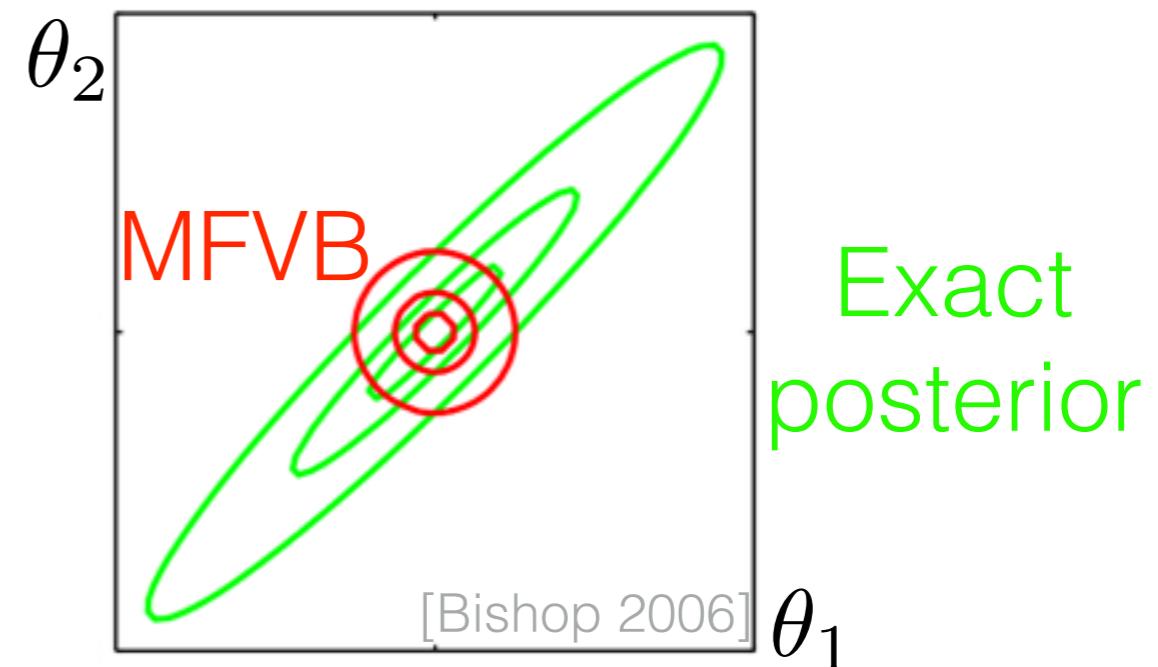
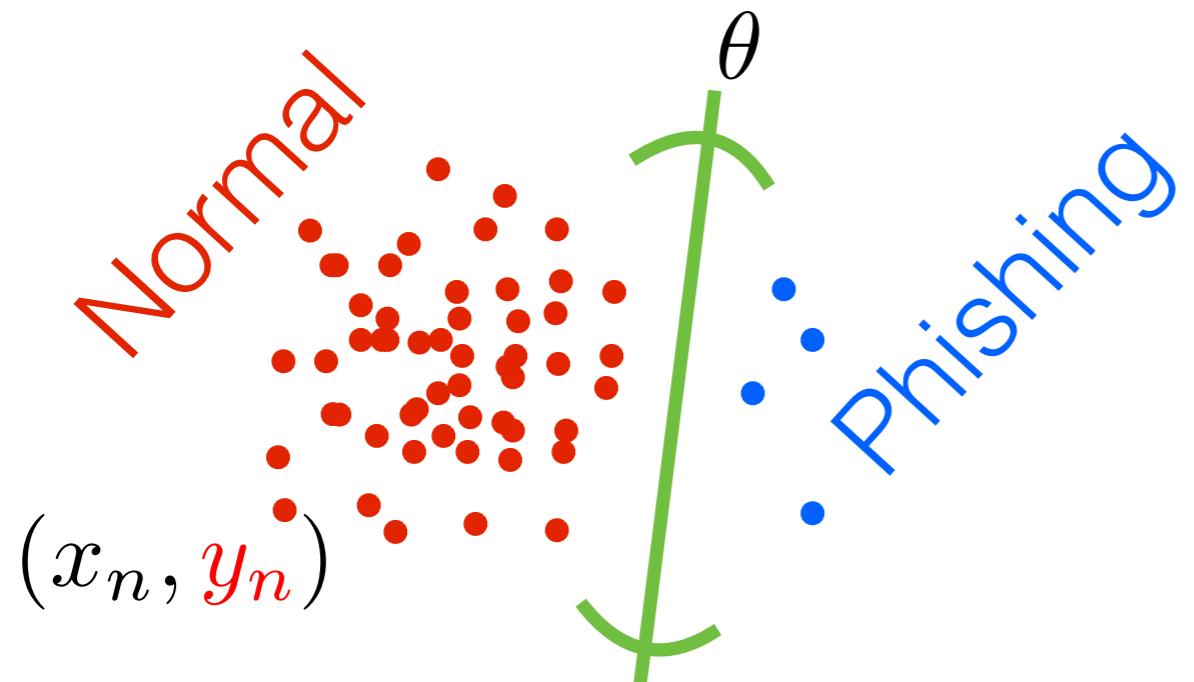


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[MacKay 2003; Bishop 2006; Wang, Titterington 2004; Turner, Sahani 2011; Fosdick 2013; Dunson 2014; Bardenet, Doucet, Holmes 2017; Opper, Winther 2003; Giordano, Broderick, Jordan 2015, 2017]

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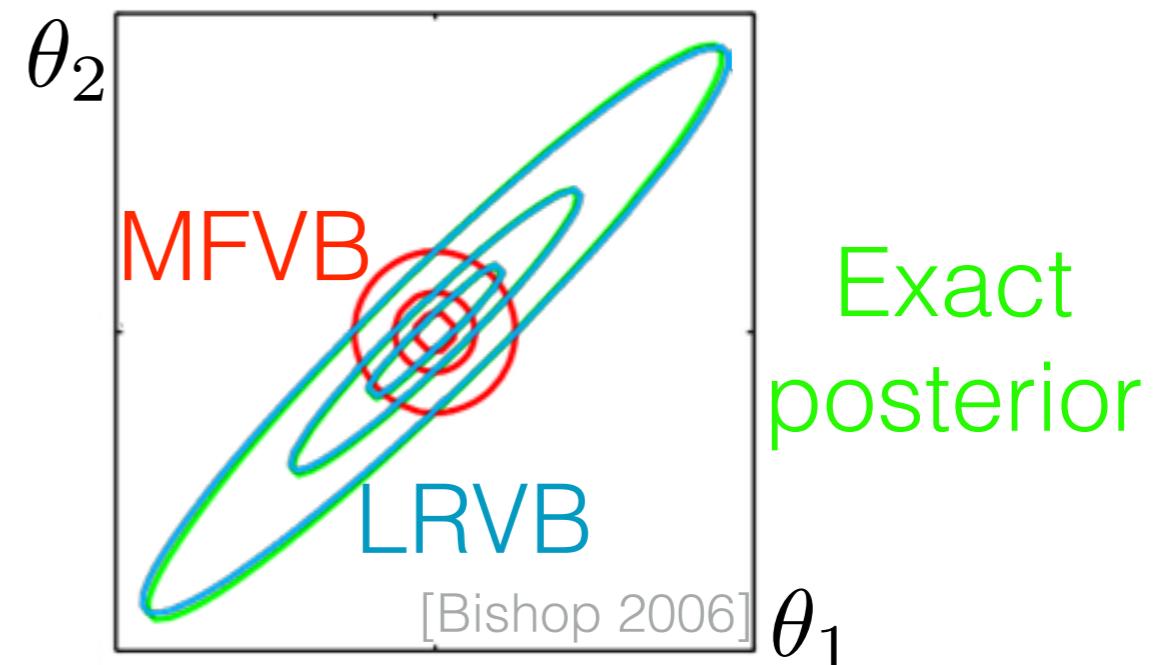
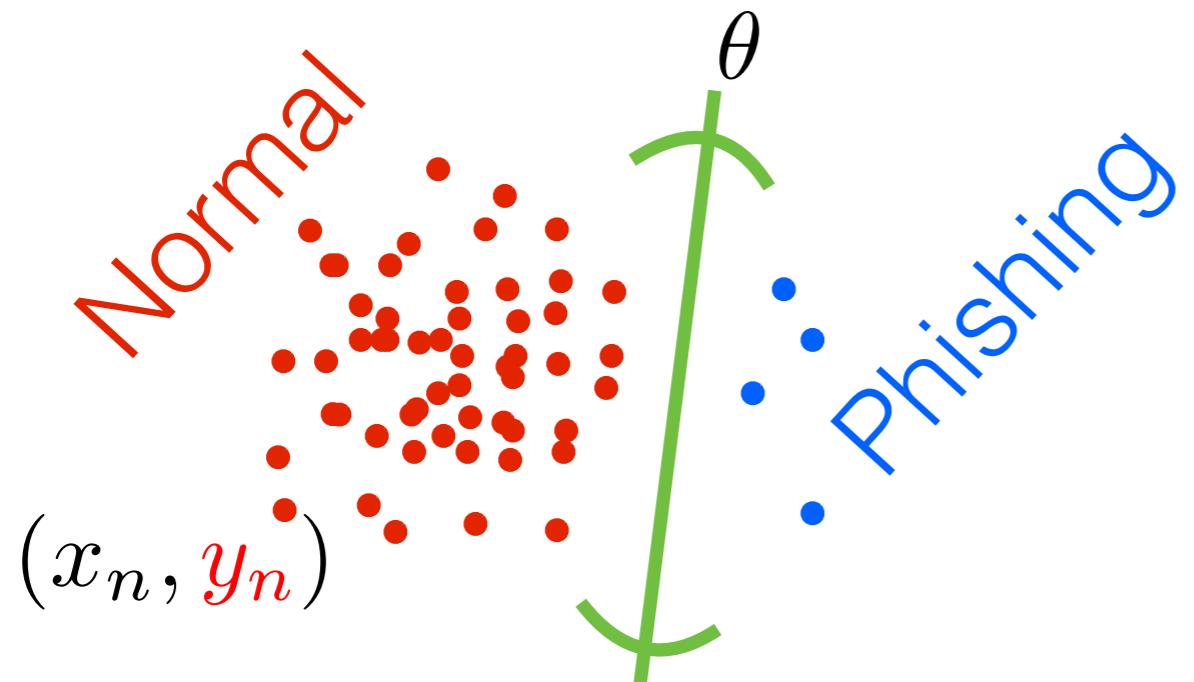


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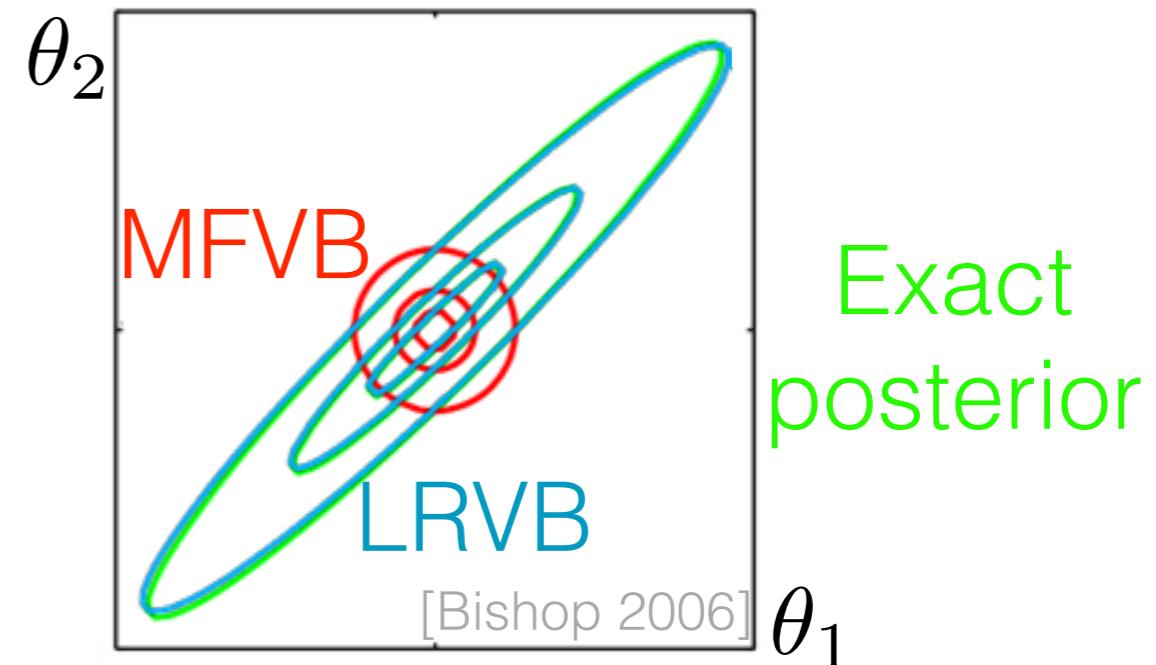
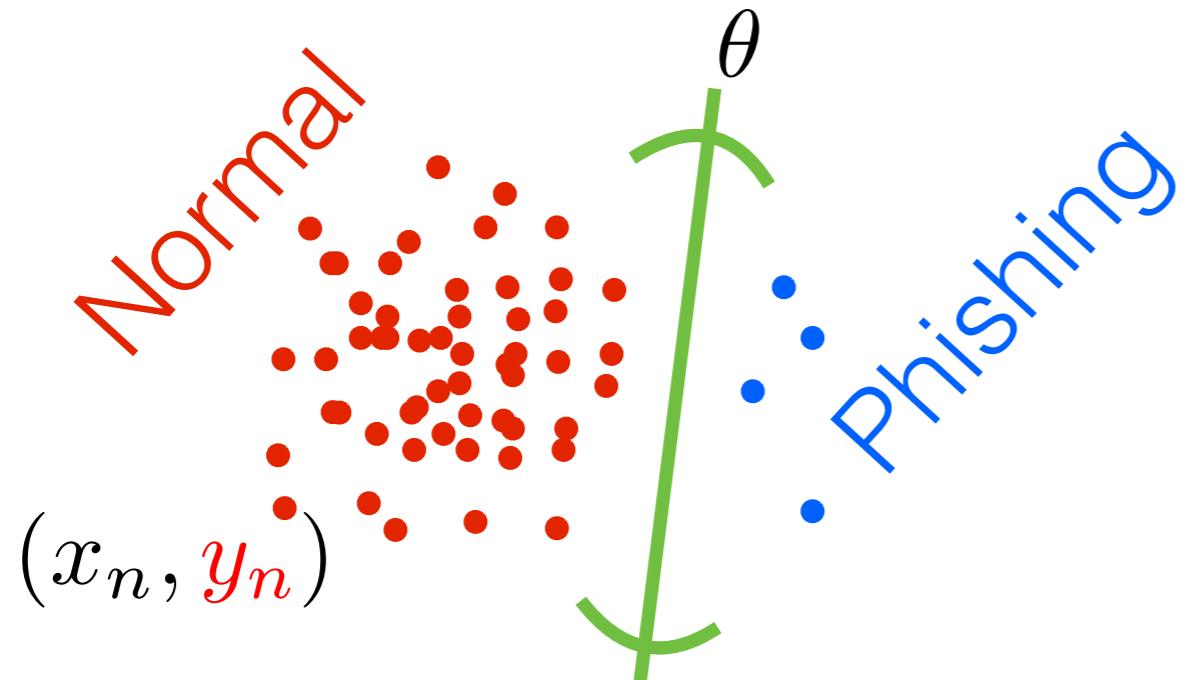


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- Automation: e.g. Stan, NUTS, ADVI

[<http://mc-stan.org/> ; Hoffman, Gelman 2014; Kucukelbir, Tran, Ranganath, Gelman, Blei 2017]

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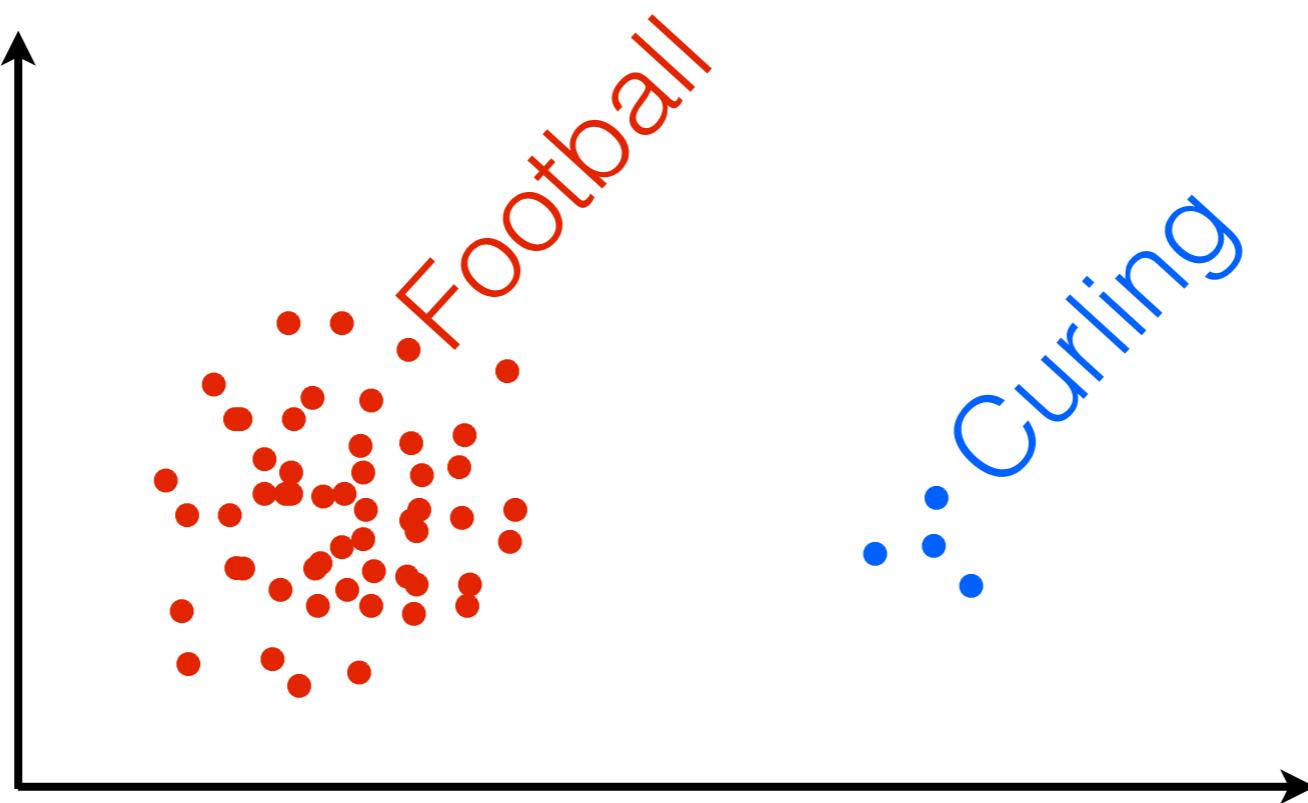
Bayesian coresets

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- Observe: redundancies can exist even if data isn't "tall"

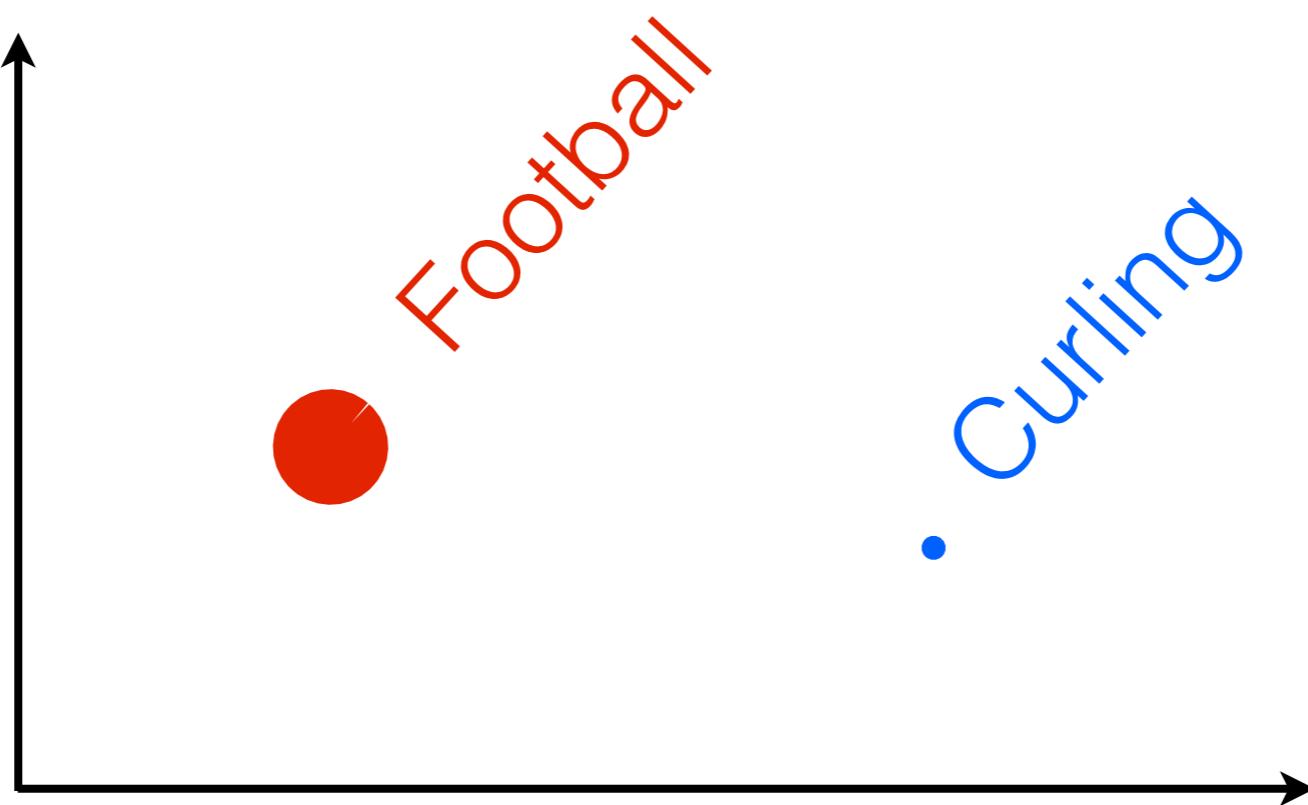
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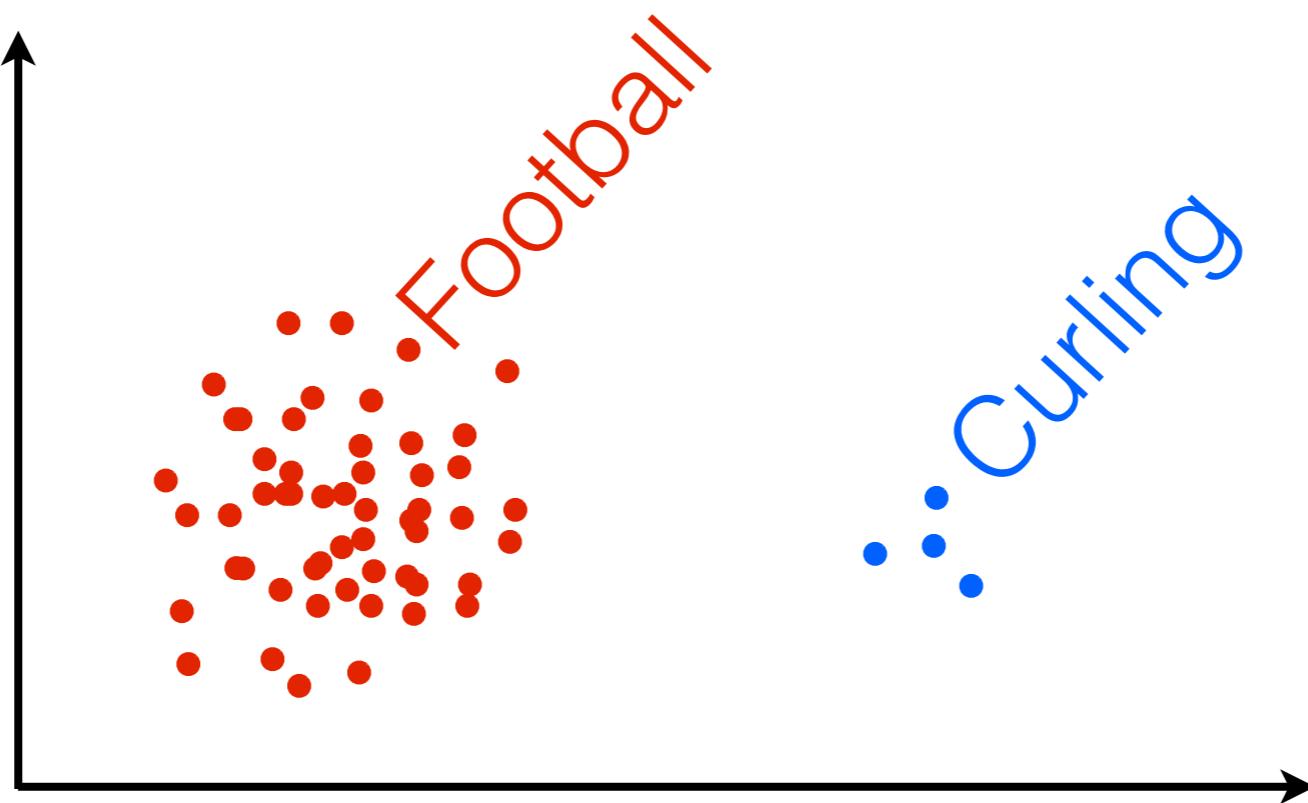
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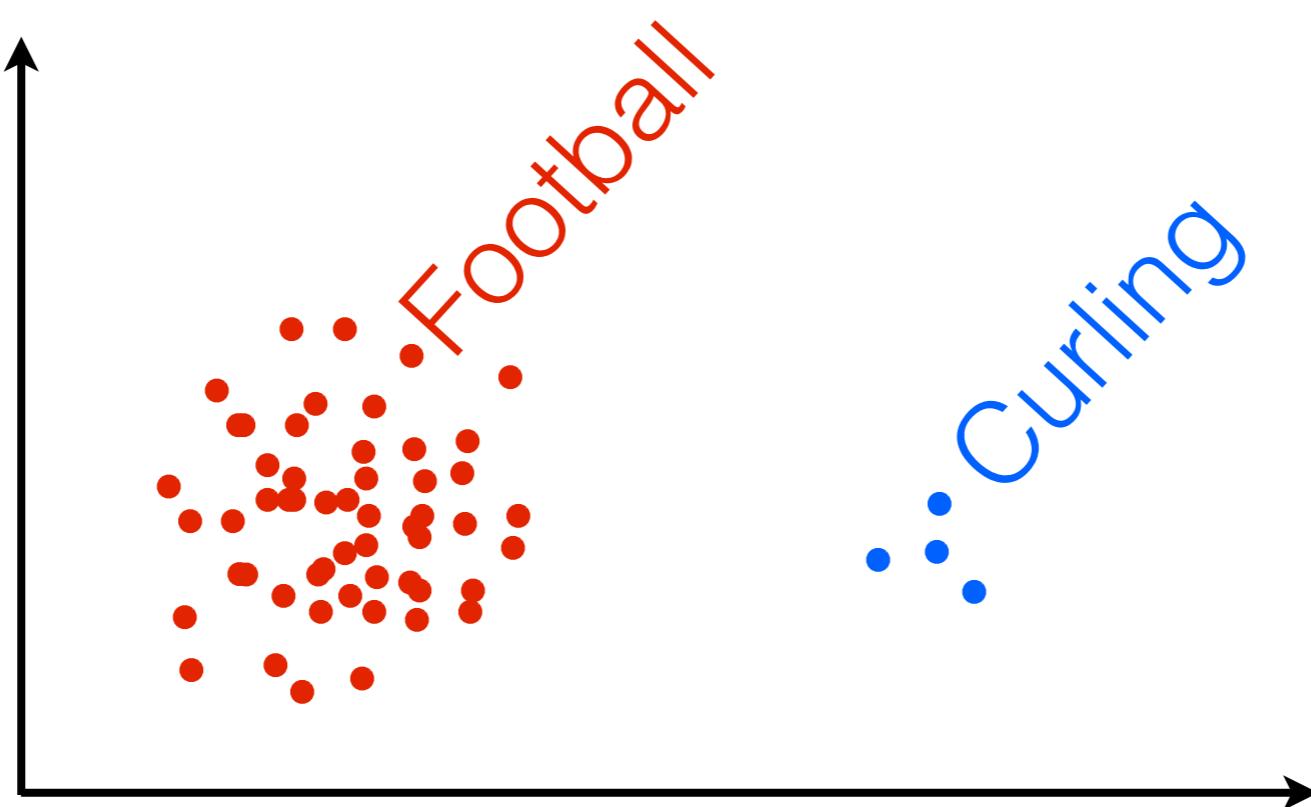
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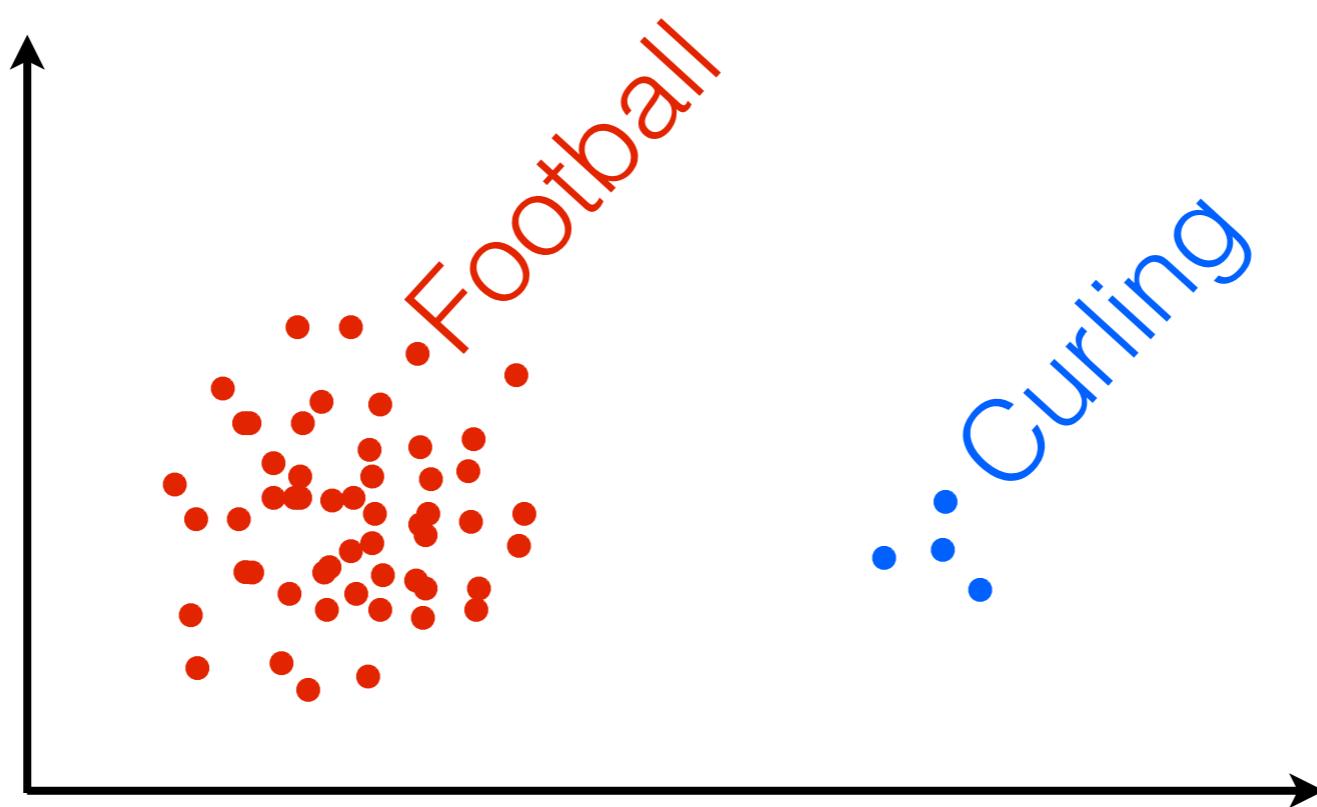
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- Coresets: pre-process data to get a smaller, weighted data set



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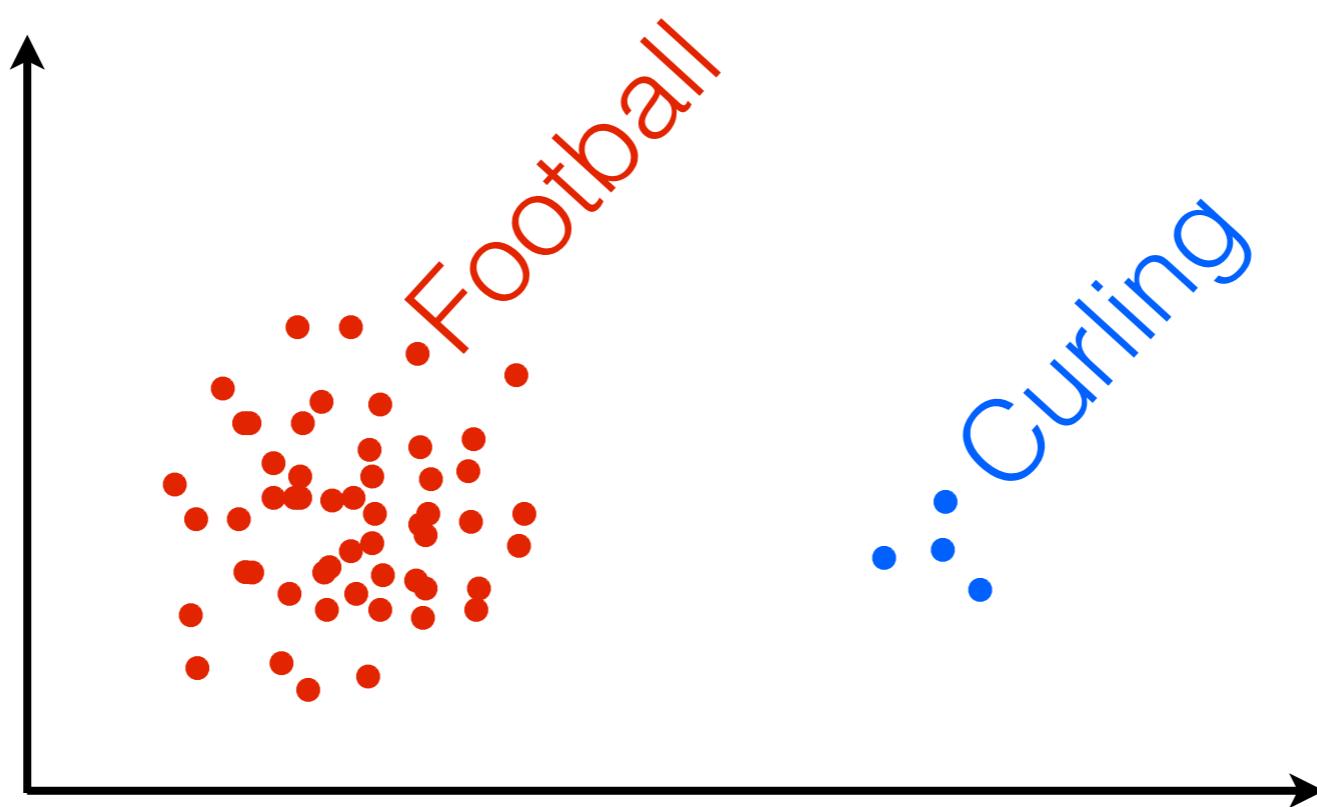
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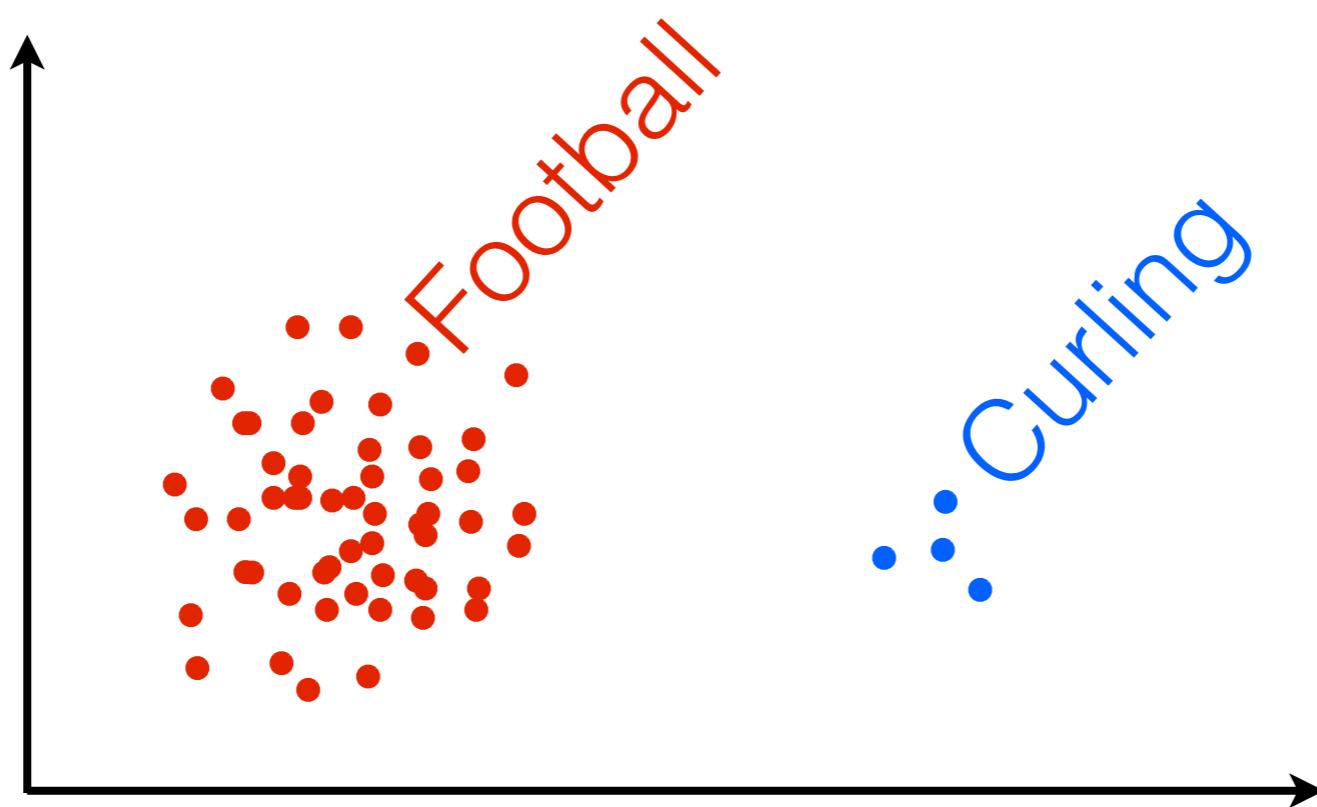
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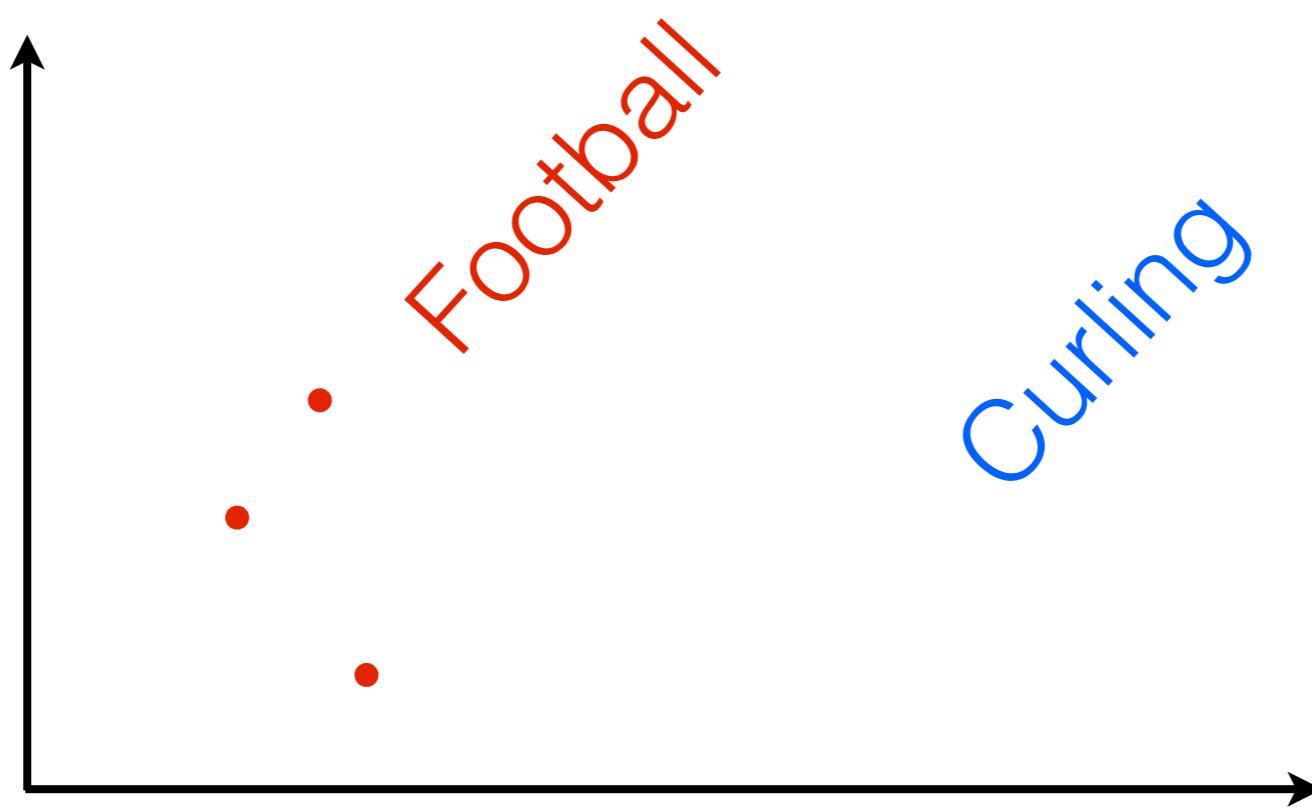
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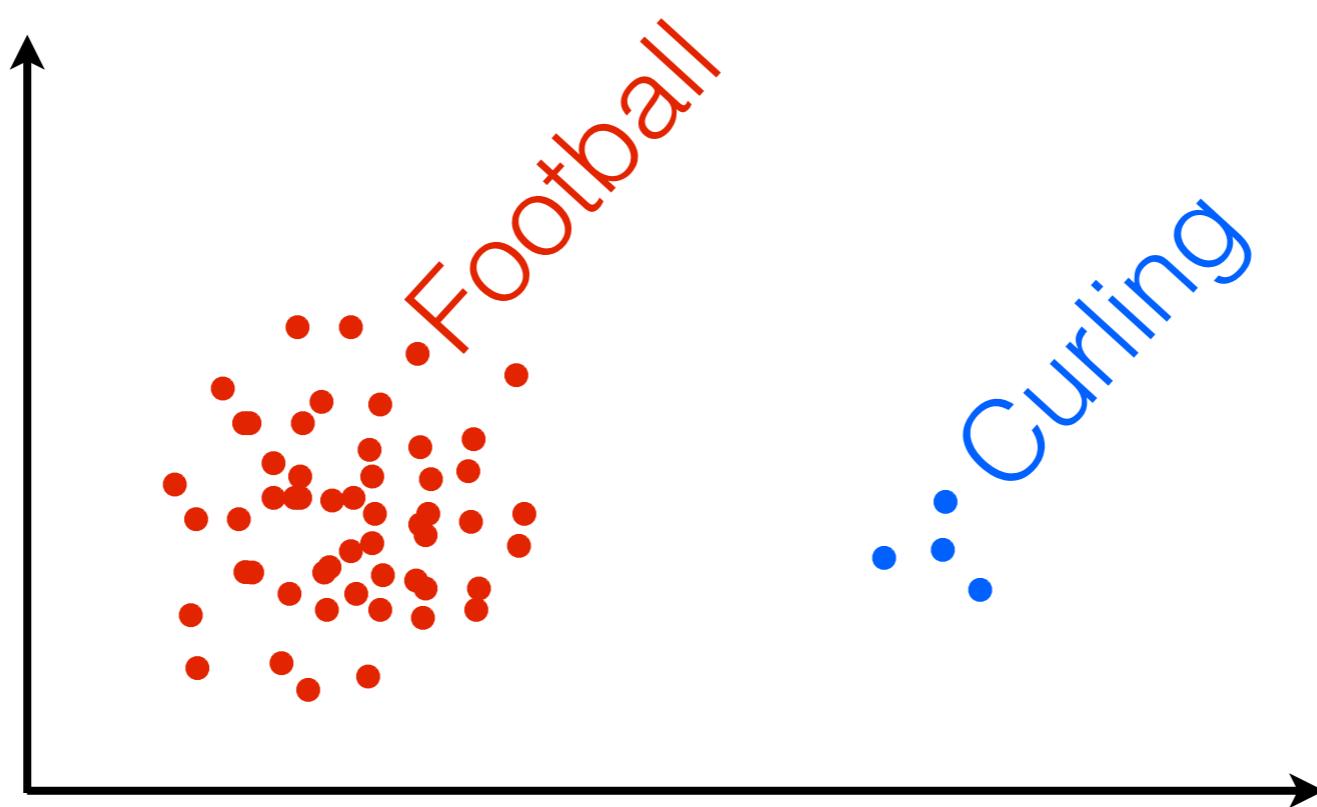
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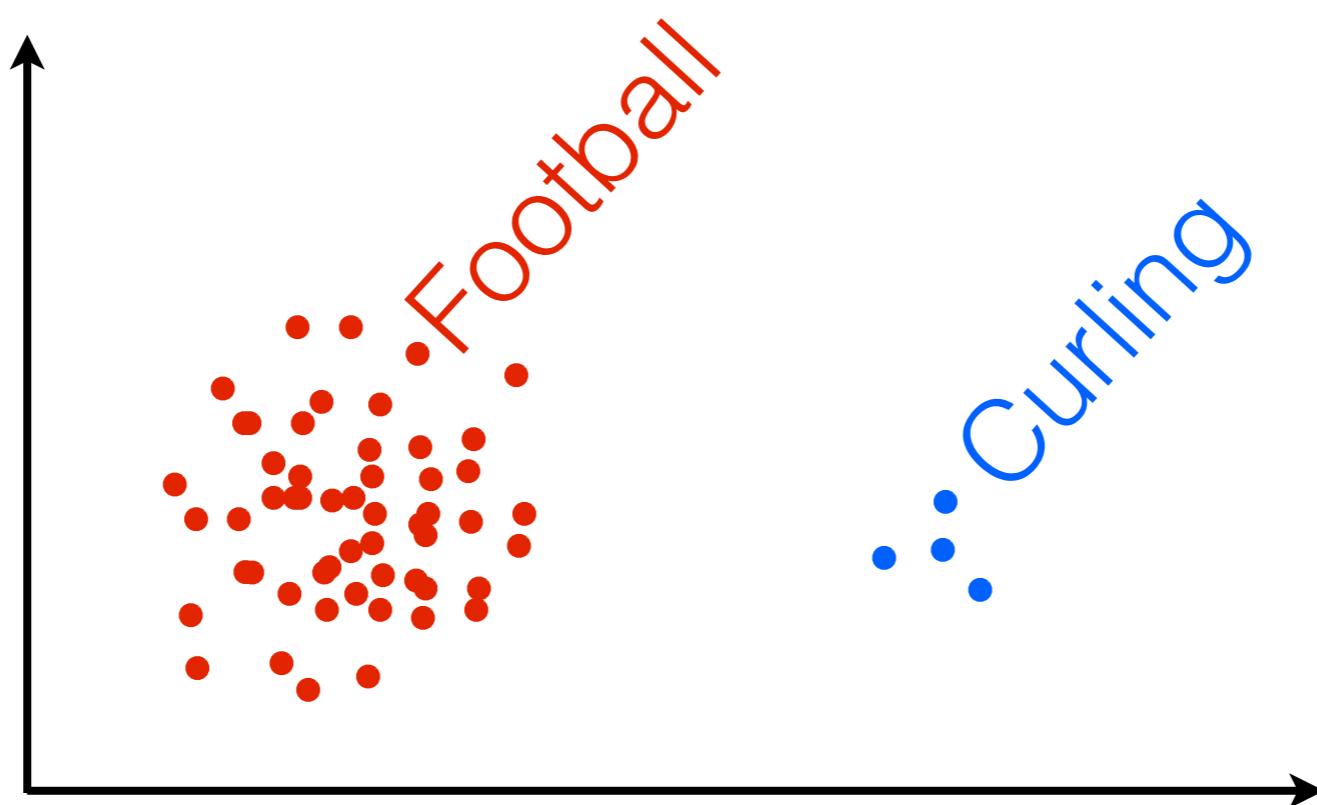
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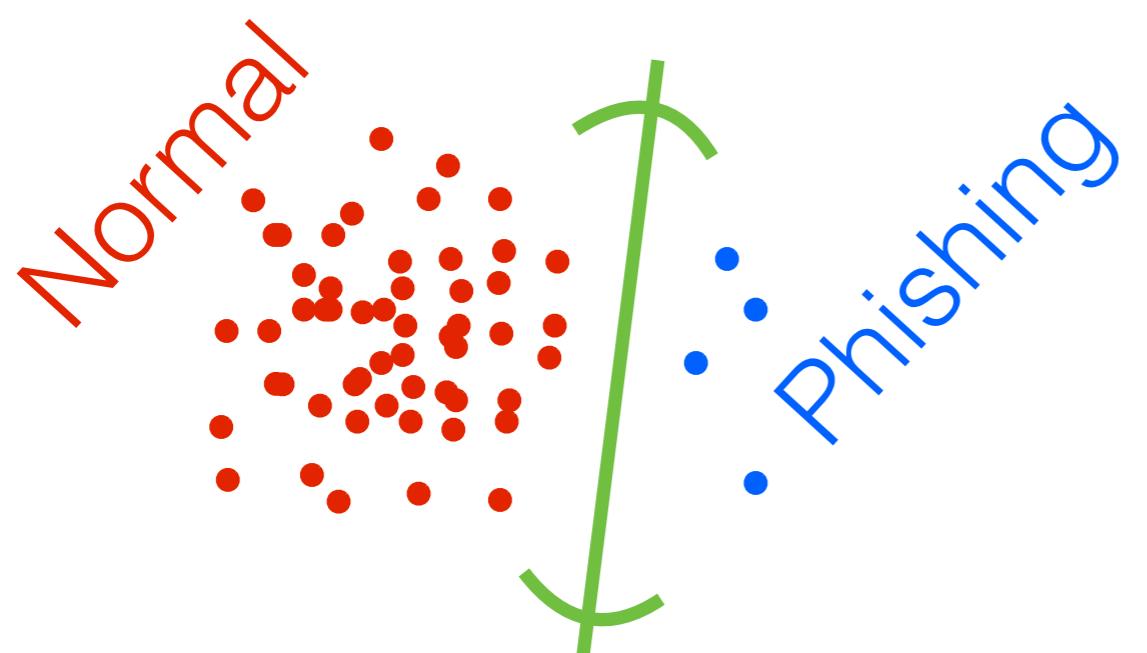


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- How to develop coresets for Bayes?

[Agarwal et al 2005; Feldman & Langberg 2011; DuMouchel et al 1999; Madigan et al 2002; Huggins, Campbell, Broderick 2016; Campbell, Broderick 2017; Campbell, Broderick 2018]

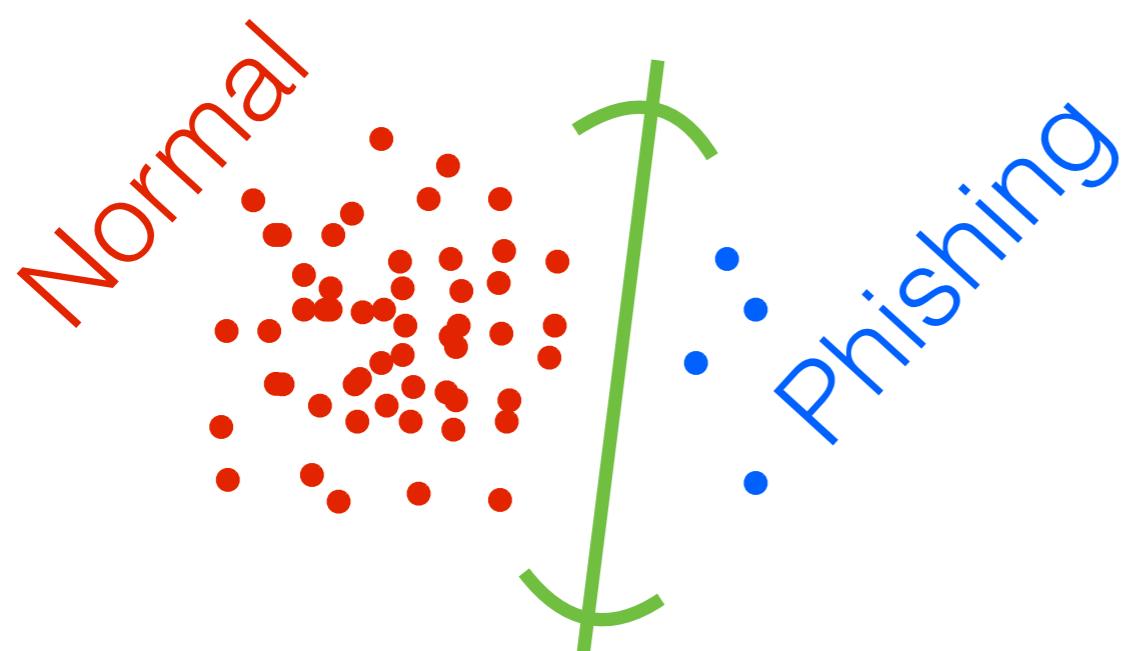
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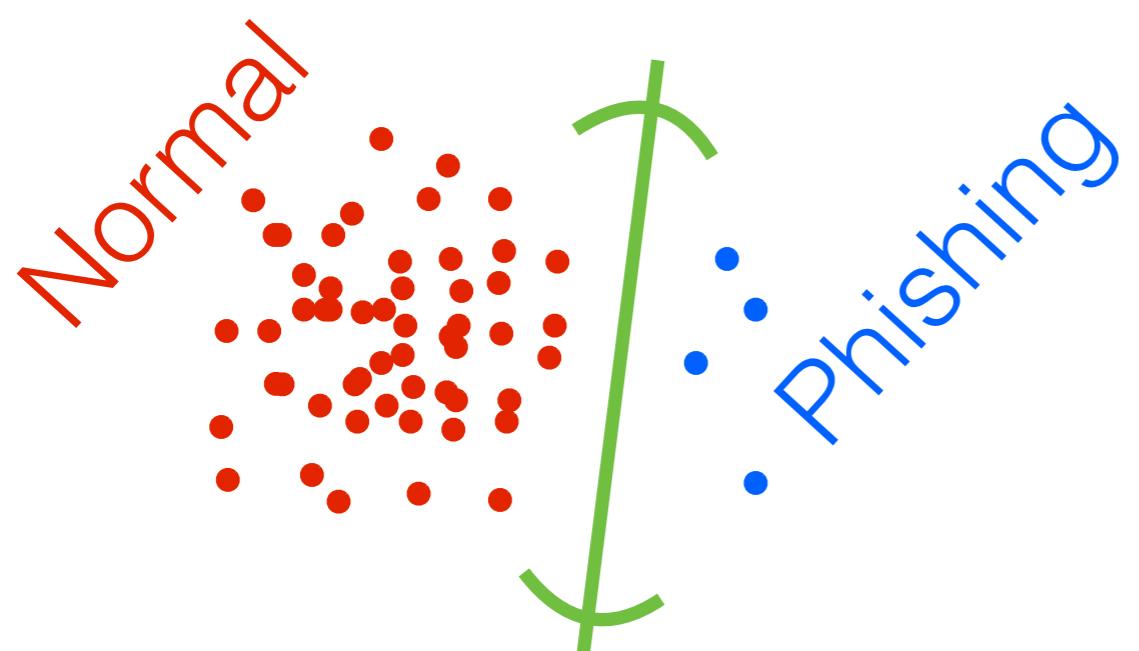
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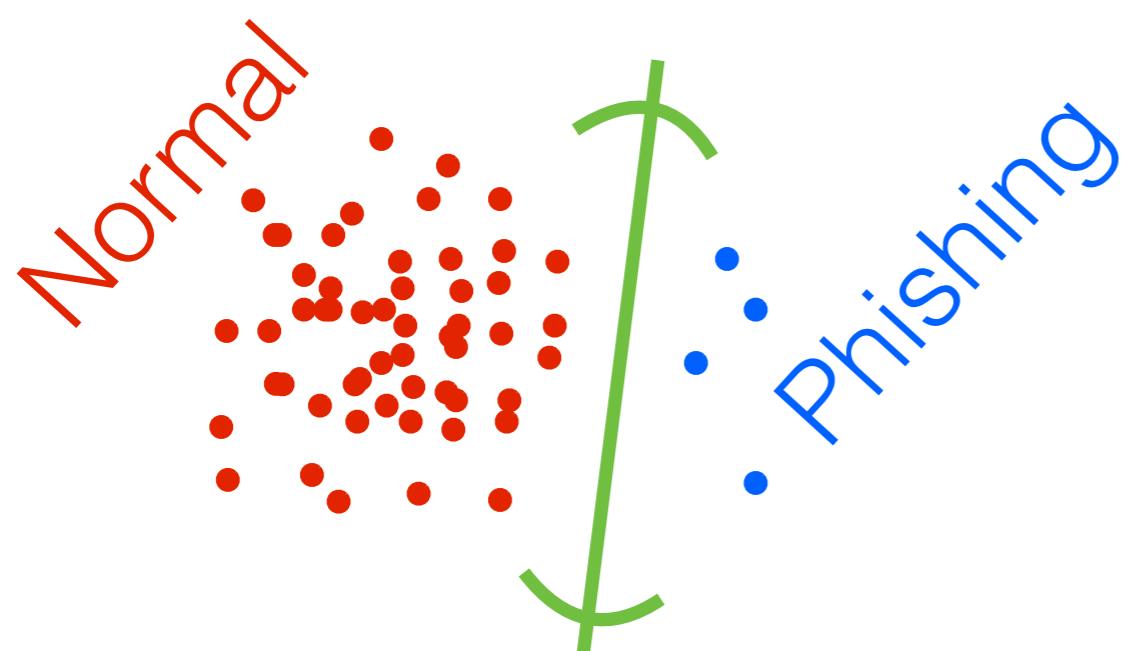
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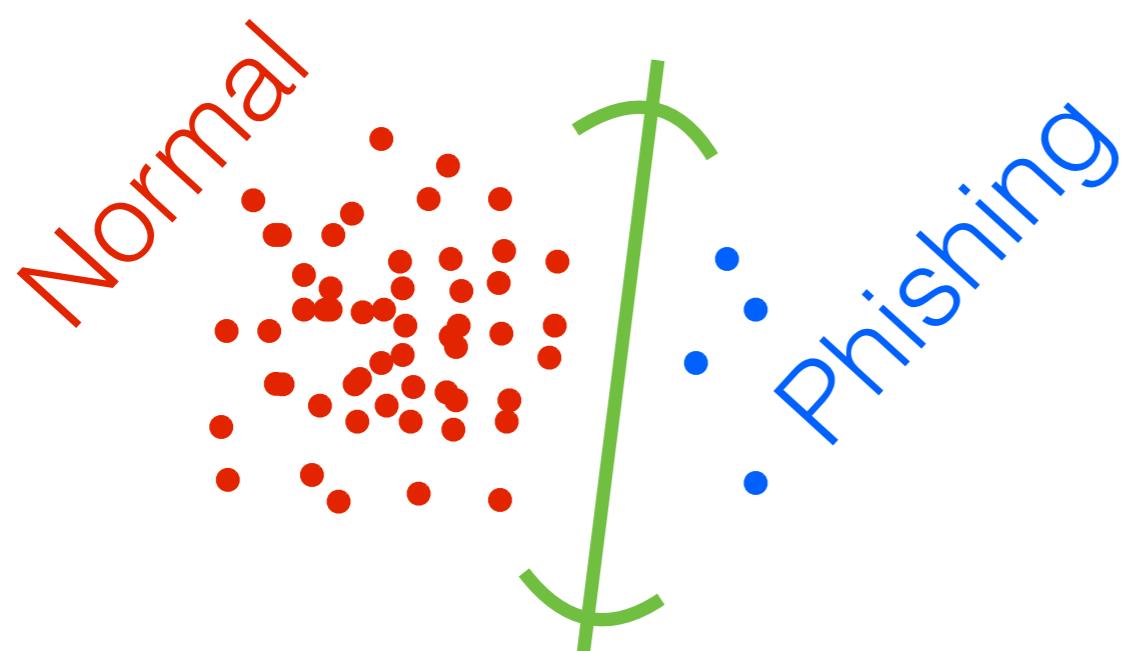
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- Coreset log likelihood $\|w\|_0 \ll N$



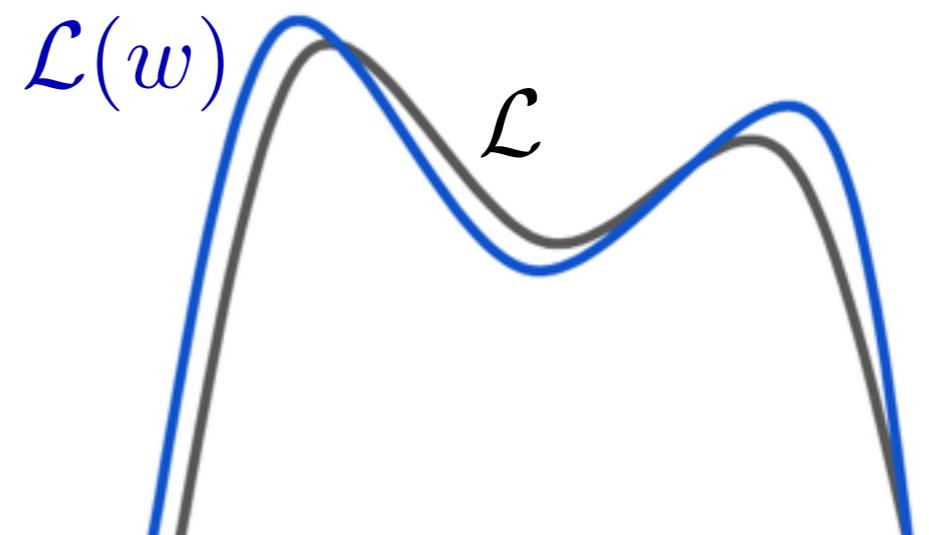
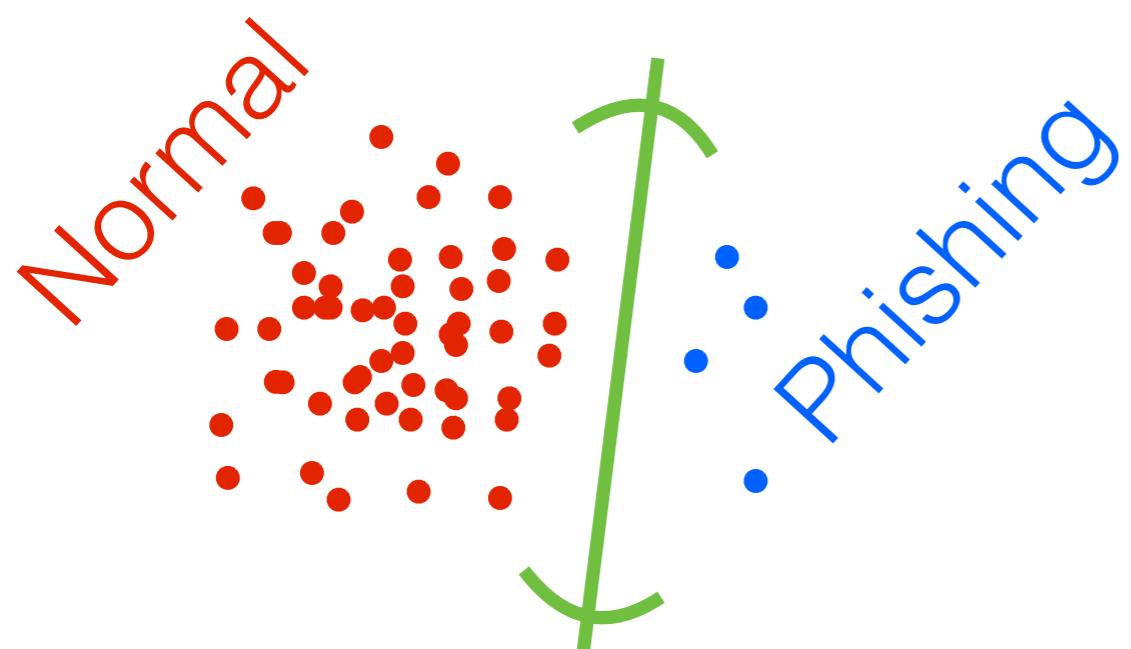
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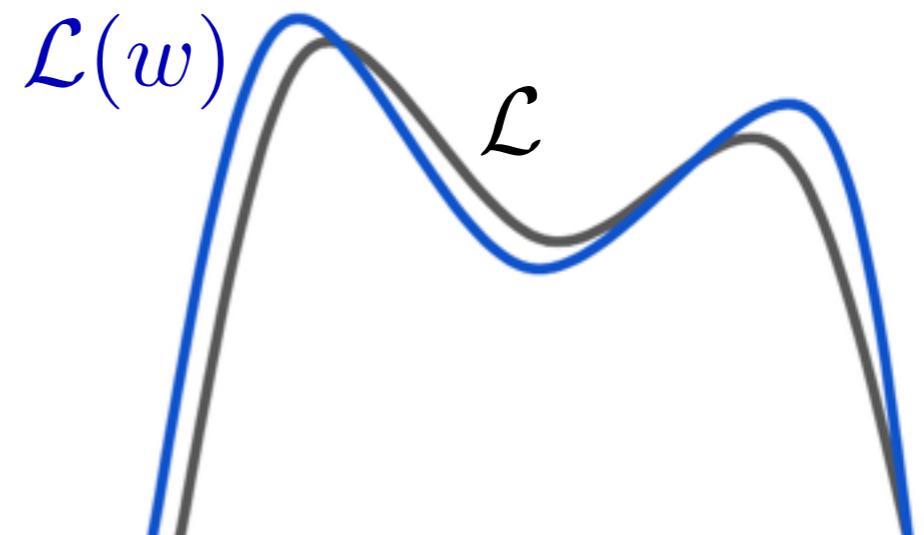
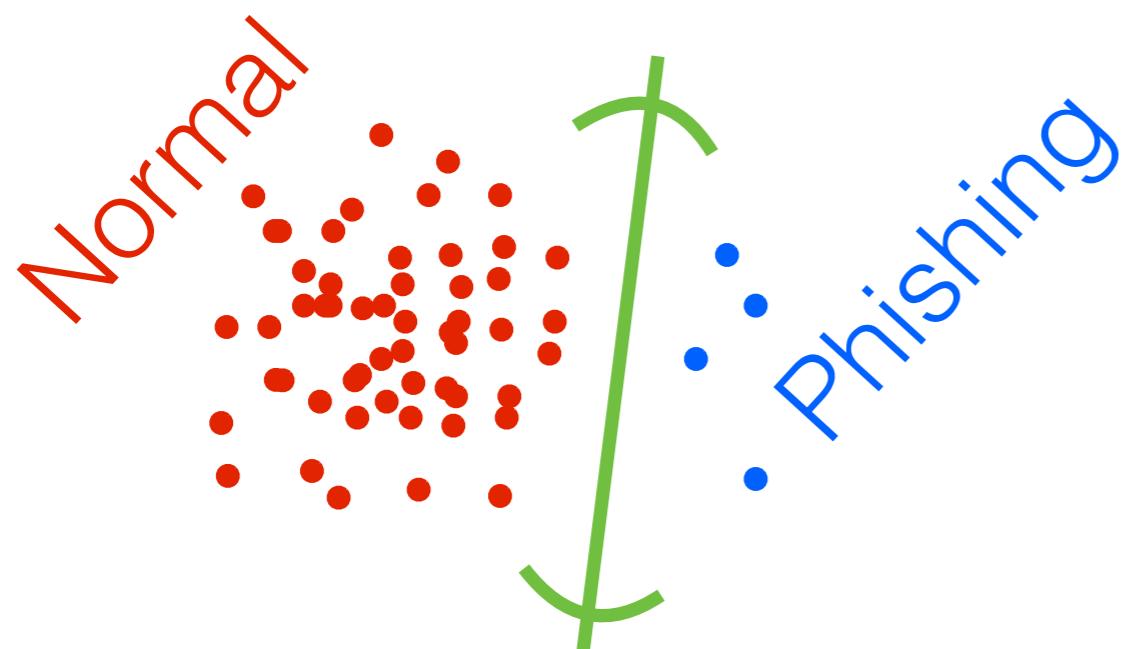
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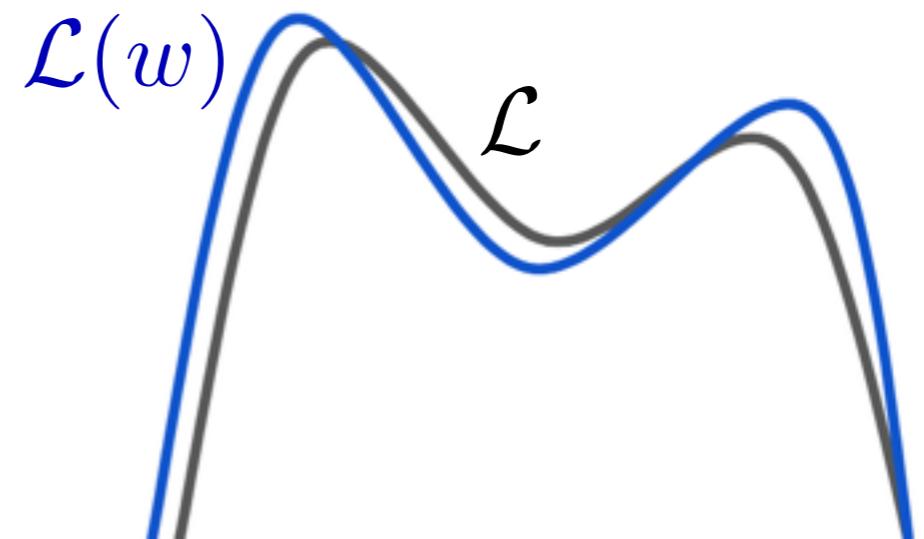
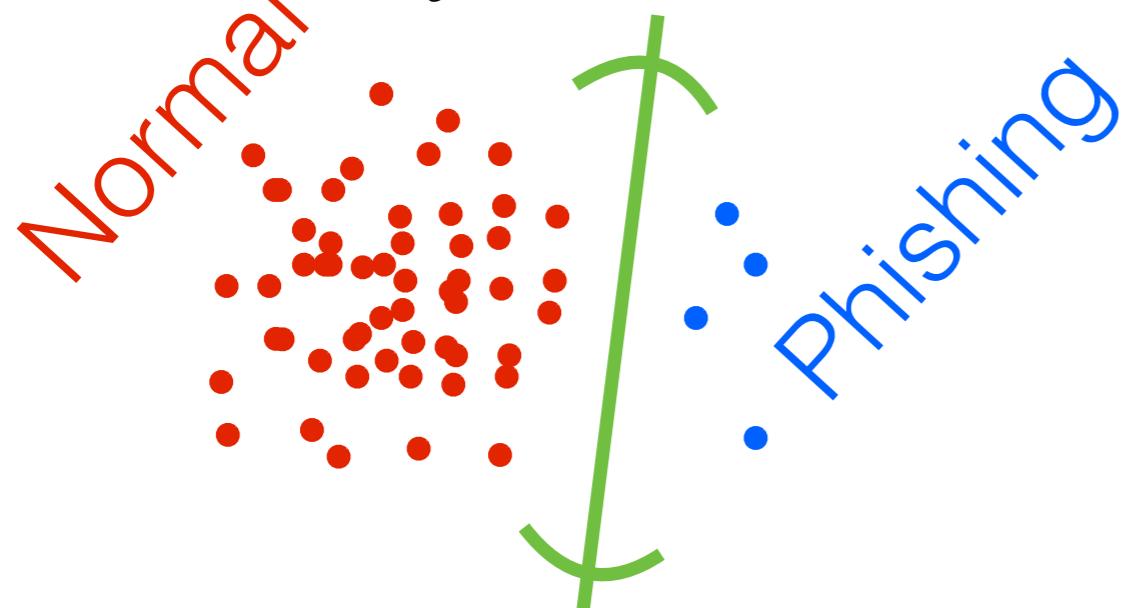
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- ϵ -coreset: $\|\mathcal{L}(w) - \mathcal{L}\| \leq \epsilon$



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- Posterior $p(\theta|y) \propto p(y|\theta)p(\theta)$
- Log likelihood $\mathcal{L}_n(\theta) := \log p(y_n|\theta)$, $\mathcal{L}(\theta) := \sum_{n=1}^N \mathcal{L}_n(\theta)$
- Coreset log likelihood $\mathcal{L}(w, \theta) := \sum_{n=1}^N w_n \mathcal{L}_n(\theta)$ s.t. $\|w\|_0 \ll N$
- ϵ -coreset: $\|\mathcal{L}(w) - \mathcal{L}\| \leq \epsilon$
 - Approximate posterior close in Wasserstein distance
 $d_{W_j}(p_w(\cdot|y), p(\cdot|y)) \leq C_j \|\mathcal{L}(w) - \mathcal{L}\|_{WFID}, j \in \{1, 2\}$



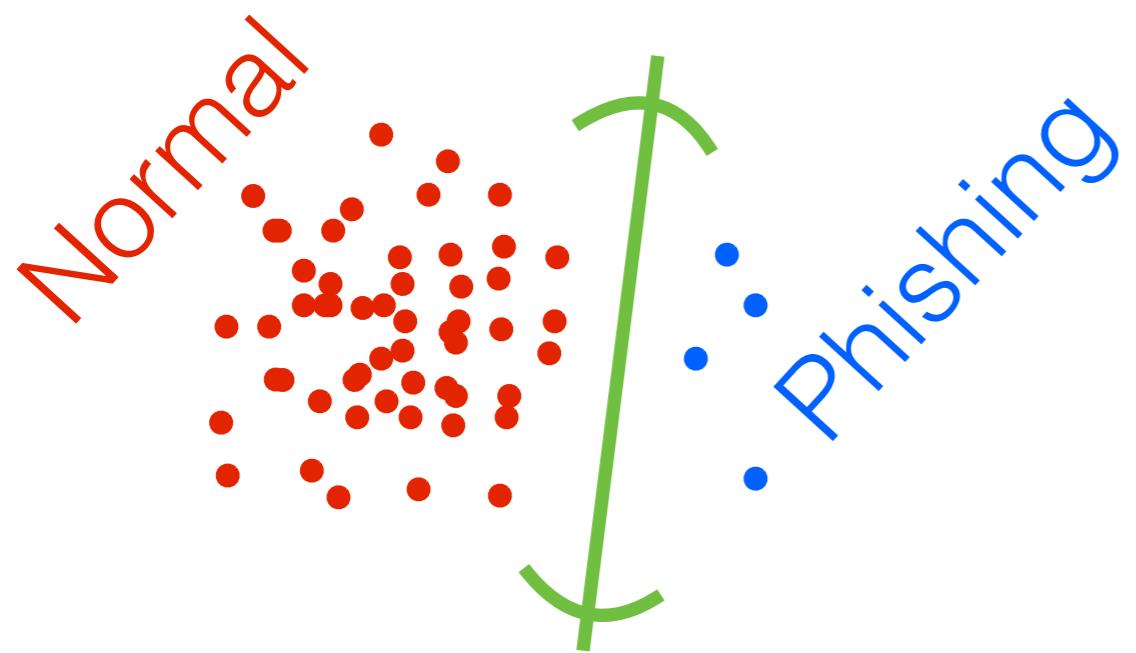
Roadmap

- Approximate Bayes review
- The “core” of the data set
- Uniform data subsampling isn’t enough
- Importance sampling for “coresets”
- Optimization for “coresets”
- Approximate sufficient statistics

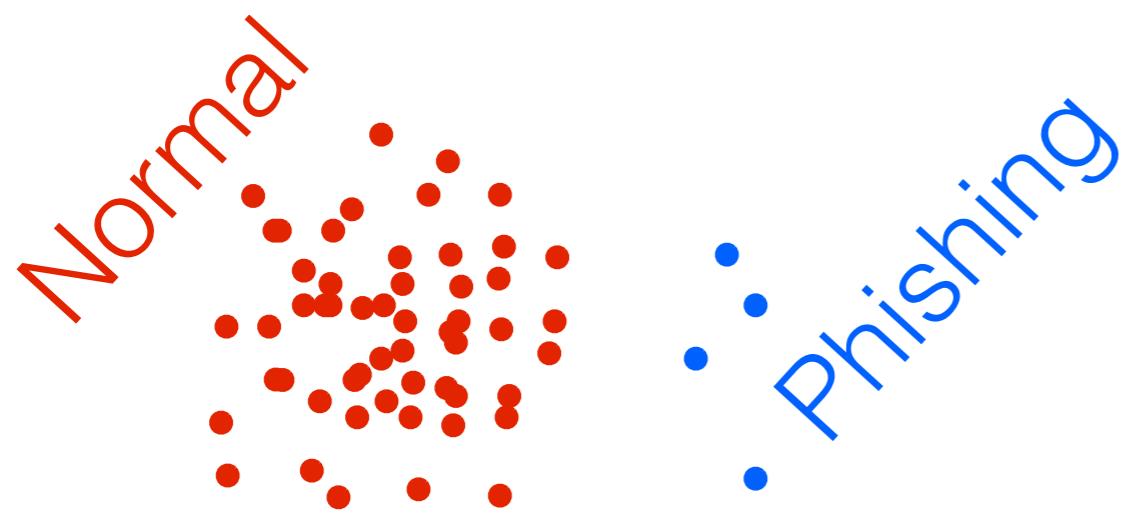
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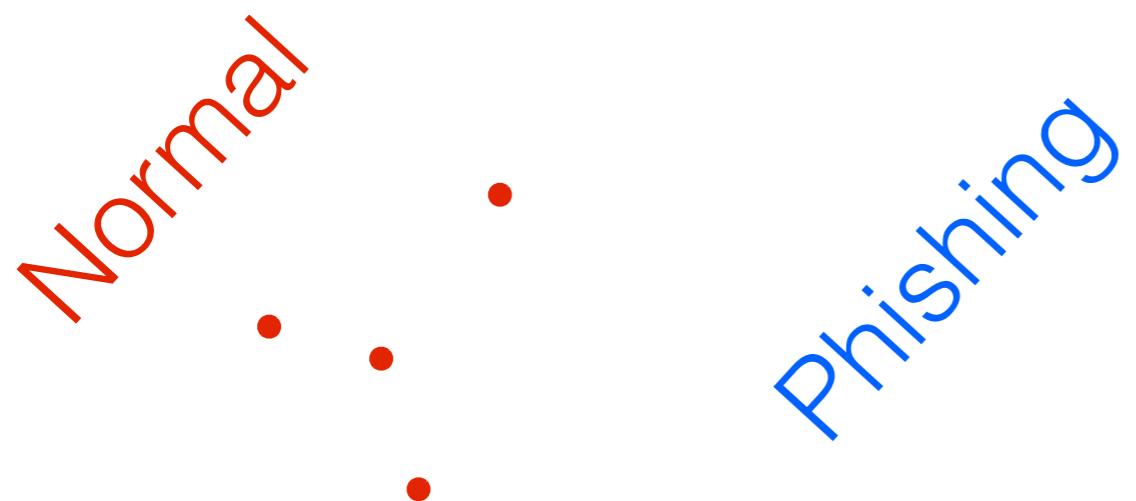
Uniform subsampling revisited



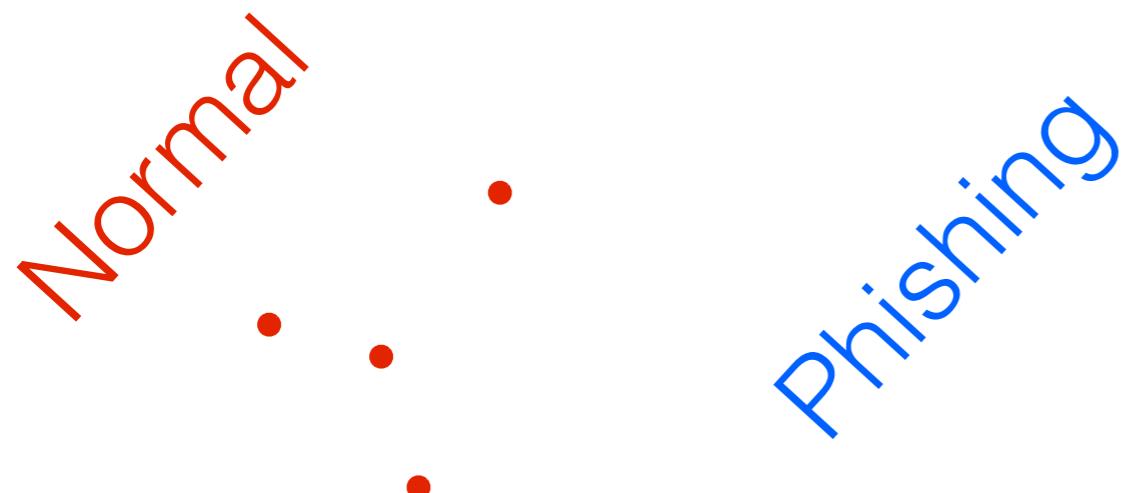
Uniform subsampling revisited



Uniform subsampling revisited

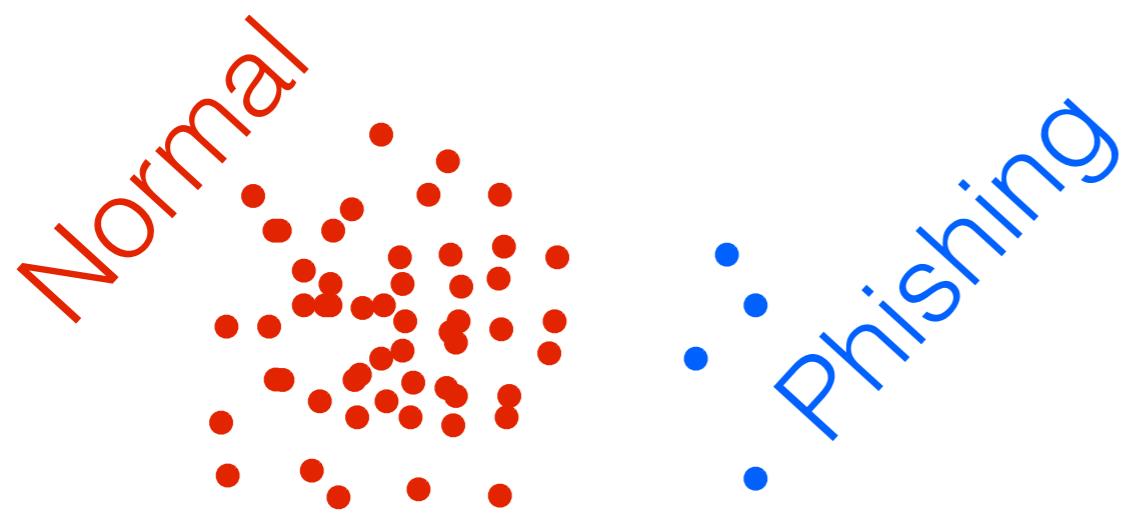


Uniform subsampling revisited



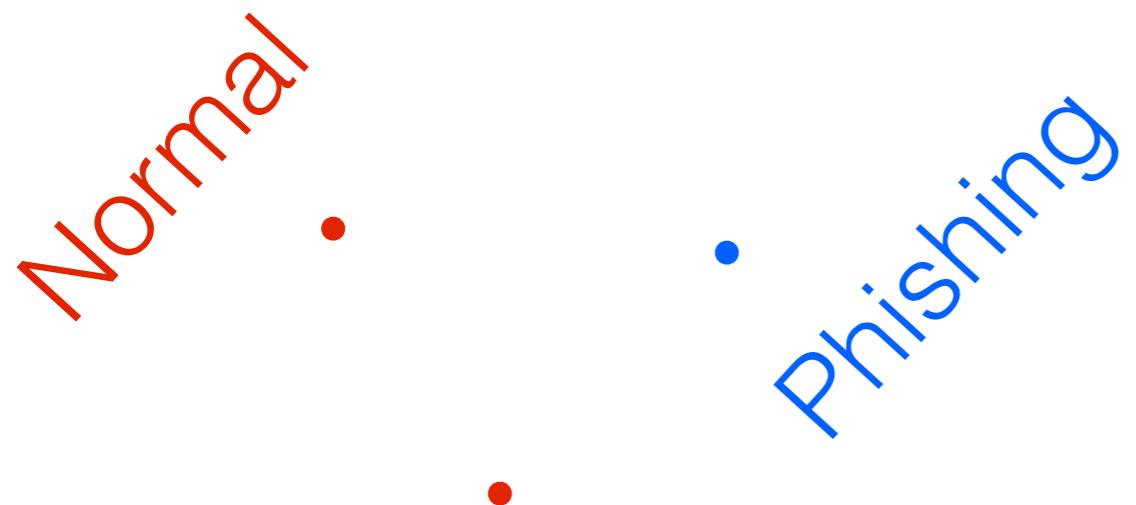
- Might miss important data

Uniform subsampling revisited



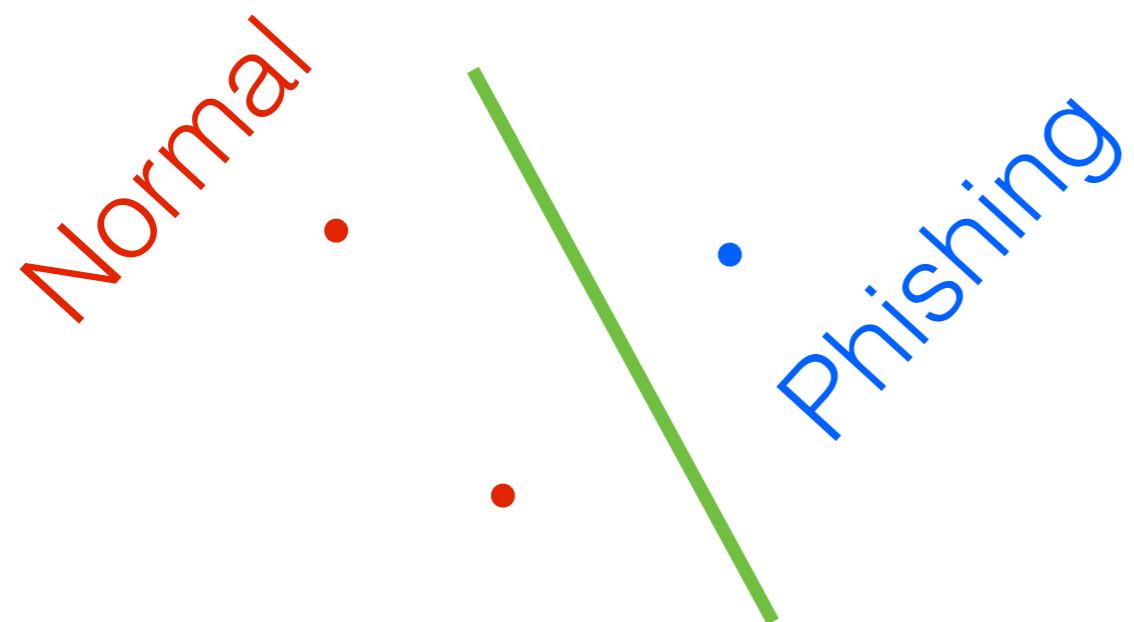
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Uniform subsampling revisited



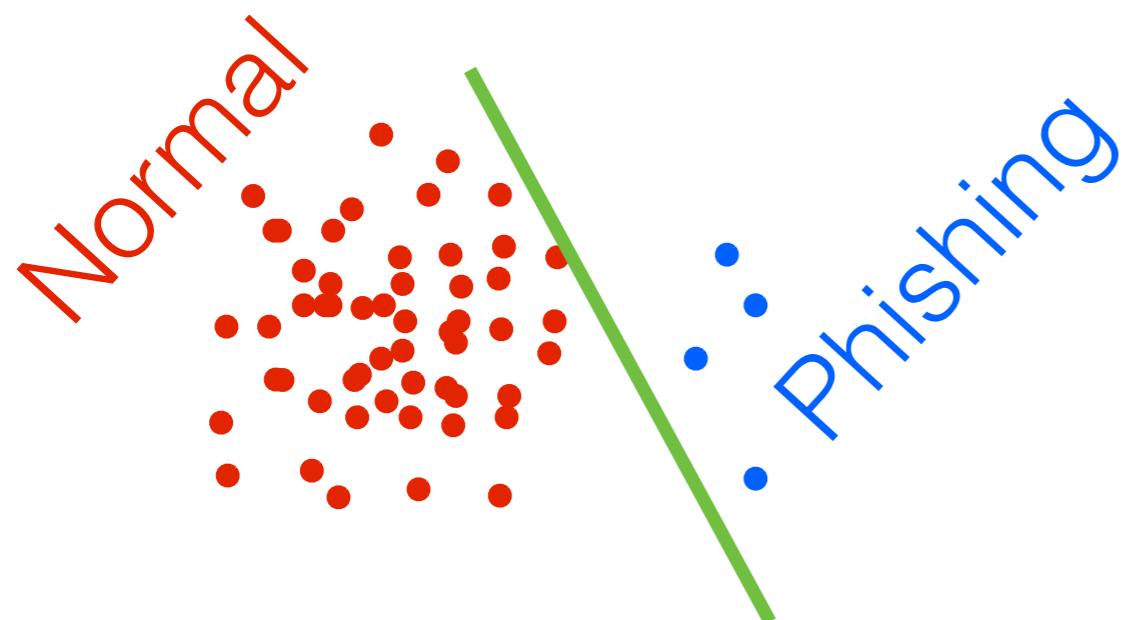
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Uniform subsampling revisited



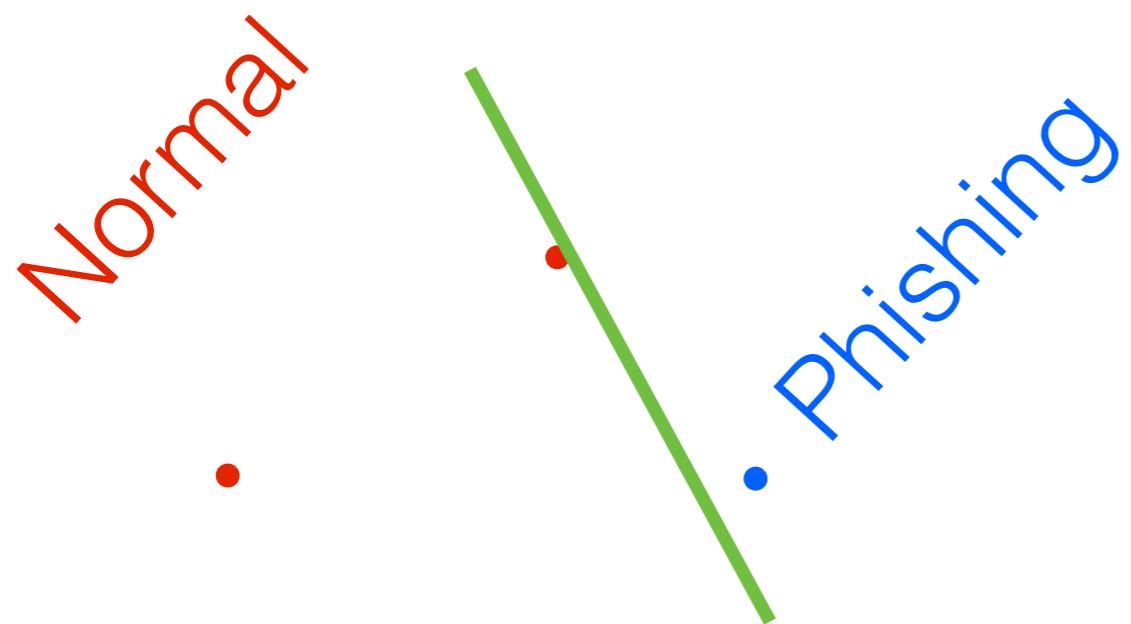
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Uniform subsampling revisited



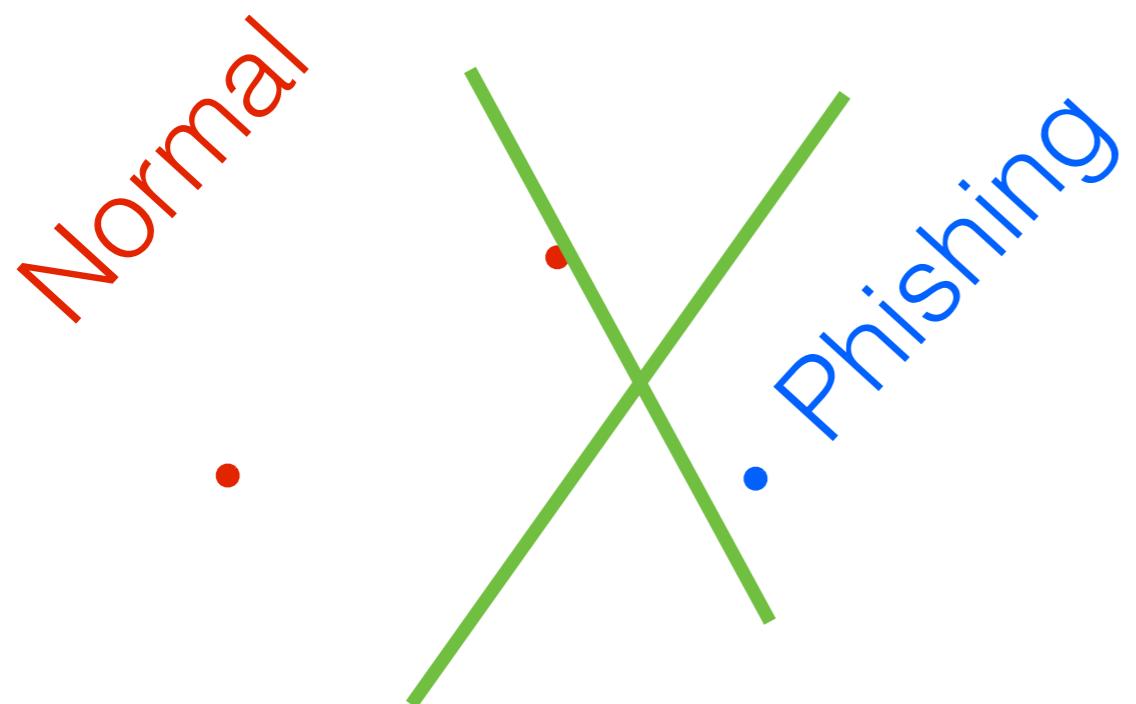
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Uniform subsampling revisited



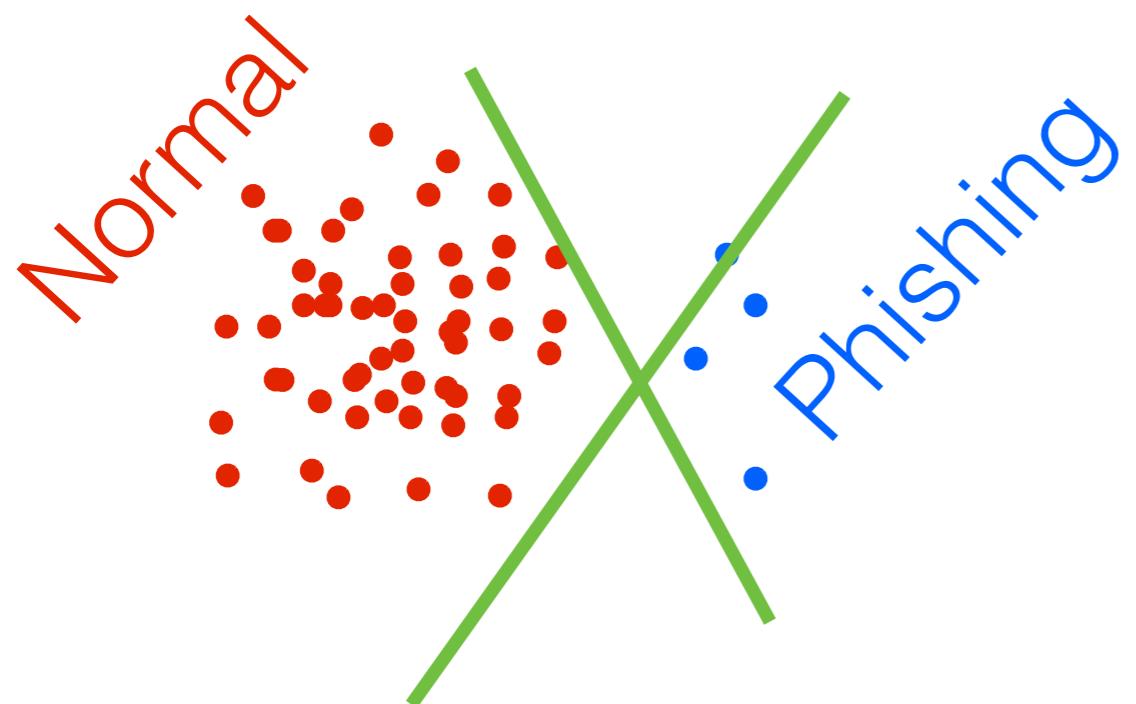
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Uniform subsampling revisited



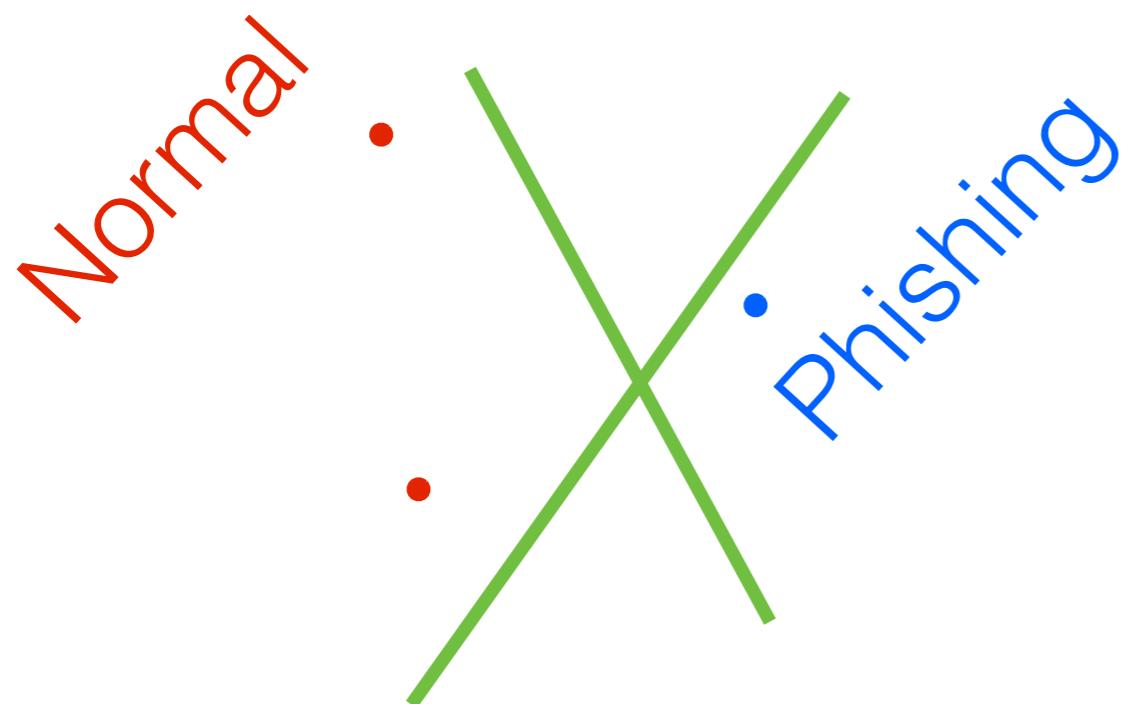
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Uniform subsampling revisited



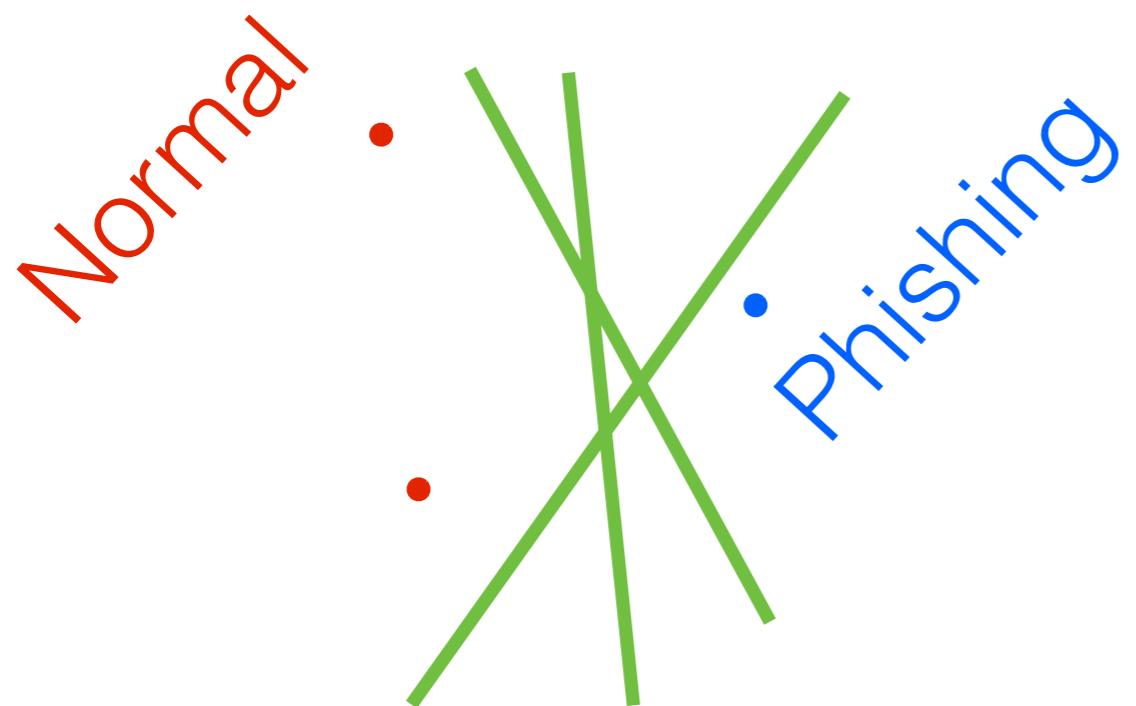
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Uniform subsampling revisited



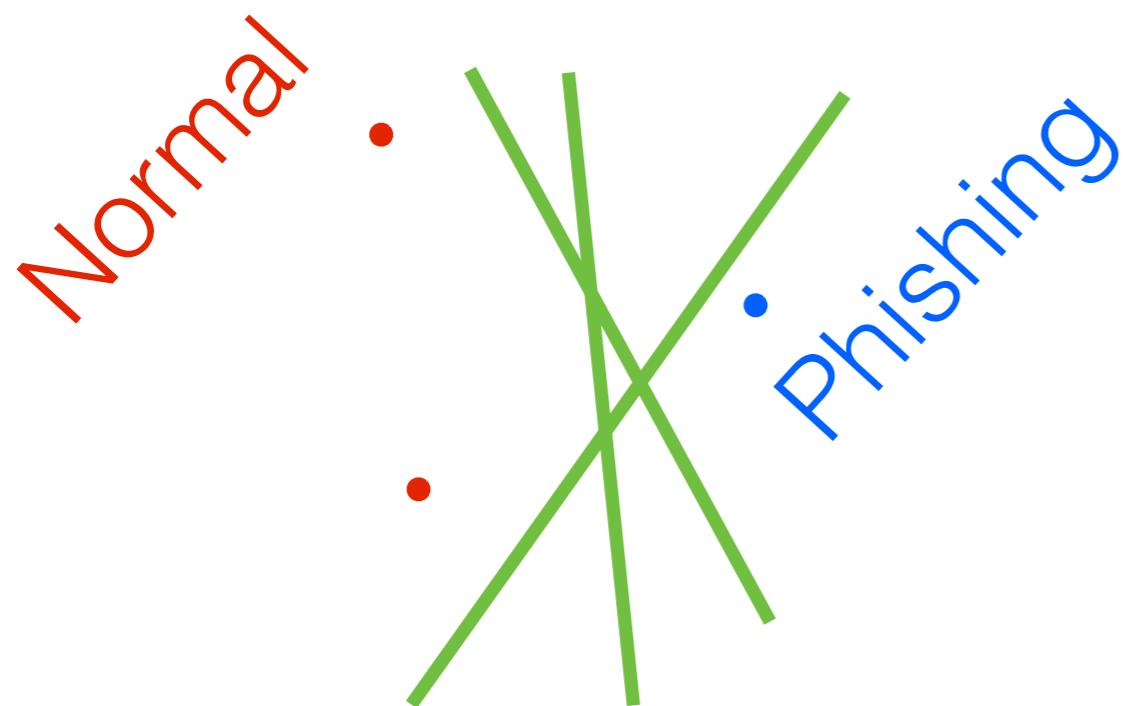
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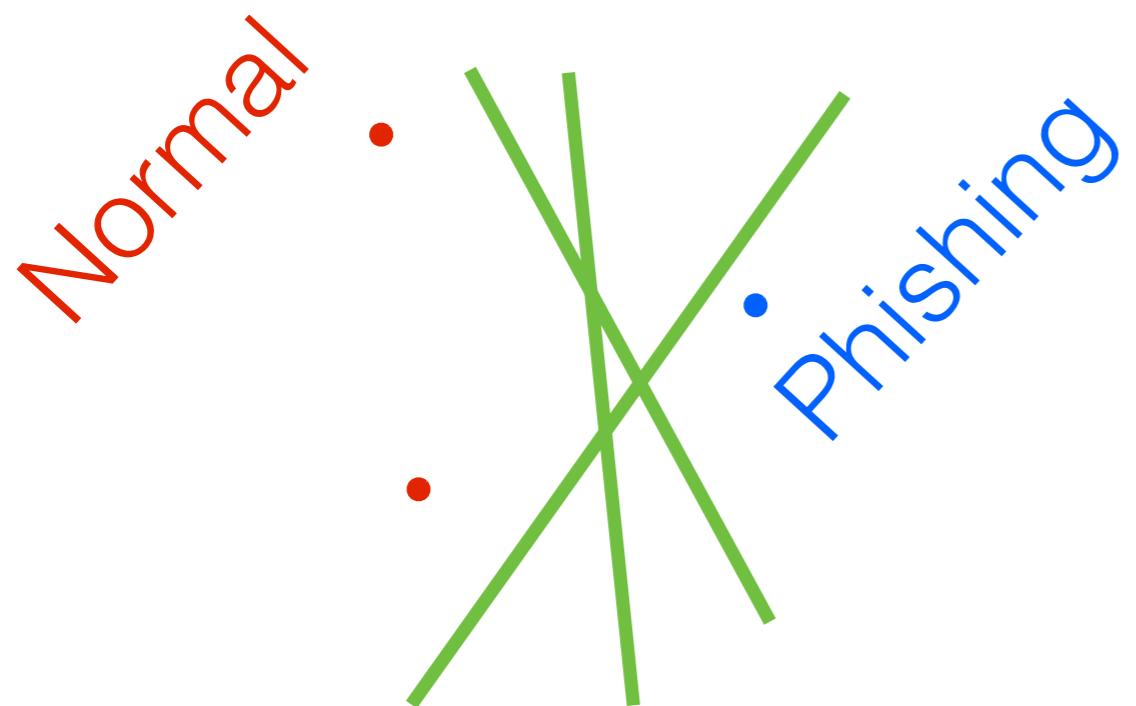
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Uniform subsampling revisited

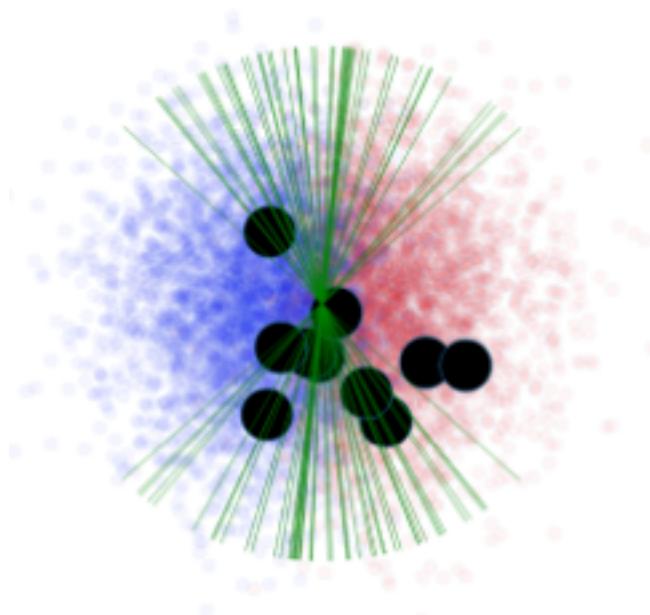


- Might miss important data
- Noisy estimates

Uniform subsampling revisited

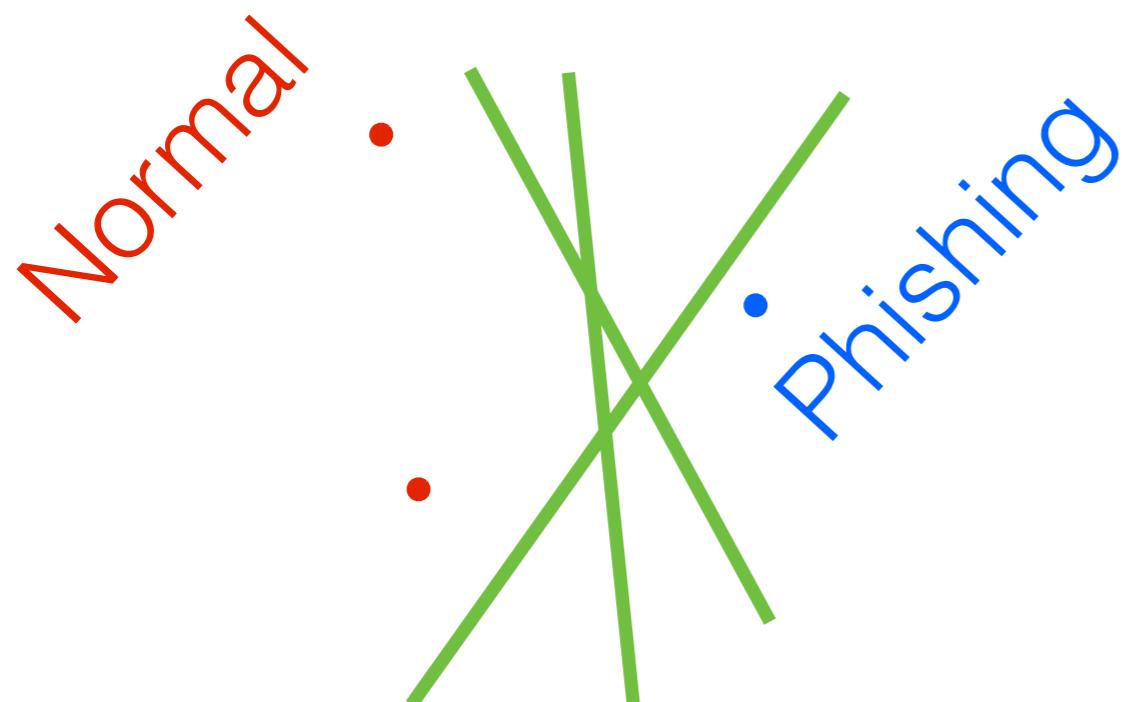


- Might miss important data
- Noisy estimates

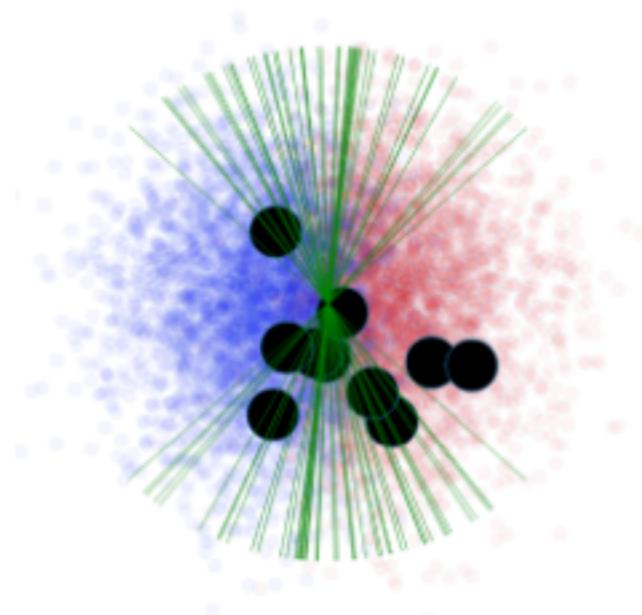


$$M = 10$$

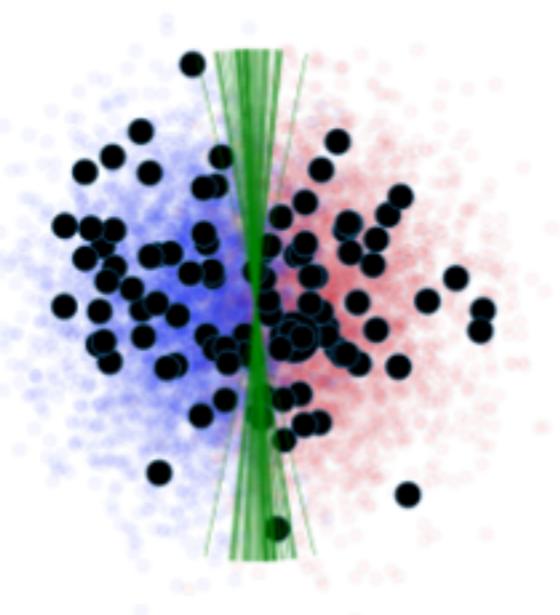
Uniform subsampling revisited



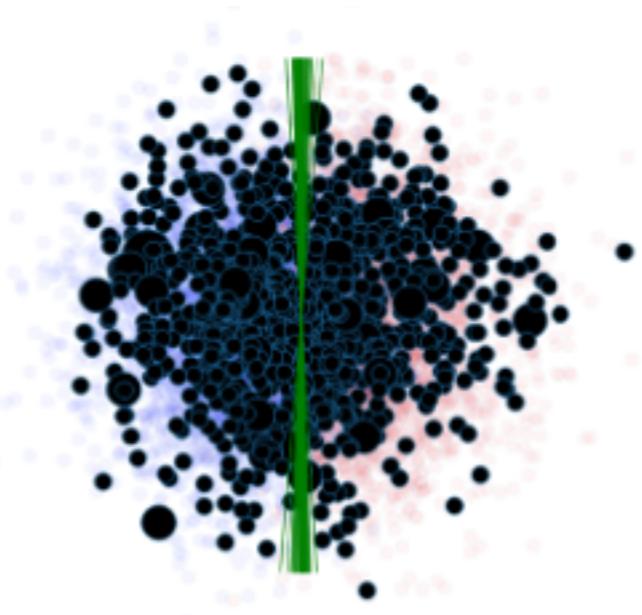
- Might miss important data
- Noisy estimates



$M = 10$



$M = 100$



$M = 1000$

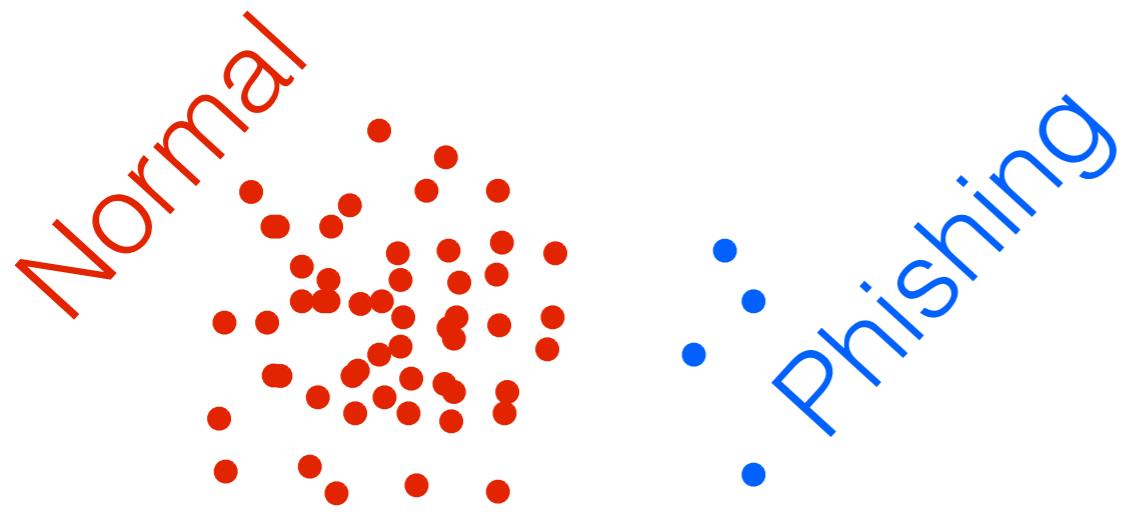
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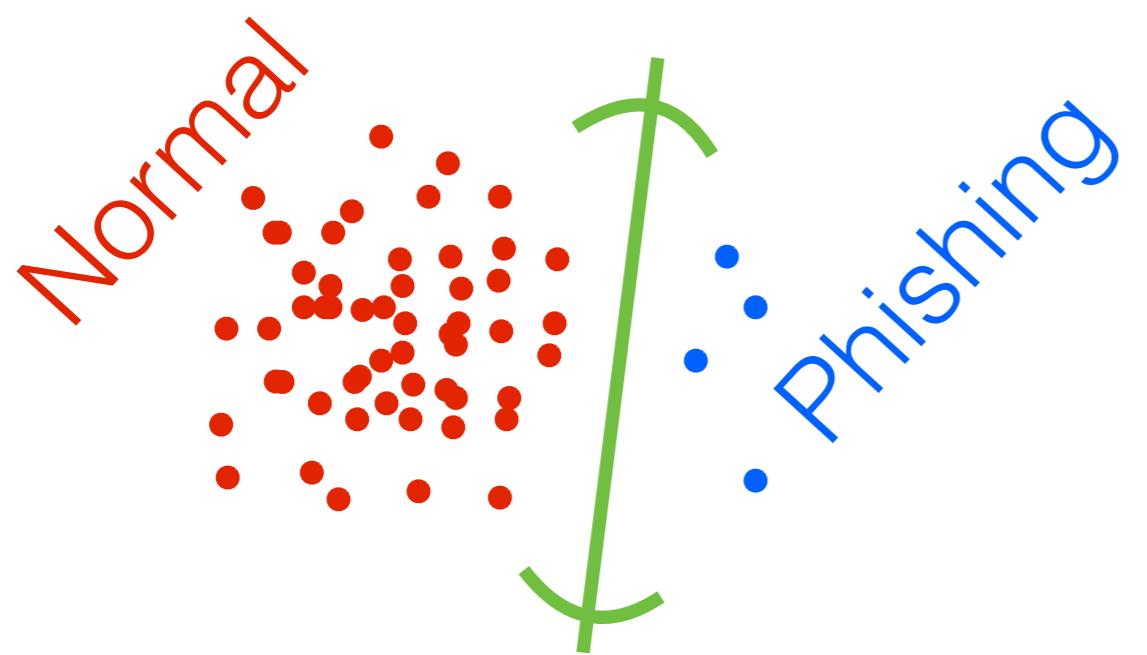
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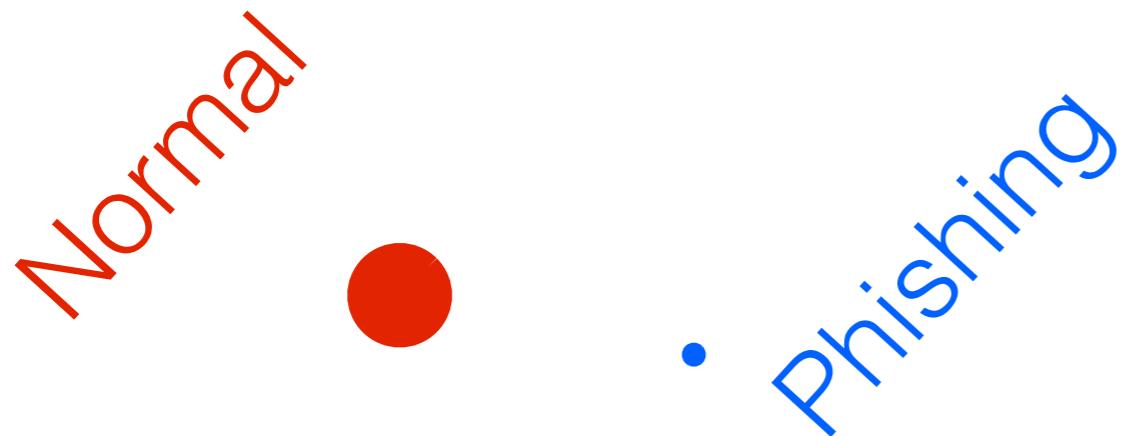
Importance sampling



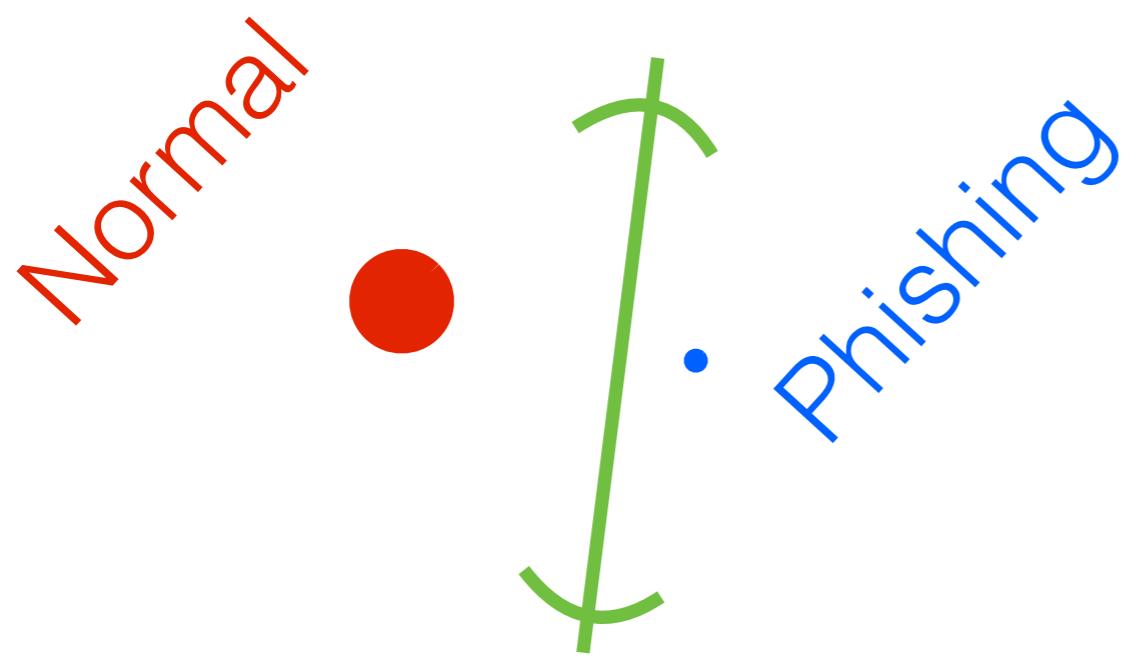
Importance sampling



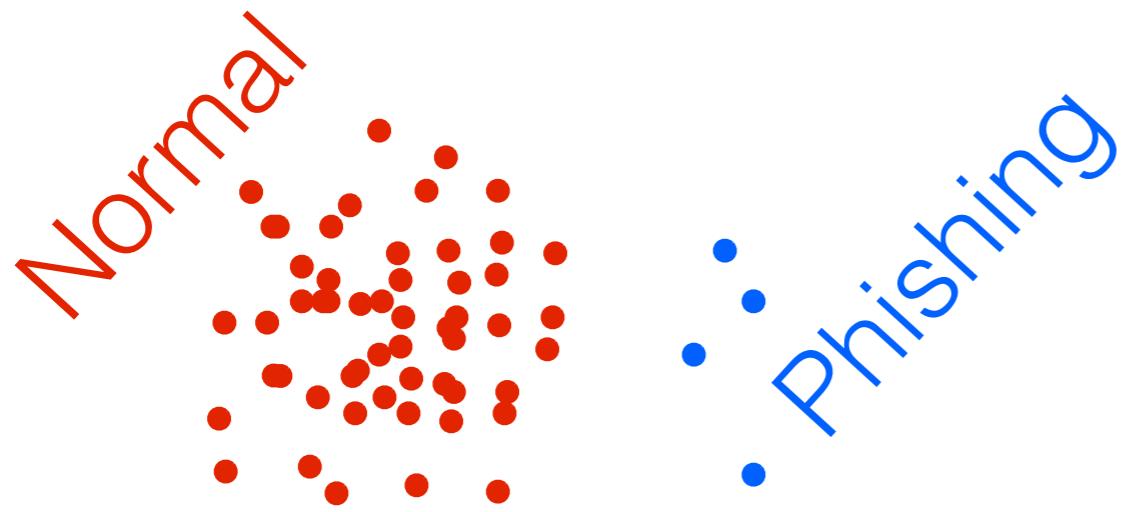
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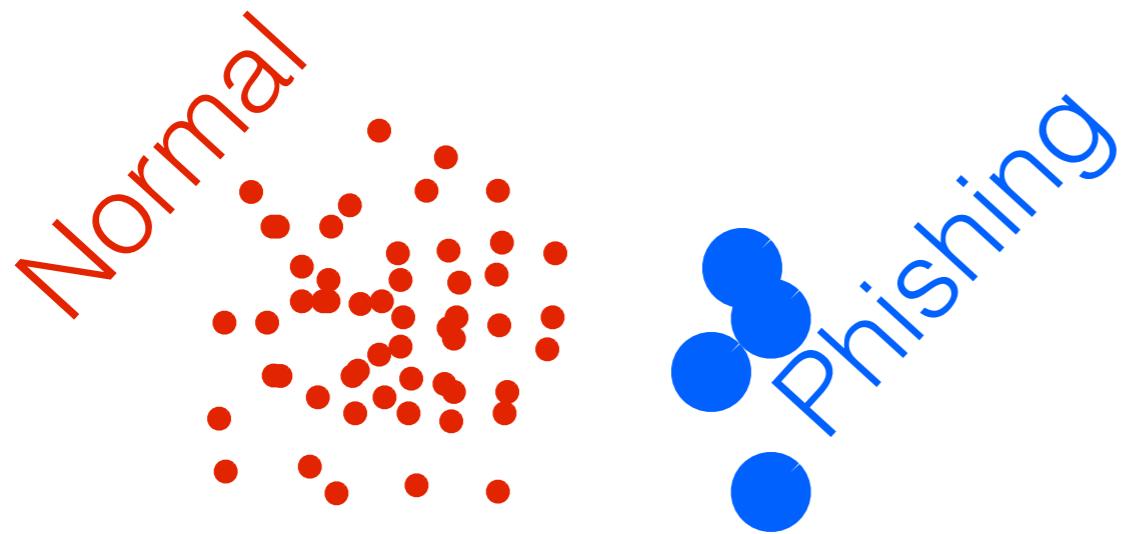
Importance sampling



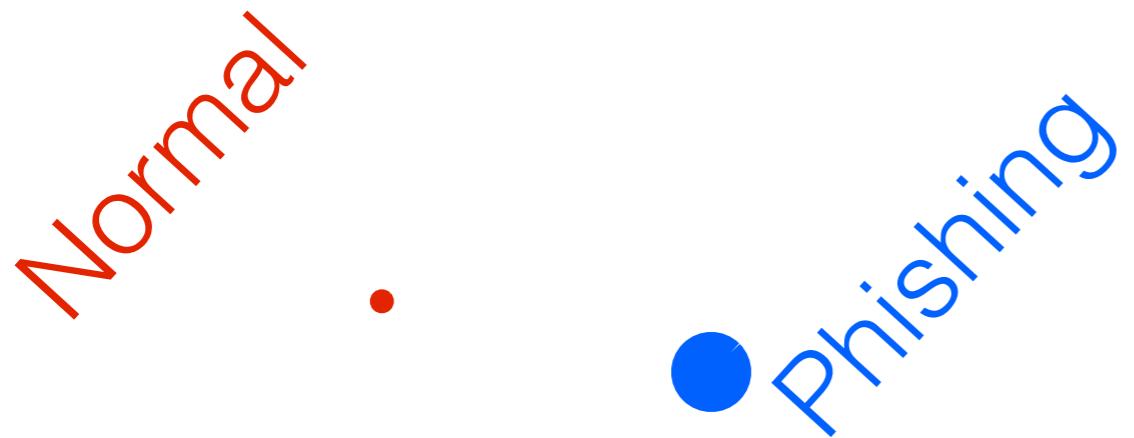
Importance sampling



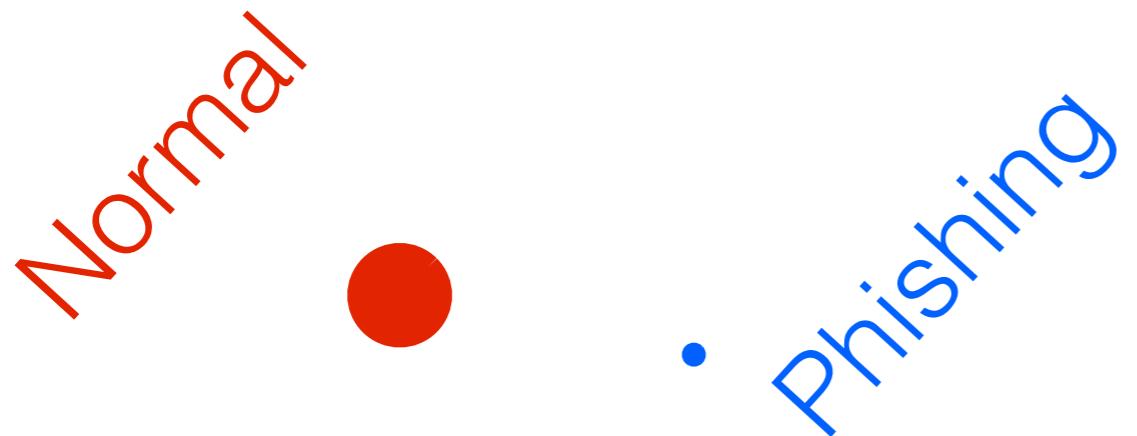
Importance sampling



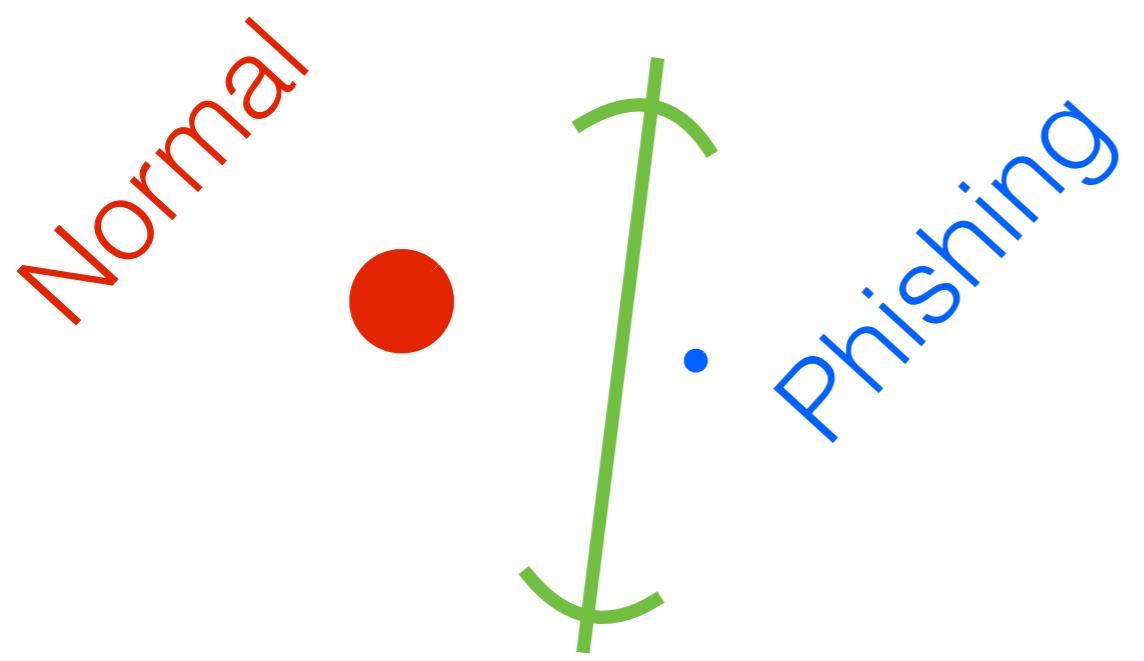
Importance sampling



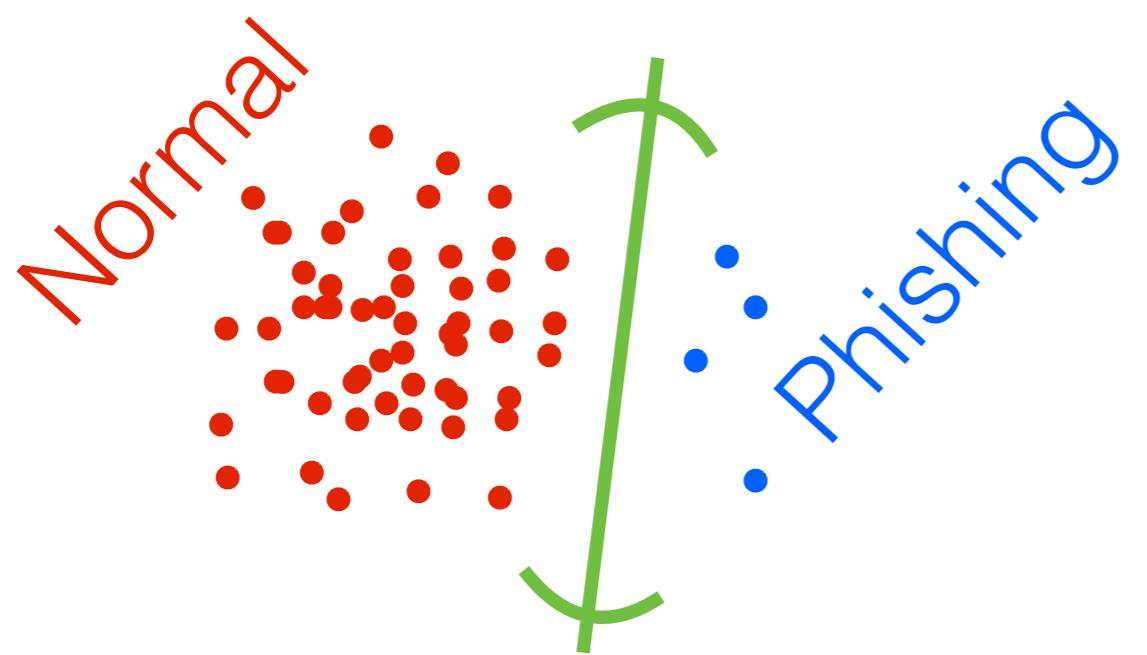
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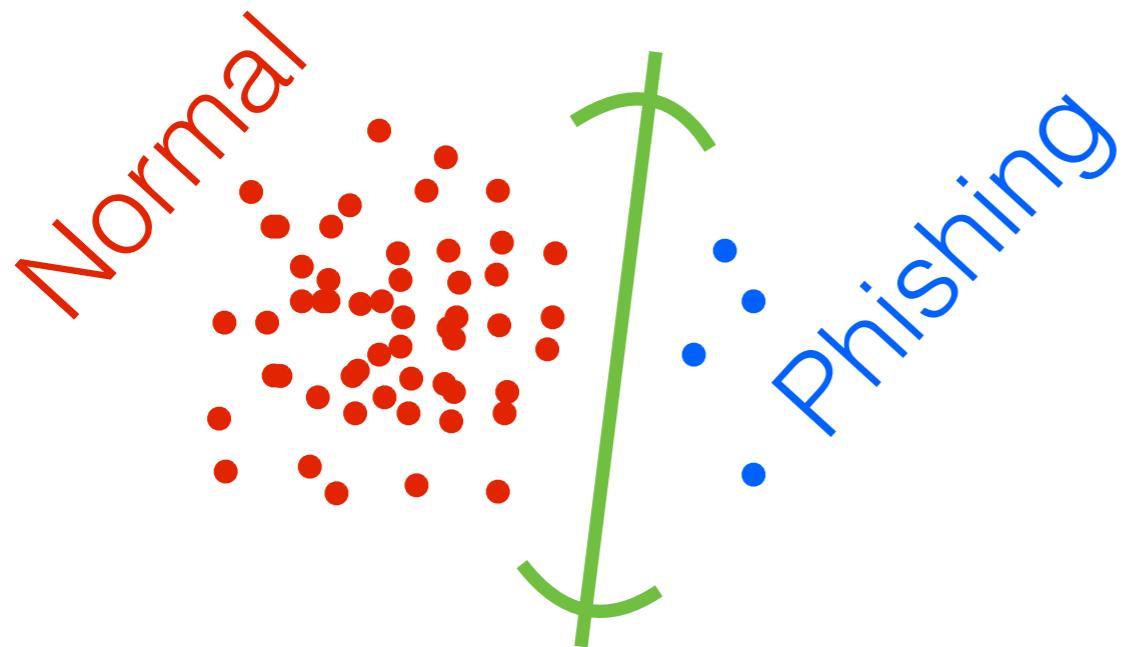
Importance sampling



Importance sampling

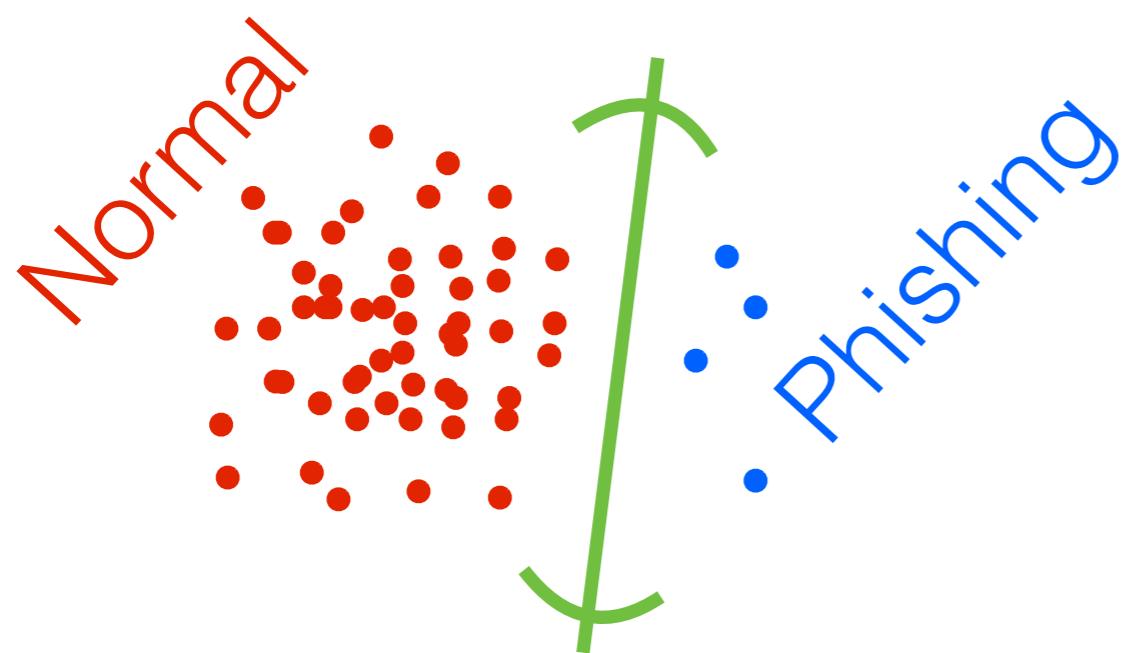


Importance sampling



$$\sigma_n \propto \|\mathcal{L}_n\|$$

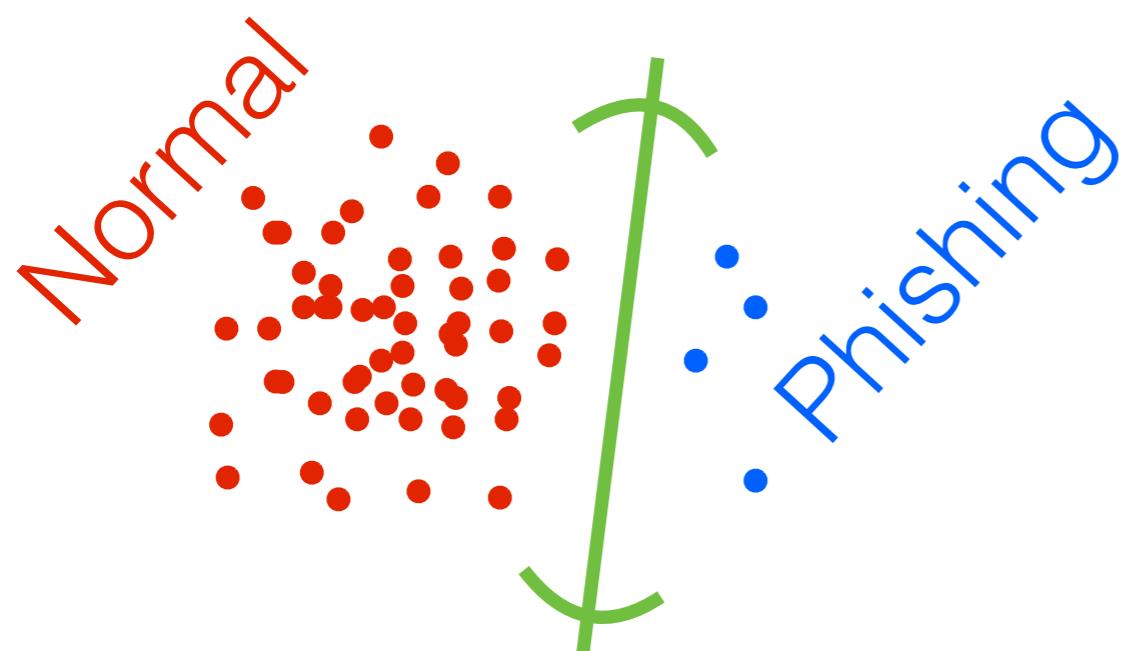
Importance sampling



$$\sigma := \sum_{n=1}^N \|\mathcal{L}_n\|$$

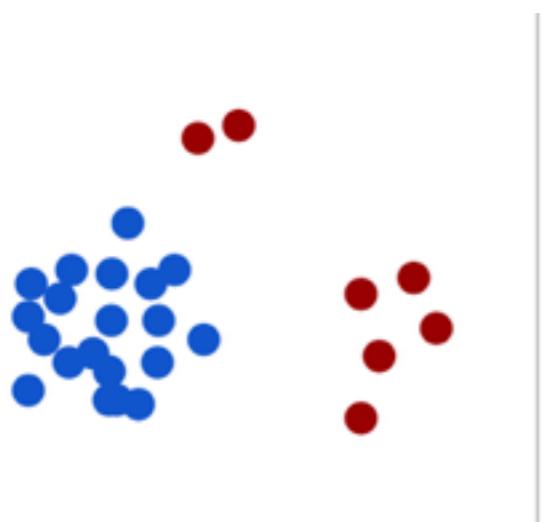
$$\sigma_n := \|\mathcal{L}_n\|/\sigma$$

Importance sampling

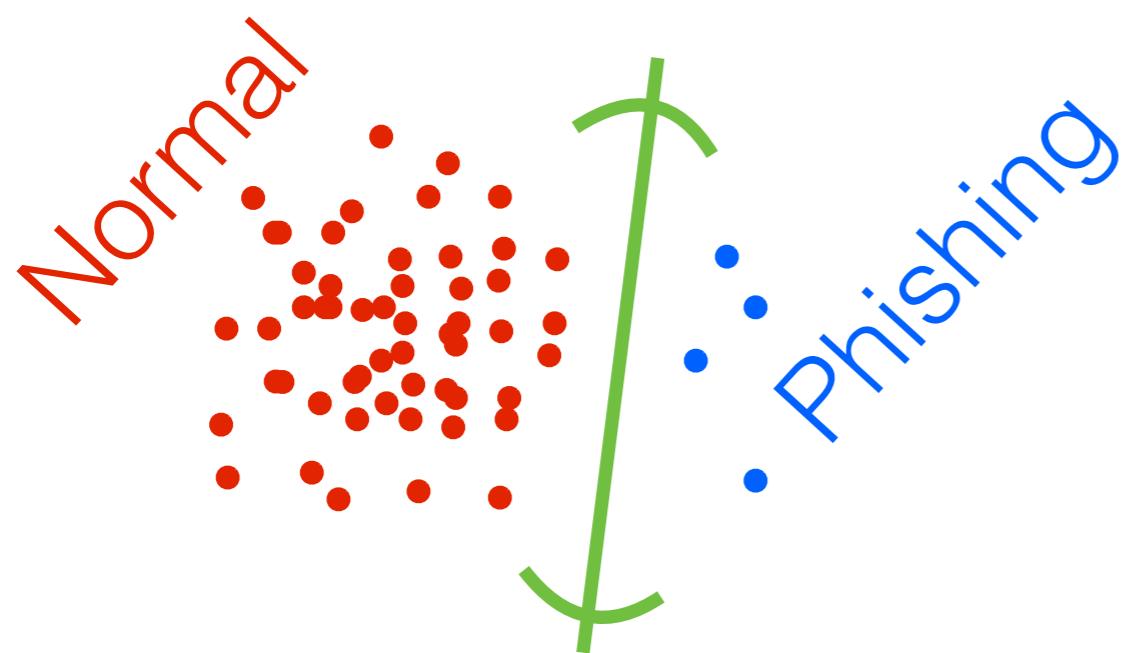


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1. data

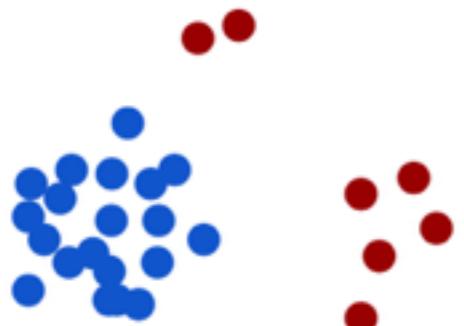


Importance sampling

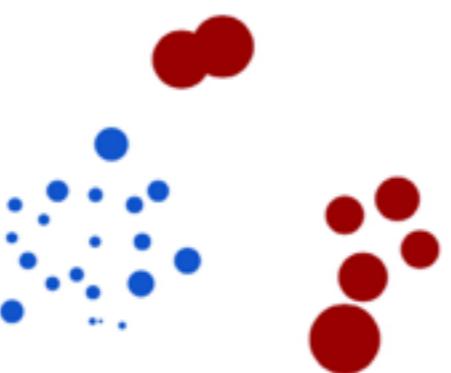


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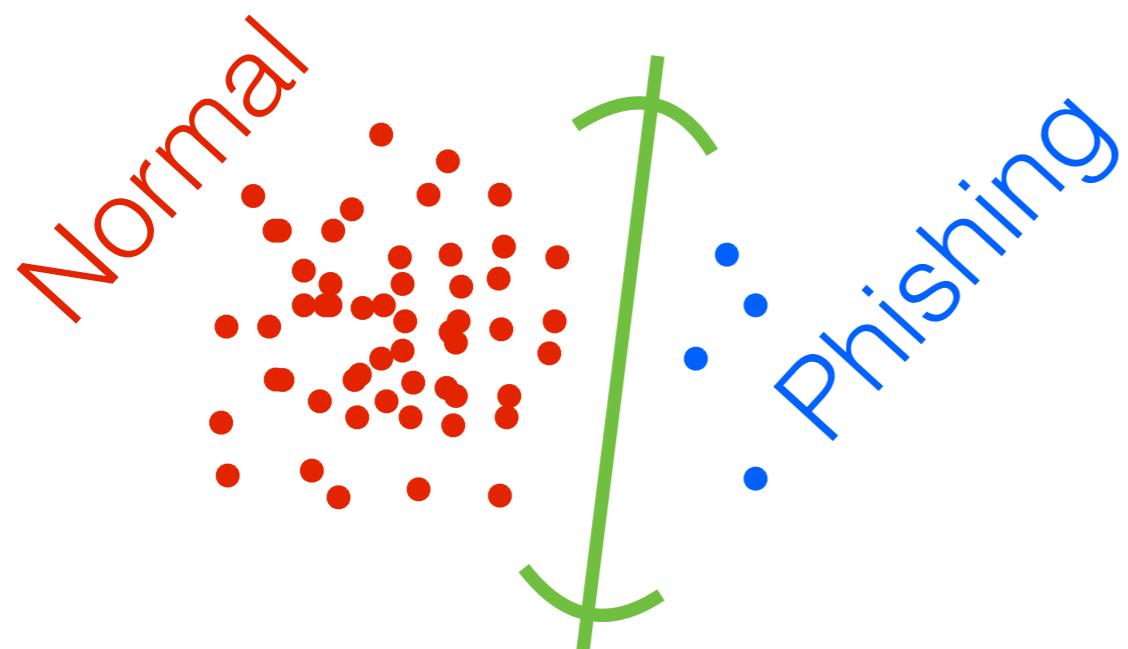
1. data



2. importance weights

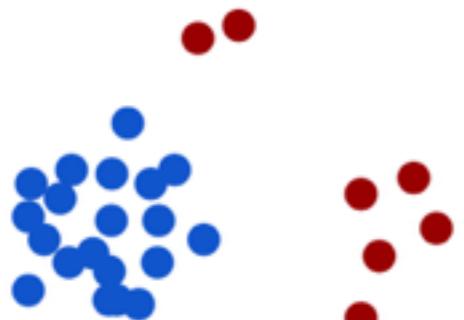


Importance sampling

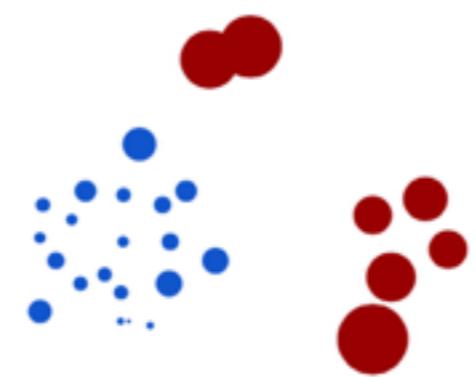


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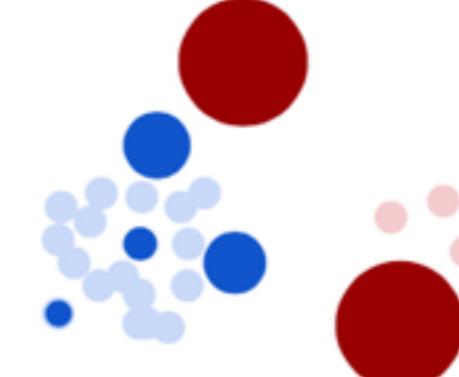
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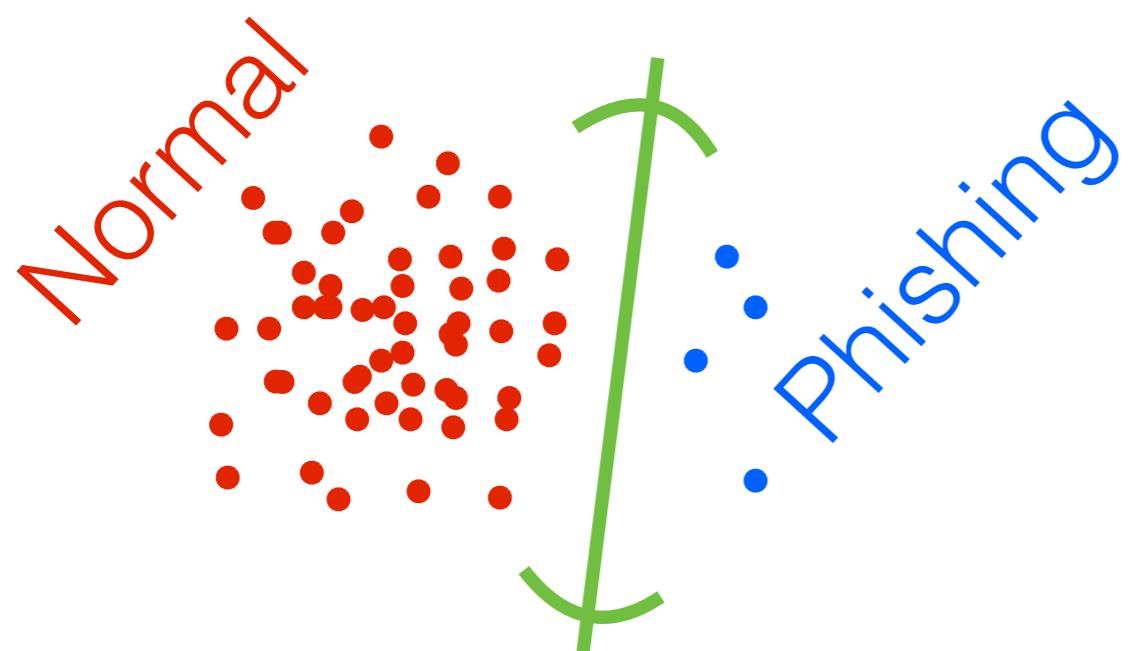
2. importance weights



3. importance sample



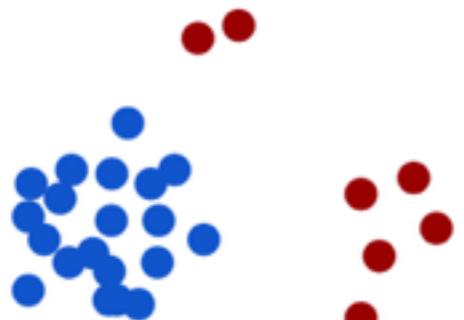
Importance sampling



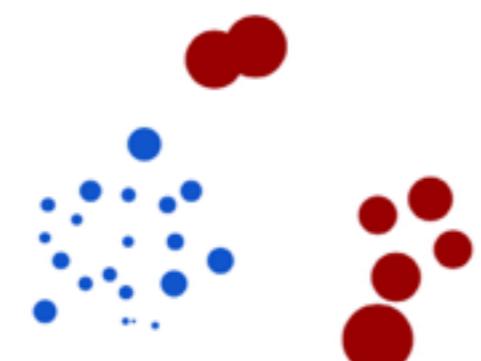
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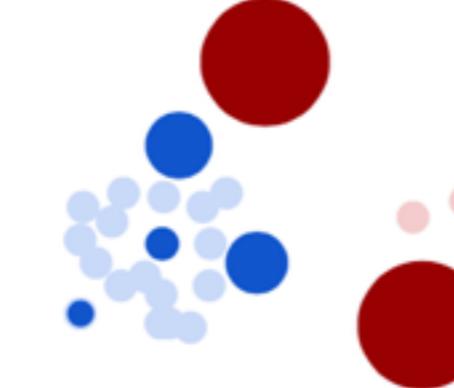
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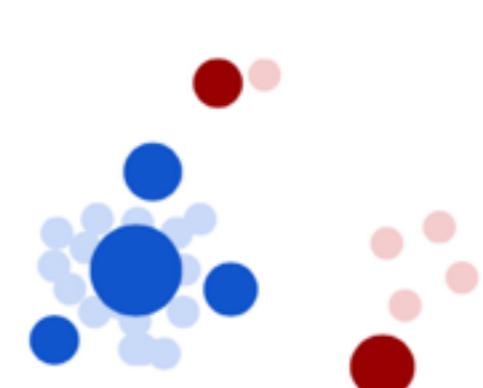
2. importance weights



3. importance sample



4. invert weights



Importance sampling

Thm sketch (CB). $\delta \in (0,1)$. W.p. $\geq 1 - \delta$, after M iterations,

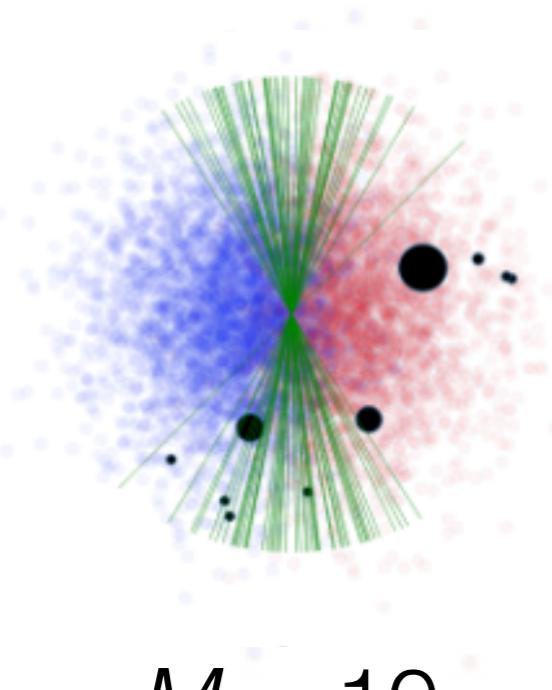
$$\|\mathcal{L}(w) - \mathcal{L}\| \leq \frac{\sigma\bar{\eta}}{\sqrt{M}} \left(1 + \sqrt{2 \log \frac{1}{\delta}} \right)$$

Importance sampling

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- Still noisy estimates



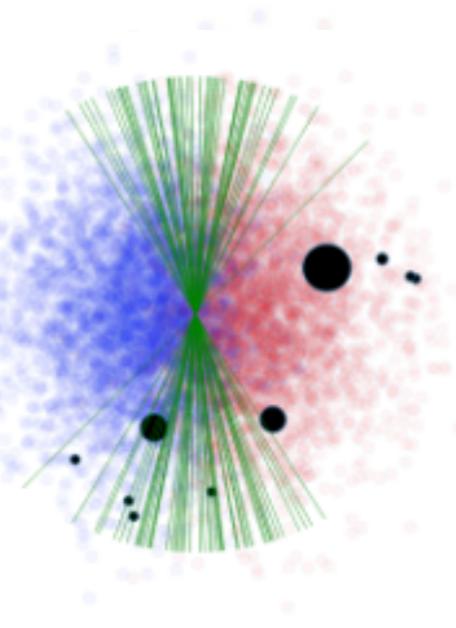
$$M = 10$$

Importance sampling

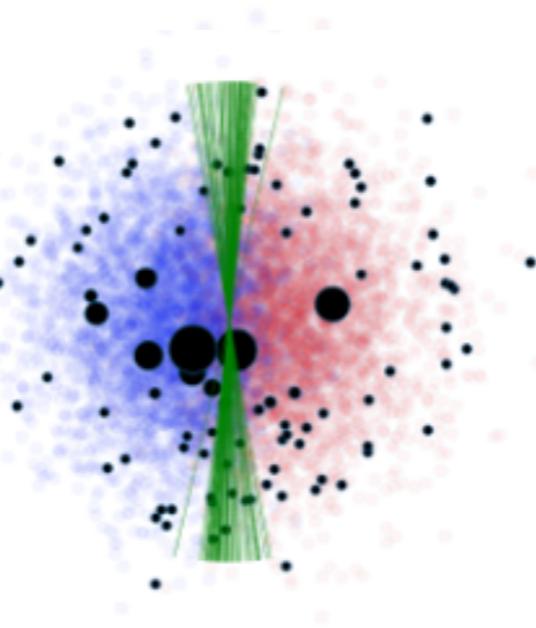
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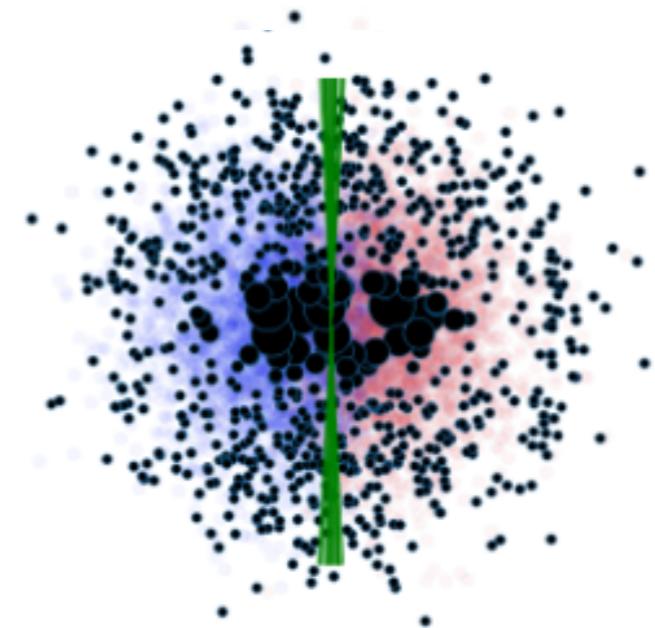
- Still noisy estimates



$M = 10$



$M = 100$



$M = 1000$

Hilbert coresets

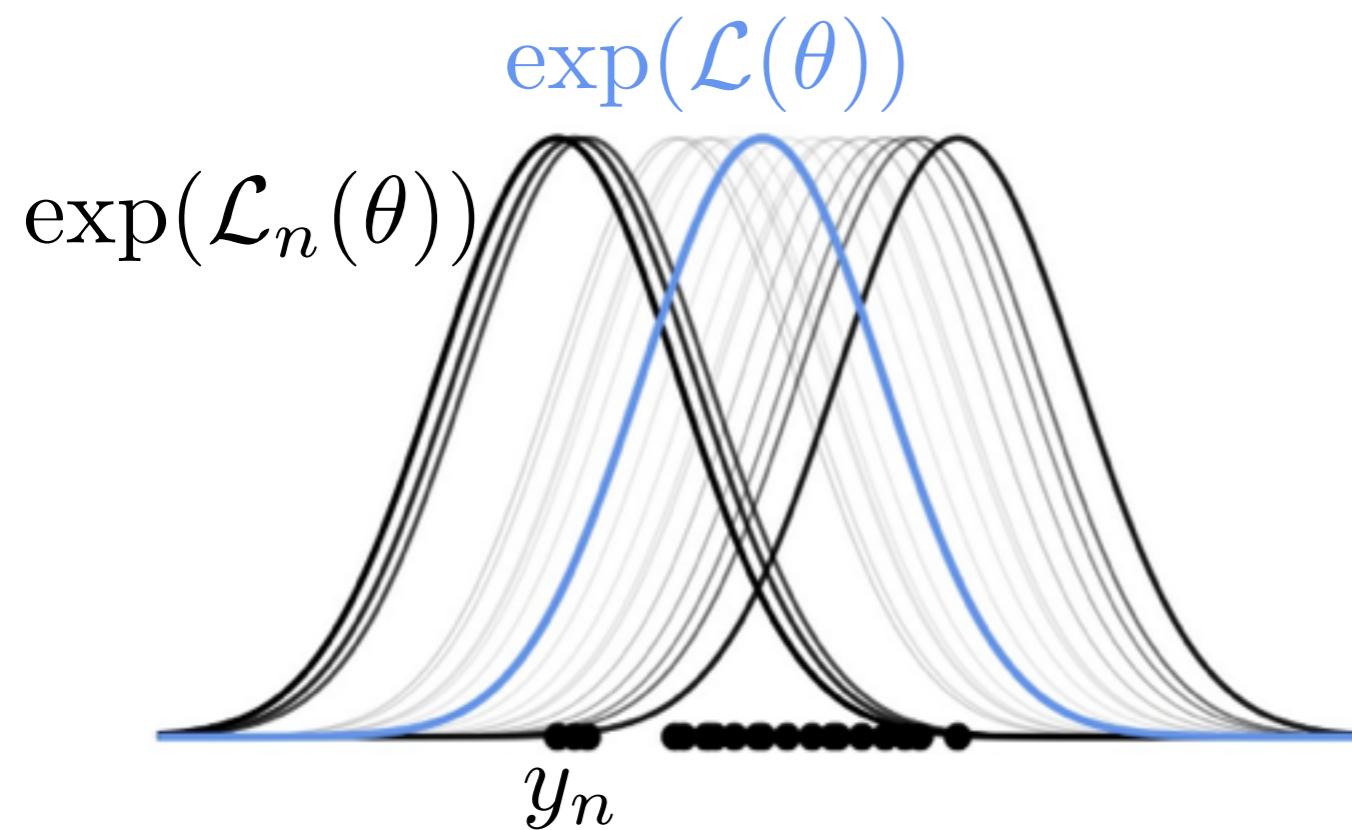
- Want a good coreset:
$$\min_{w \in \mathbb{R}^N} \|\mathcal{L}(w) - \mathcal{L}\|$$

s.t. $w \geq 0, \|w\|_0 \leq M$

Hilbert coresets

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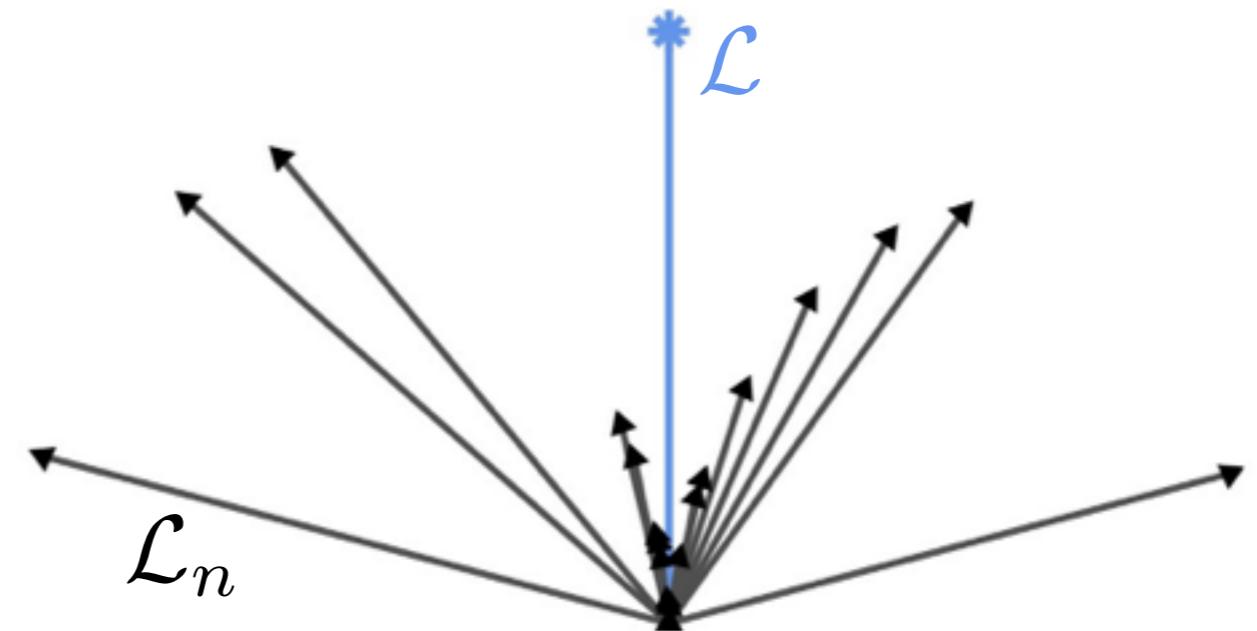
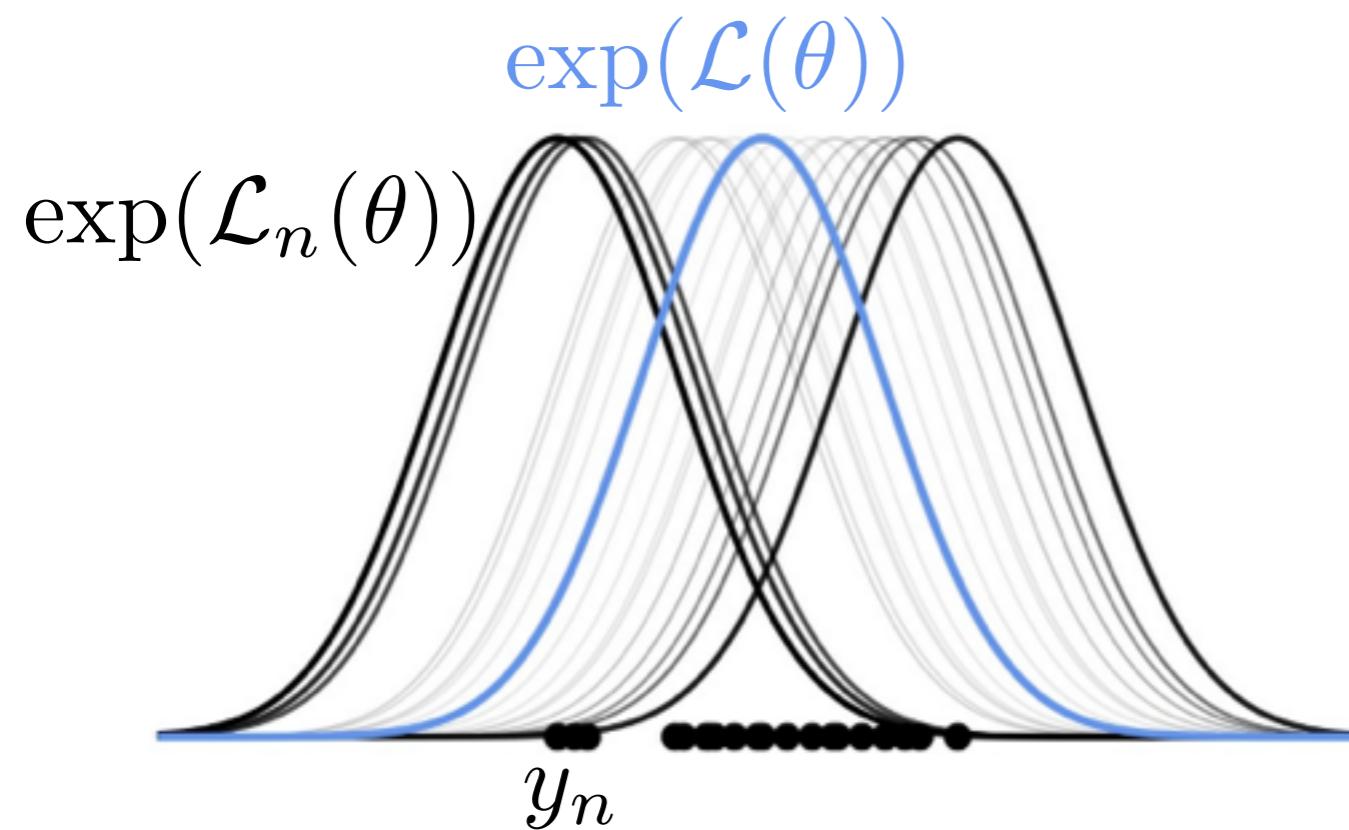
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Hilbert coresets

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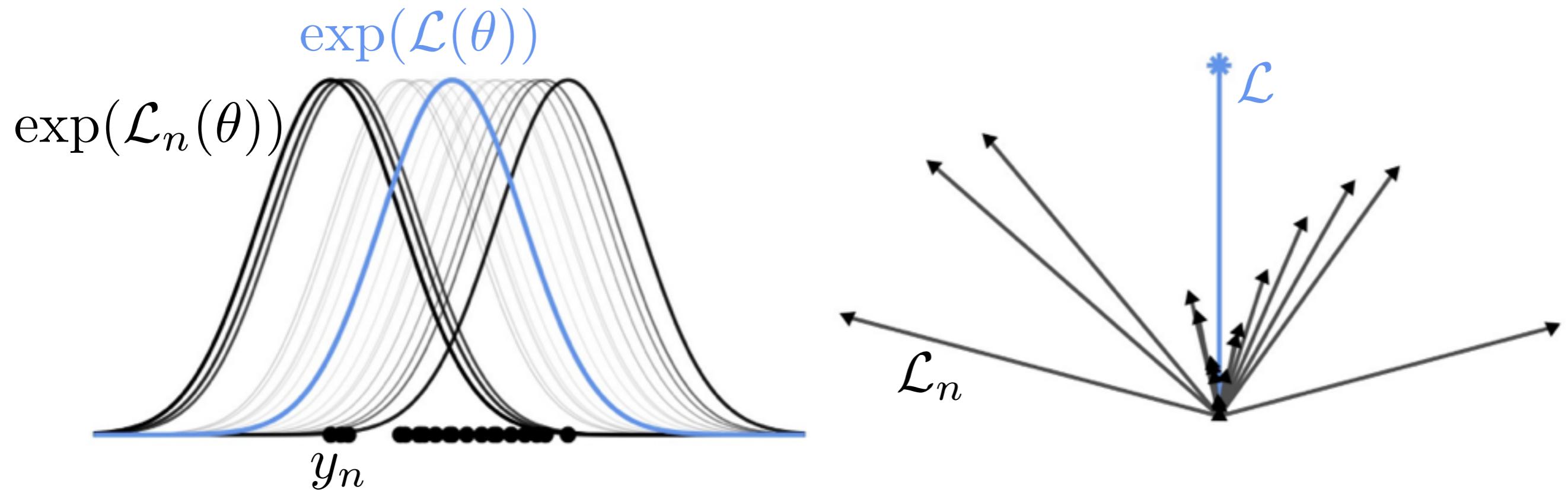
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Hilbert coresets

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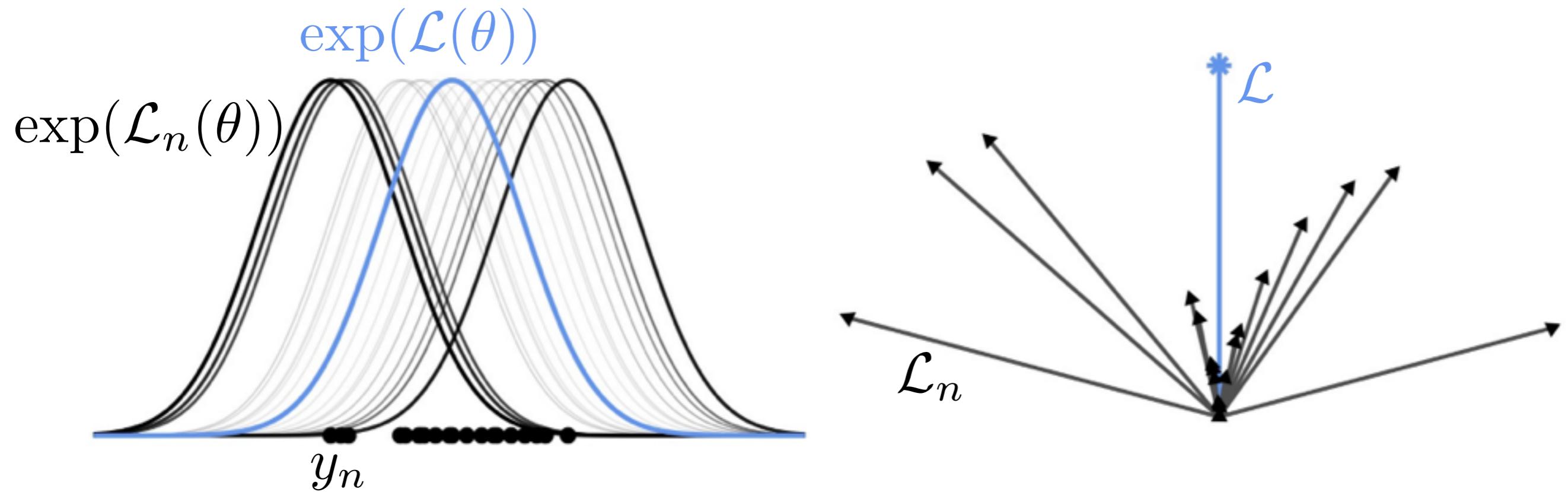


- need to consider (residual) error direction

Hilbert coresets

- Want a good coreset:
$$\min_{w \in \mathbb{R}^N} \|\mathcal{L}(w) - \mathcal{L}\|$$

s.t. $w \geq 0, \|w\|_0 \leq M$



- need to consider (residual) error direction
- sparse optimization

Roadmap

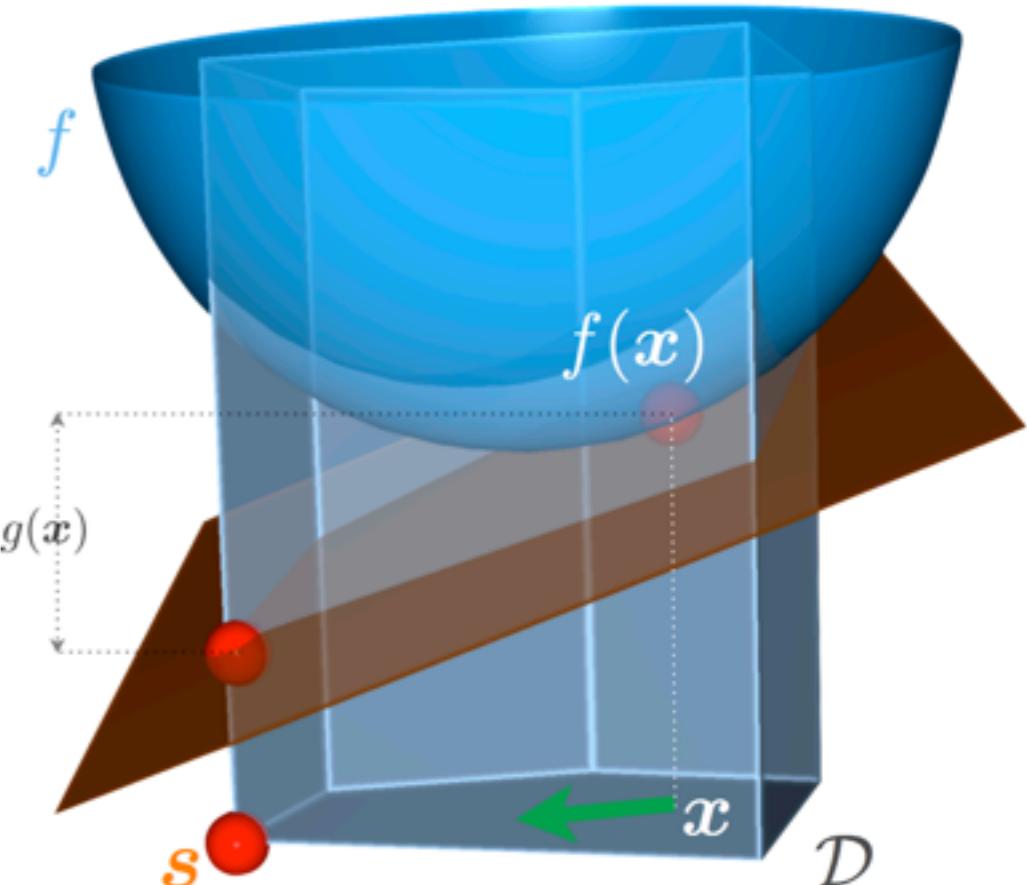
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Frank-Wolfe

Convex optimization on a polytope D

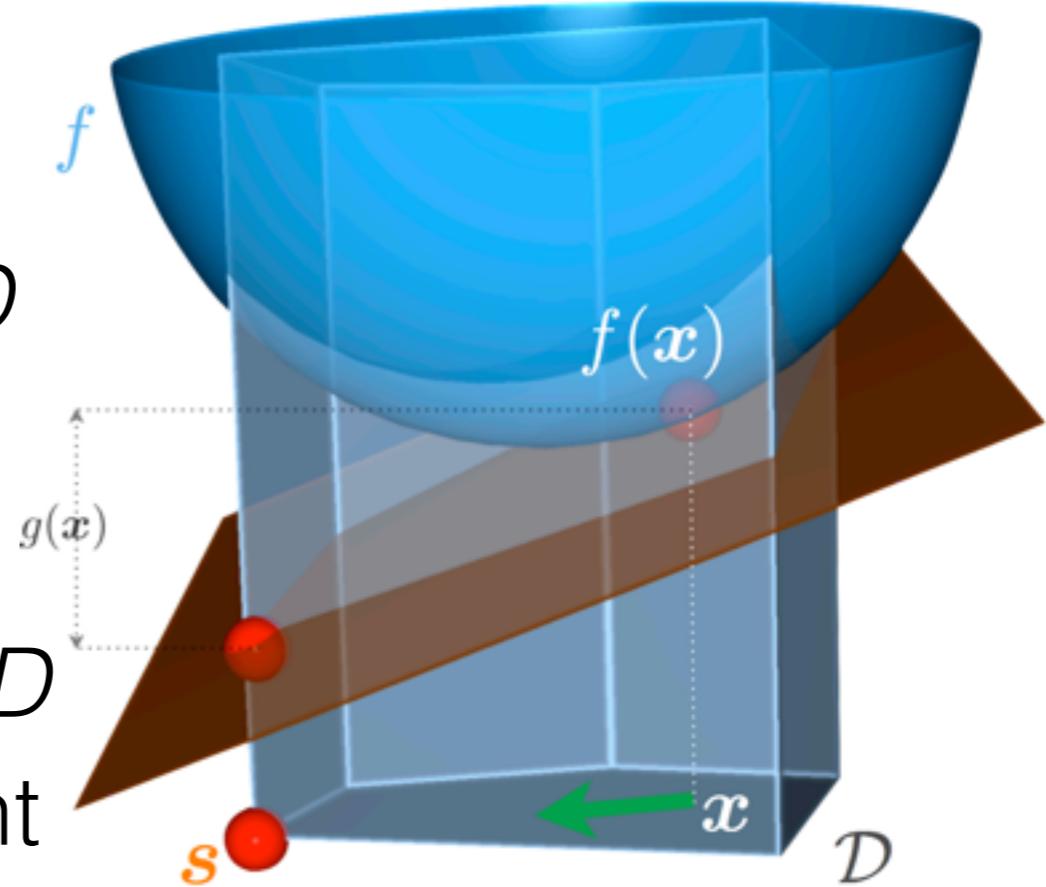


[Jaggi 2013]

Frank-Wolfe

Convex optimization on a polytope D

- Repeat:
 1. Find gradient
 2. Find argmin point on plane in D
 3. Do line search between current point and argmin point

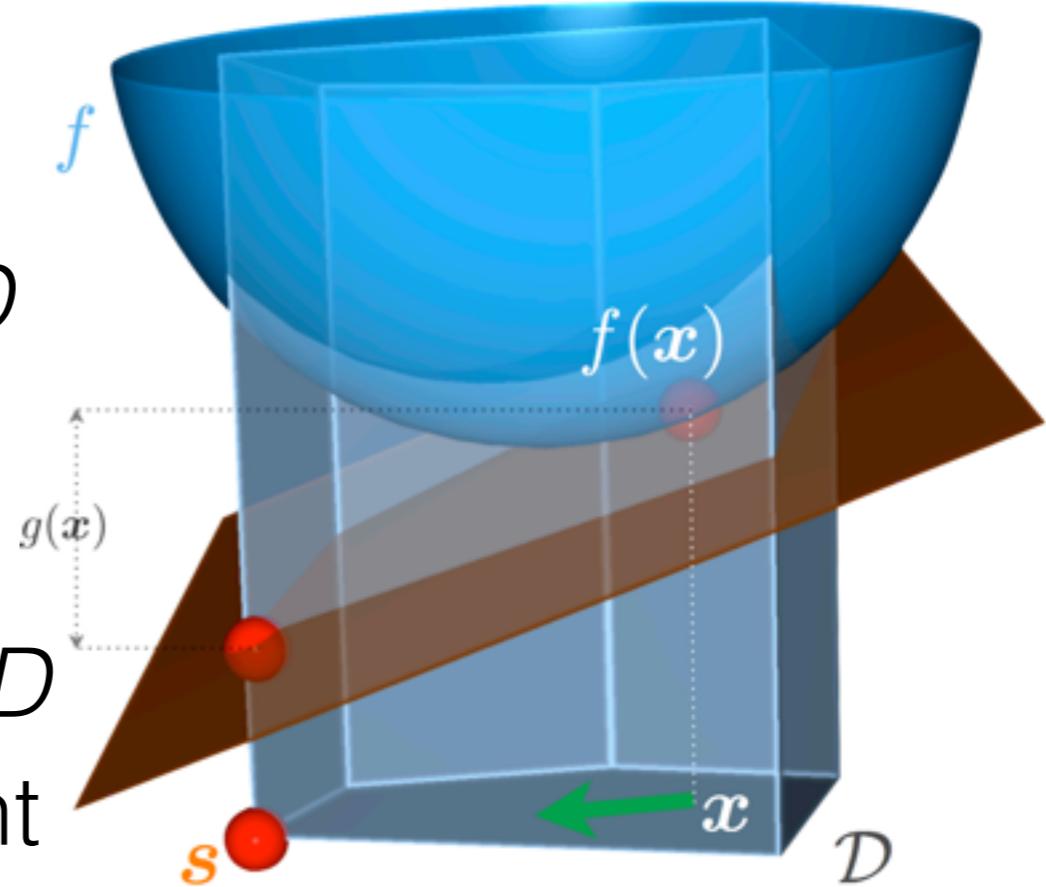


[Jaggi 2013]

Frank-Wolfe

Convex optimization on a polytope D

- Repeat:
 1. Find gradient
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- Convex combination of M vertices after $M-1$ steps

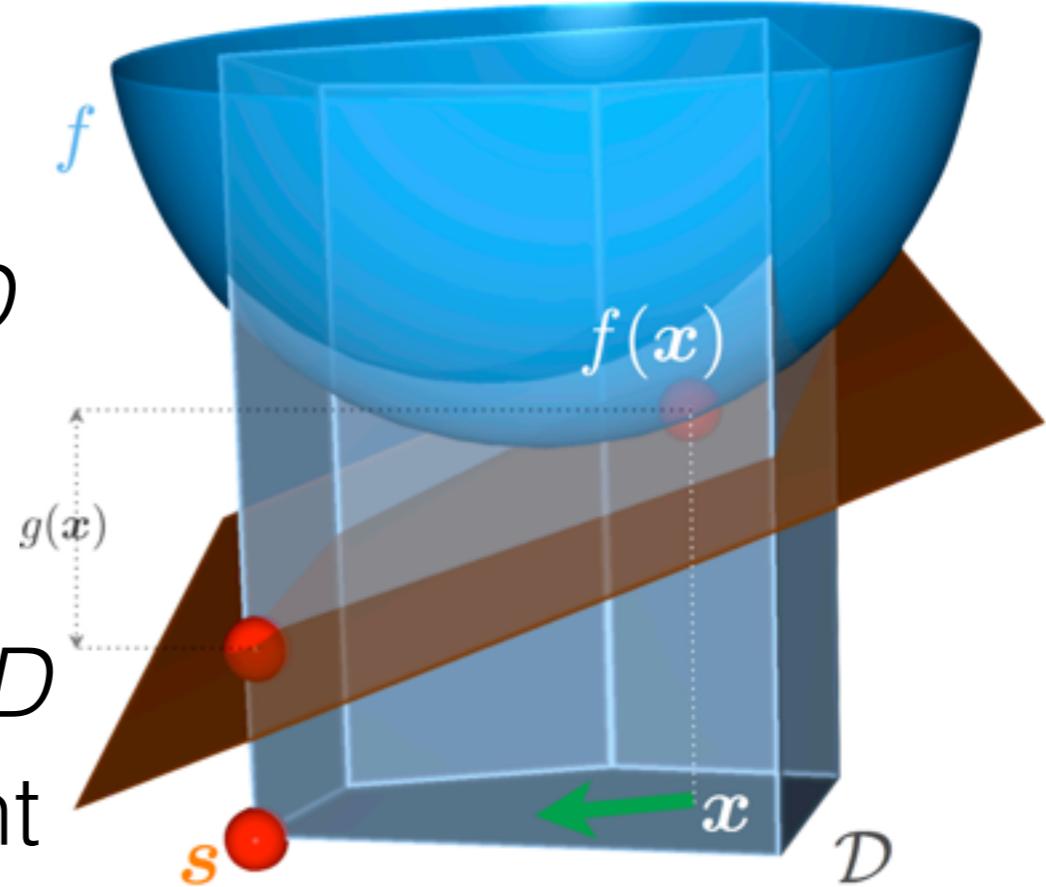


[Jaggi 2013]

Frank-Wolfe

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- Our problem: $\min_{w \in \mathbb{R}^N} \|\mathcal{L}(w) - \mathcal{L}\|$

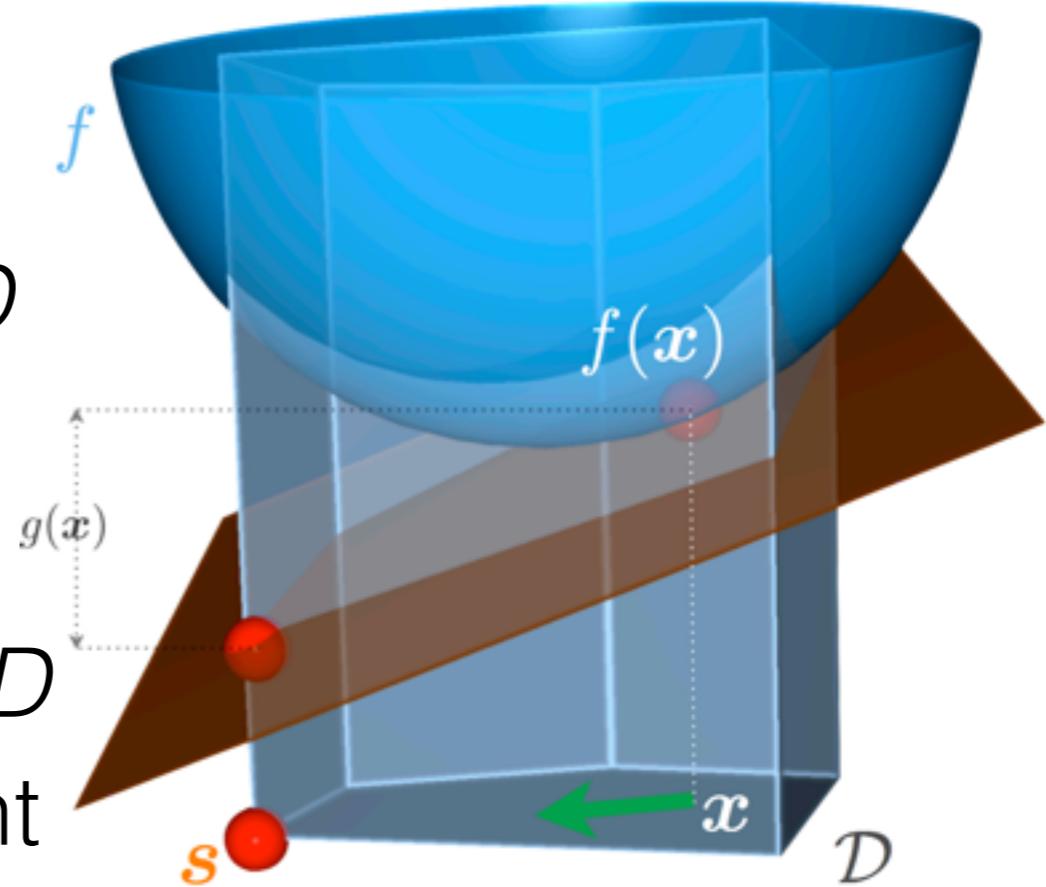


[Jaggi 2013]

Frank-Wolfe

Convex optimization on a polytope D

- Repeat:
 1. Find gradient
 2. Find argmin point on plane in D
 3. Do line search between current point and argmin point
- Convex combination of M vertices after $M-1$ steps
- Our problem: $\min_{w \in \mathbb{R}^N} \|\mathcal{L}(w) - \mathcal{L}\|^2$

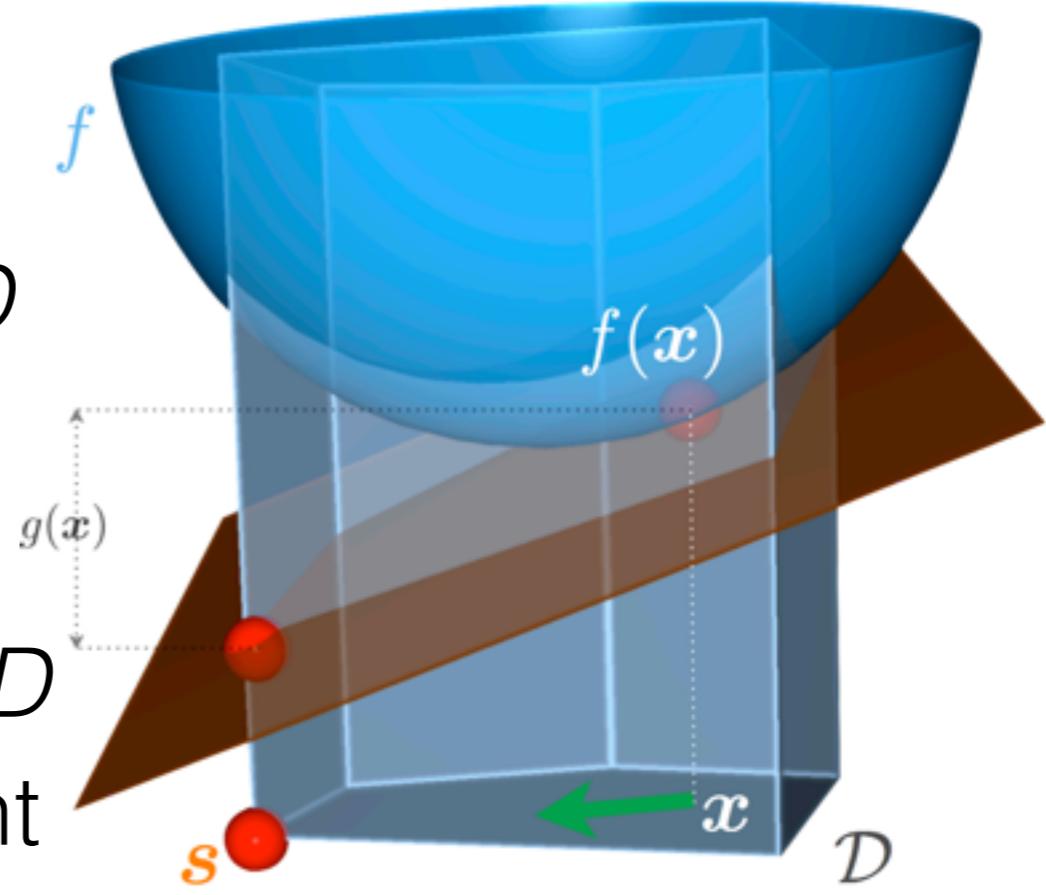


[Jaggi 2013]

Frank-Wolfe

Convex optimization on a polytope D

- Repeat:
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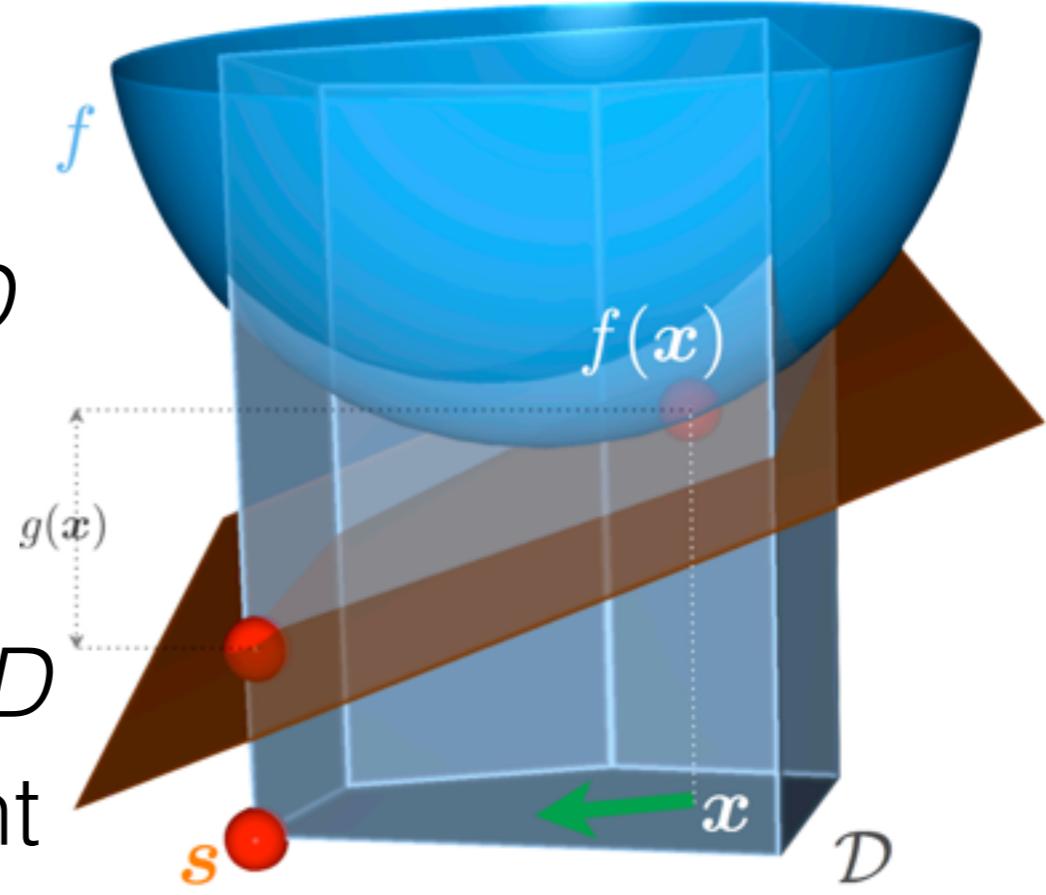
[Jaggi 2013]

- Convex combination of M vertices after $M-1$ steps
- Our problem: $\min_{w \in \mathbb{R}^N} \|\mathcal{L}(w) - \mathcal{L}\|^2$
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Frank-Wolfe

Convex optimization on a polytope D

- Repeat:
 1. Find gradient
 2. Find argmin point on plane in D
 3. Do line search between current point and argmin point



[Jaggi 2013]

- Convex combination of M vertices after $M-1$ steps
- Our problem:

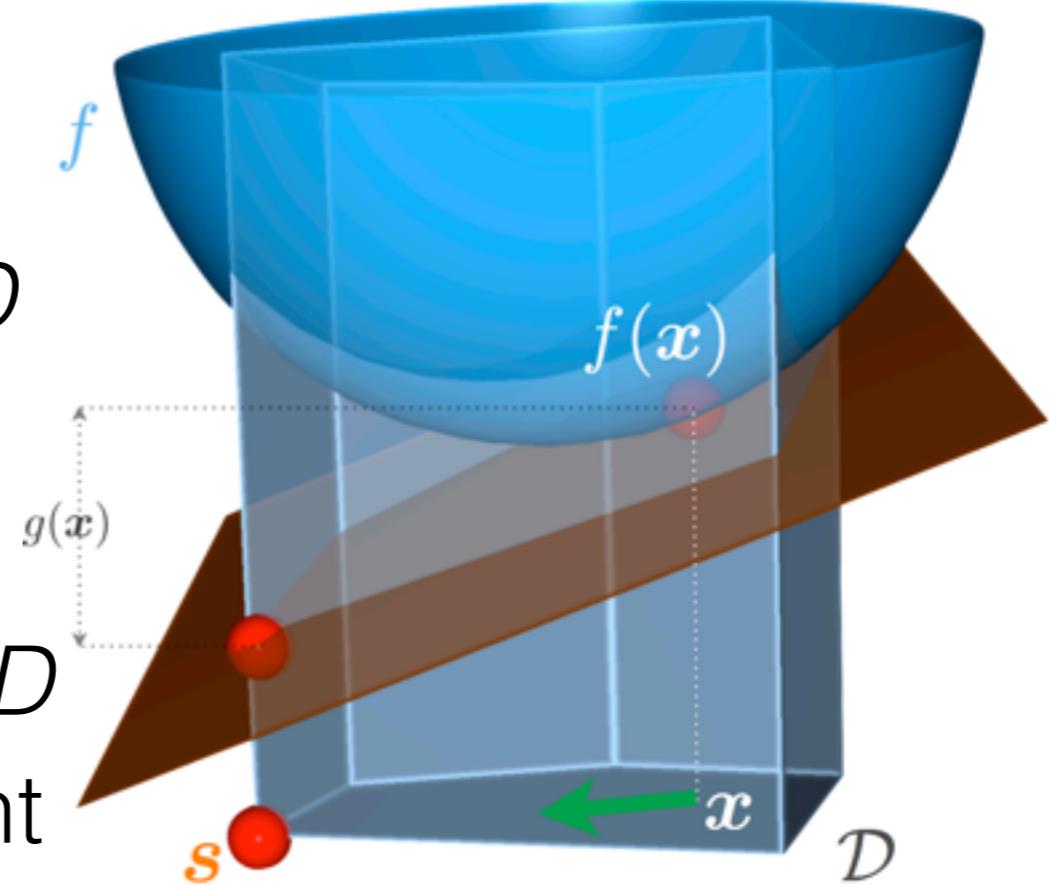
$$\min_{w \in \mathbb{R}^N} \|\mathcal{L}(w) - \mathcal{L}\|^2$$

$$\Delta^{N-1} := \left\{ w \in \mathbb{R}^N : \sum_{n=1}^N \sigma_n w_n = \sigma, w \geq 0 \right\}$$

Frank-Wolfe

Convex optimization on a polytope D

- Repeat:
 1. Find gradient
 2. Find argmin point on plane in D
 3. Do line search between current point and argmin point



[Jaggi 2013]

- Convex combination of M vertices after $M-1$ steps
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$$\Delta^{N-1} := \left\{ w \in \mathbb{R}^N : \sum_{n=1}^N \sigma_n w_n = \sigma, w \geq 0 \right\}$$

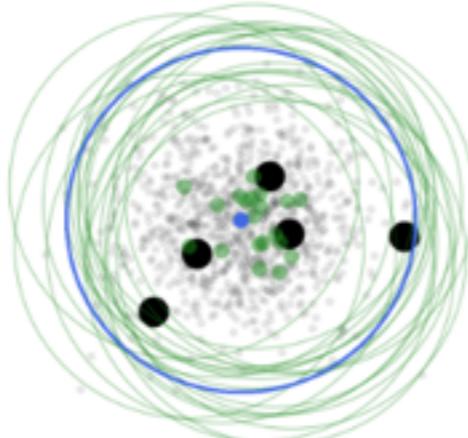
Thm sketch (CB). After M iterations,

$$\|\mathcal{L}(w) - \mathcal{L}\| \leq \frac{\sigma \bar{\eta}}{\sqrt{\alpha^{2M} + M}}$$

Gaussian model (simulated)

- 10K pts; norms, inference: closed-form

Uniform
subsampling

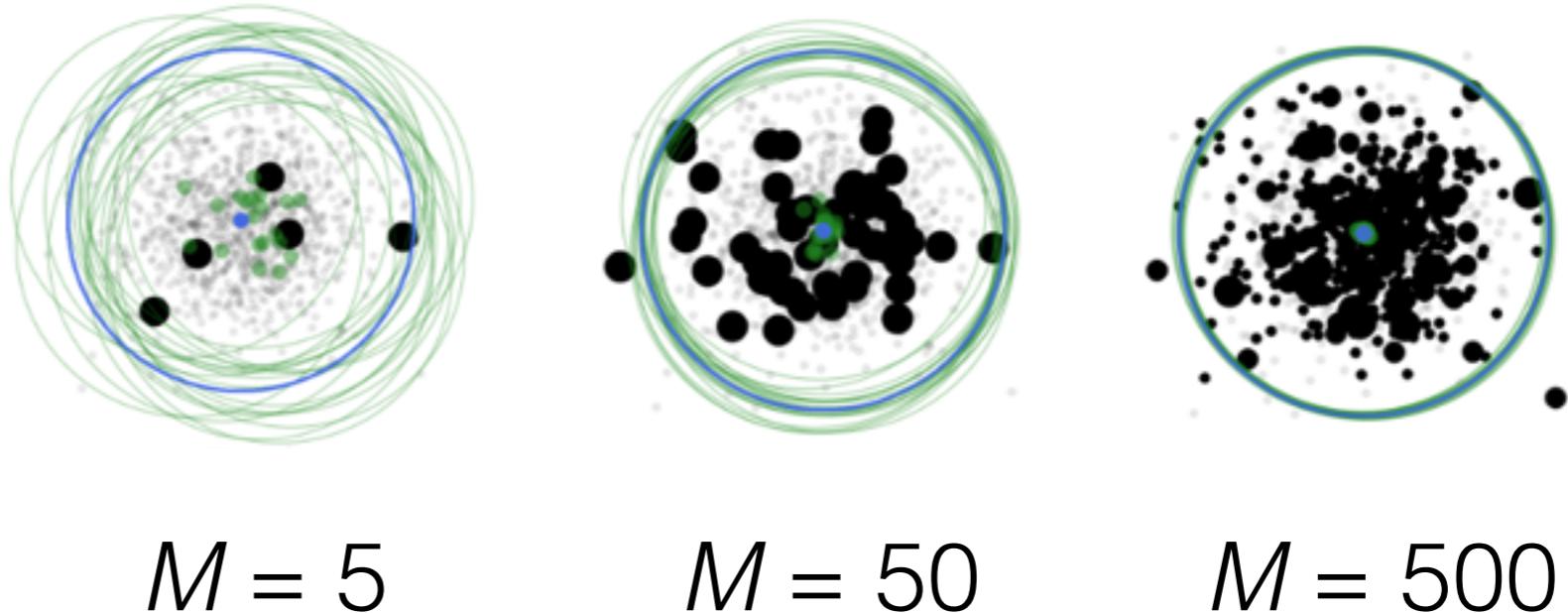


$$M = 5$$

Gaussian model (simulated)

- 10K pts; norms, inference: closed-form

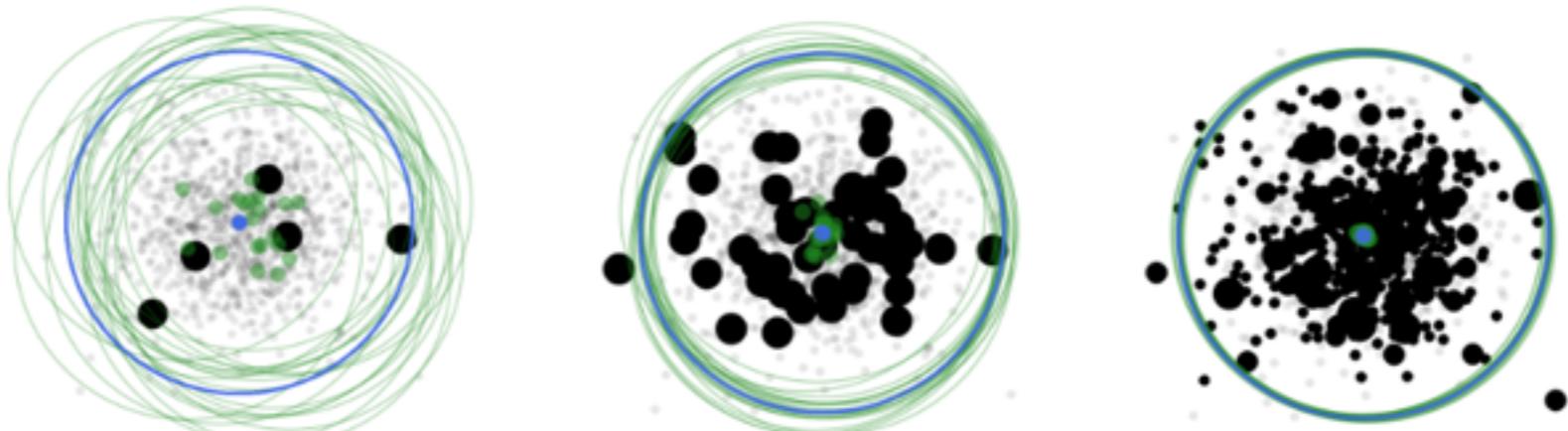
Uniform
subsampling



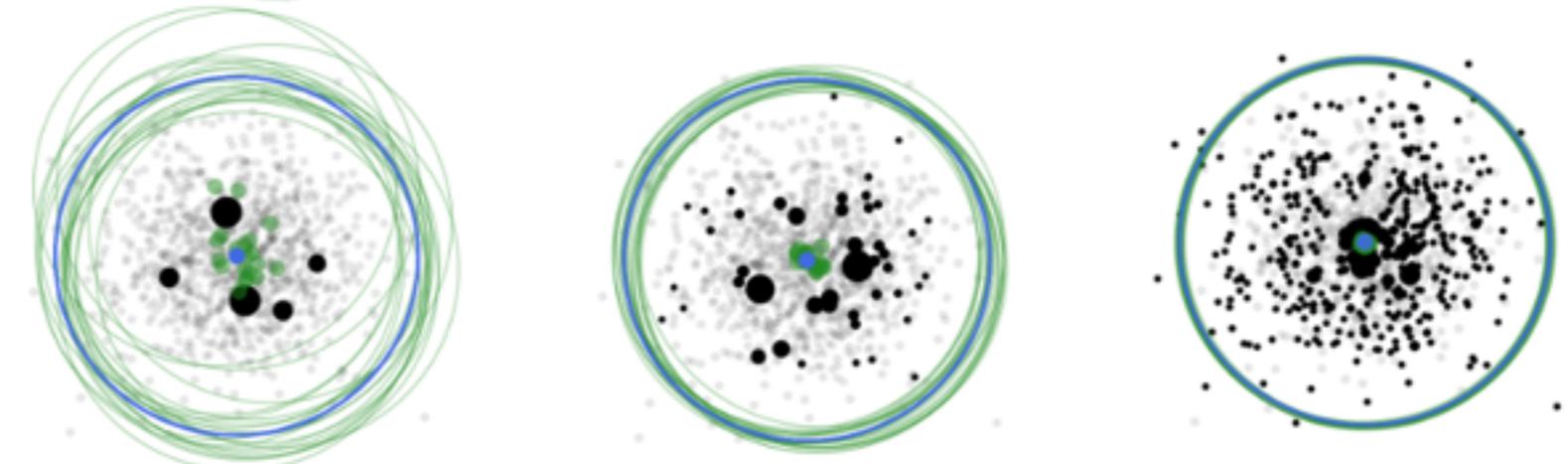
Gaussian model (simulated)

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Uniform
subsampling



Importance
sampling



$M = 5$

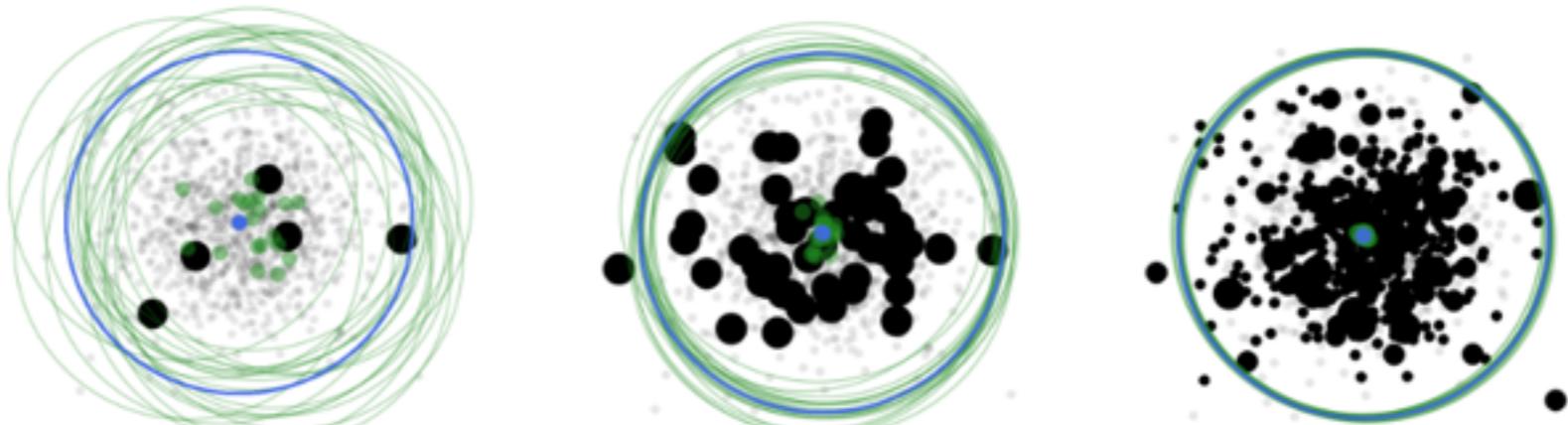
$M = 50$

$M = 500$

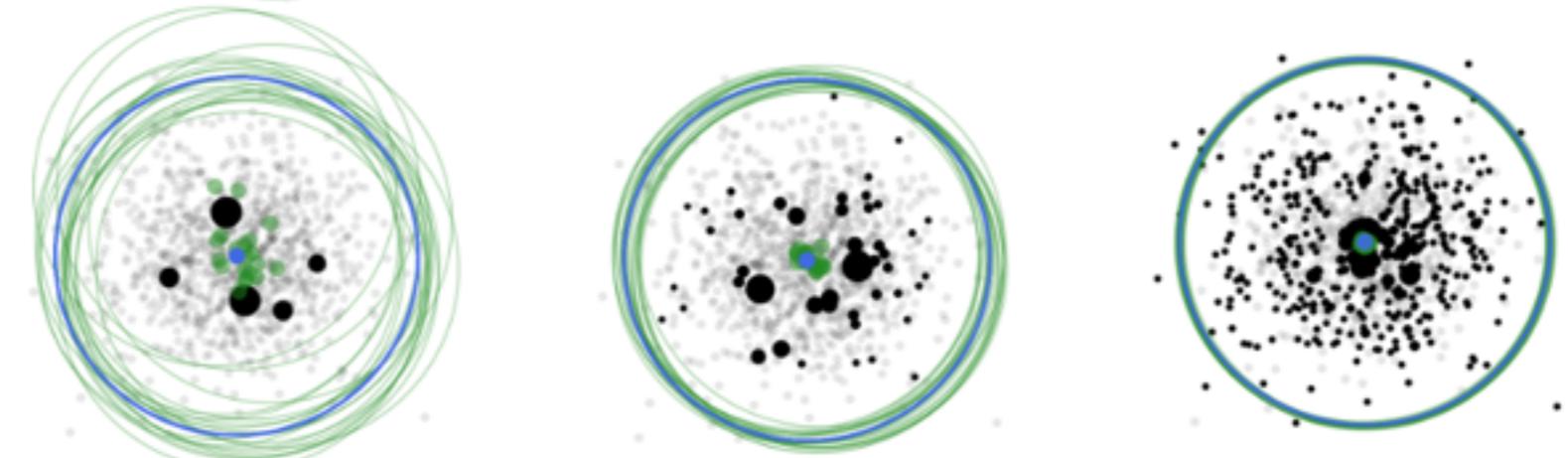
Gaussian model (simulated)

- 10K pts; norms, inference: closed-form

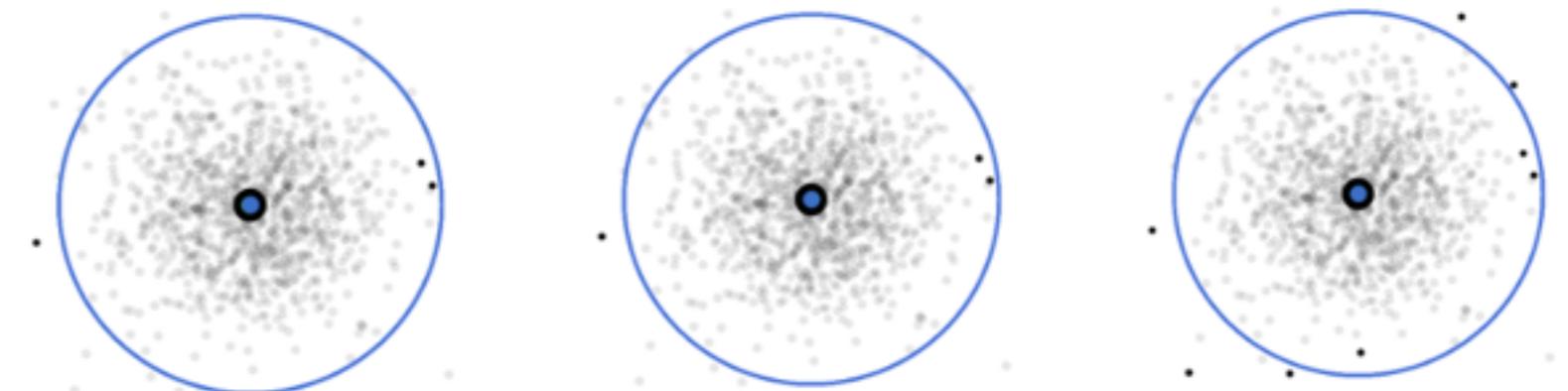
Uniform
subsampling



Importance
sampling



Frank-Wolfe



$M = 5$

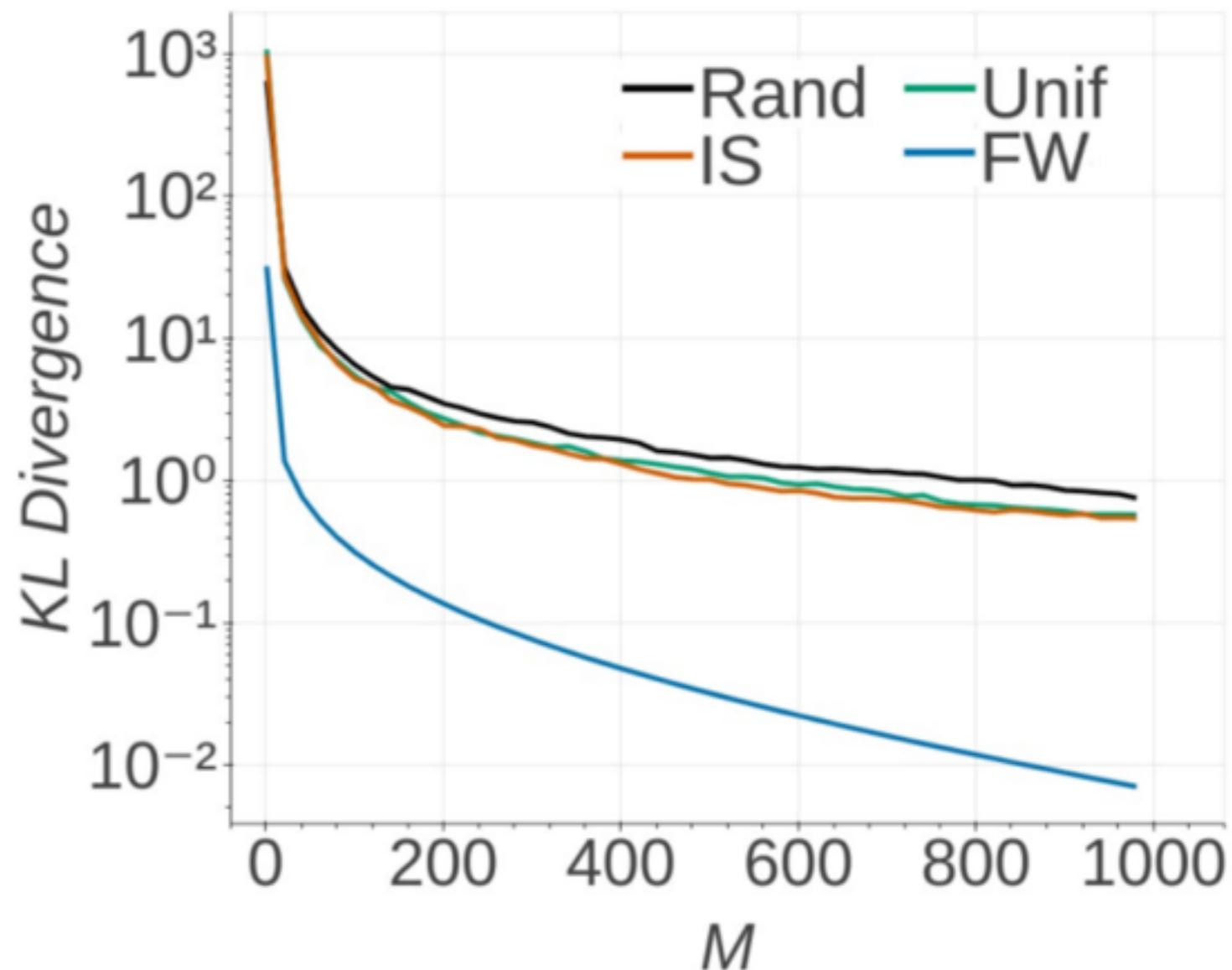
$M = 50$

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Gaussian model (simulated)

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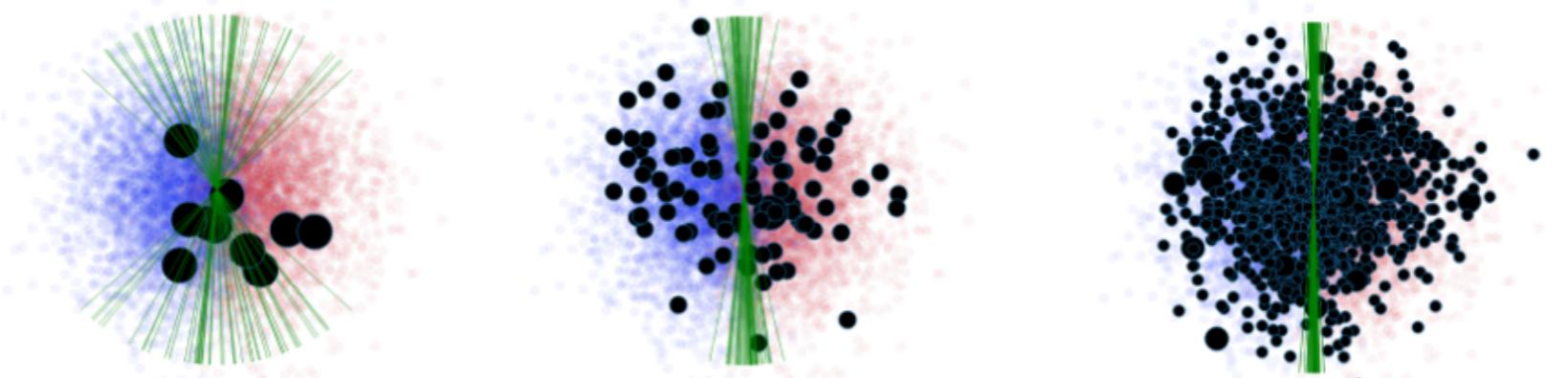
lower
error



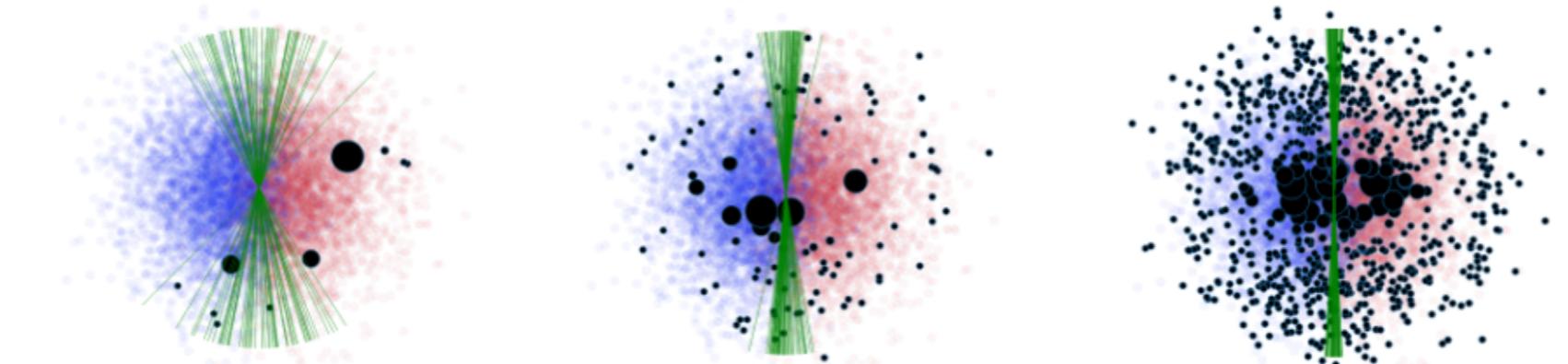
Logistic regression (simulated)

- 10K pts; general inference

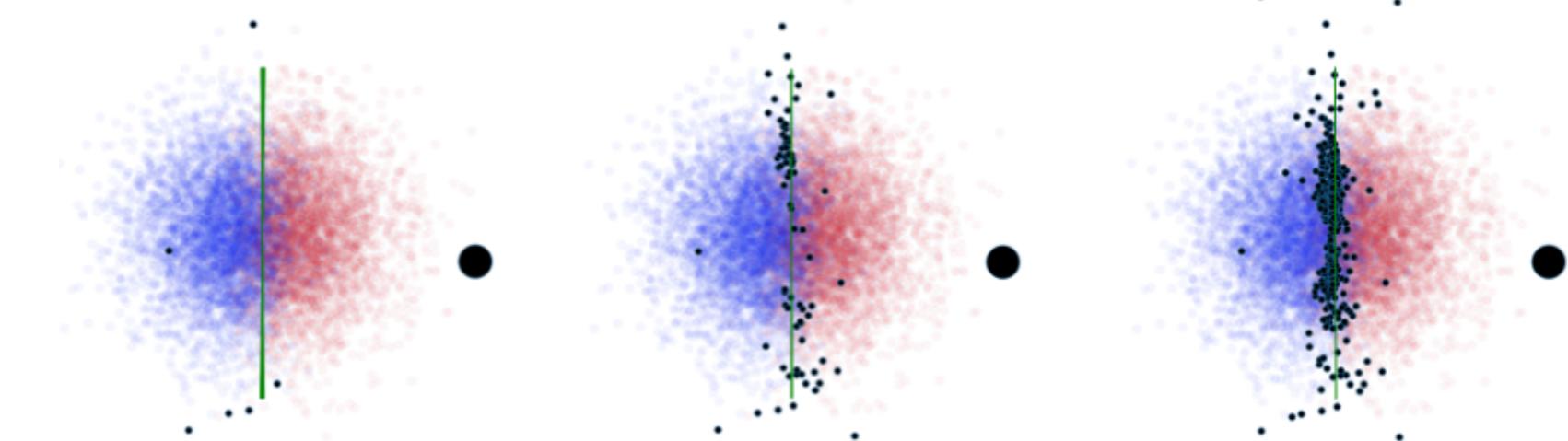
Uniform
subsampling



Importance
sampling



Frank-Wolfe



$M = 10$

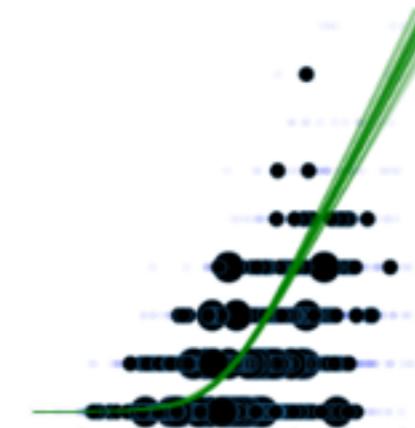
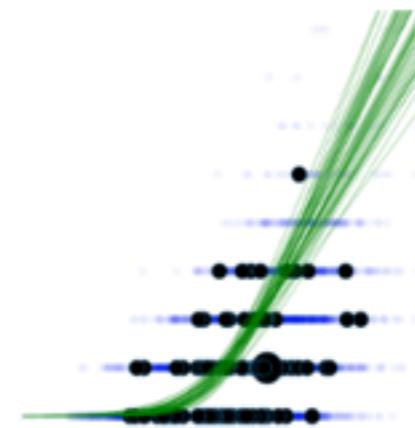
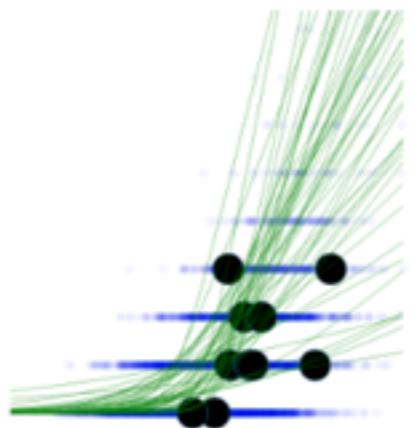
$M = 100$

$M = 1000$

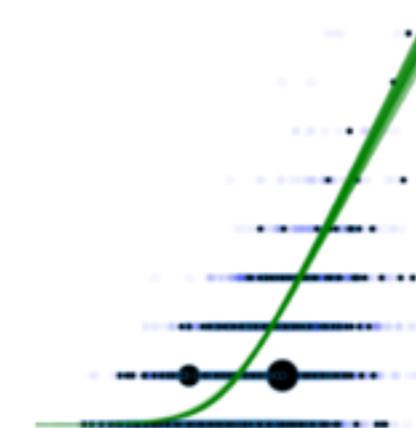
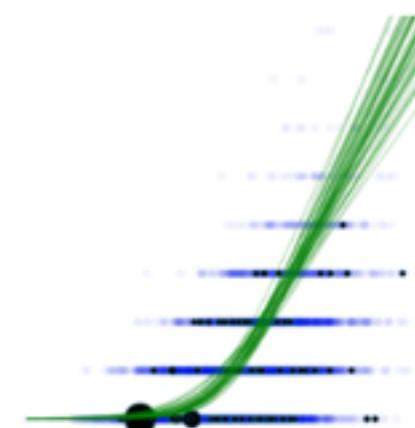
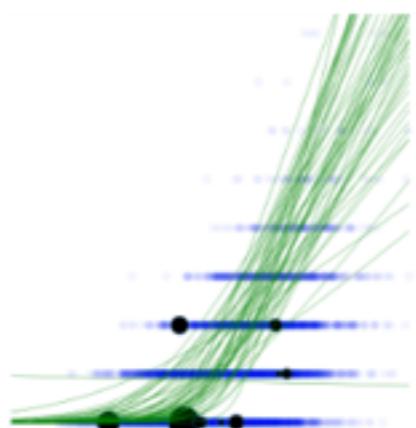
Poisson regression (simulated)

- 10K pts; general inference

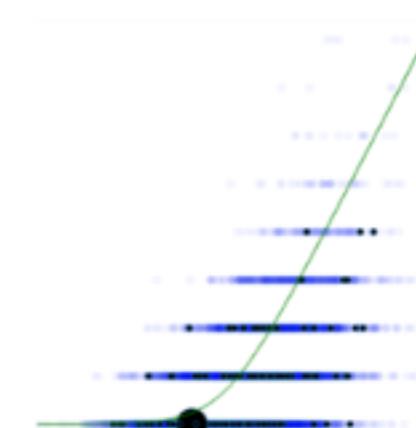
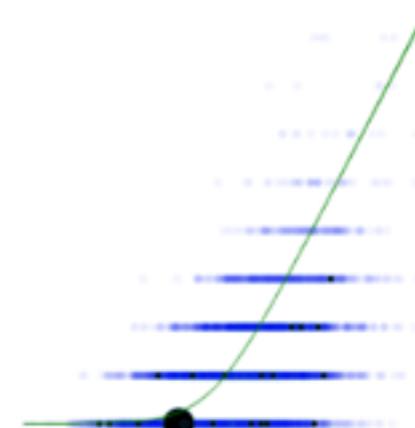
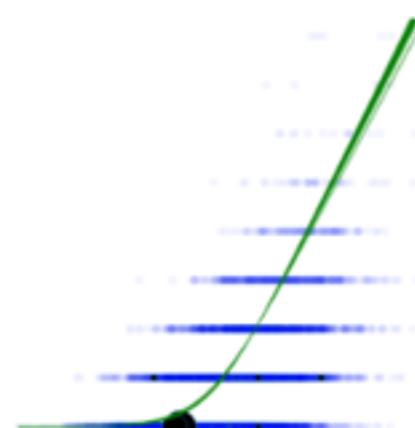
Uniform
subsampling



Importance
sampling



Frank-Wolfe



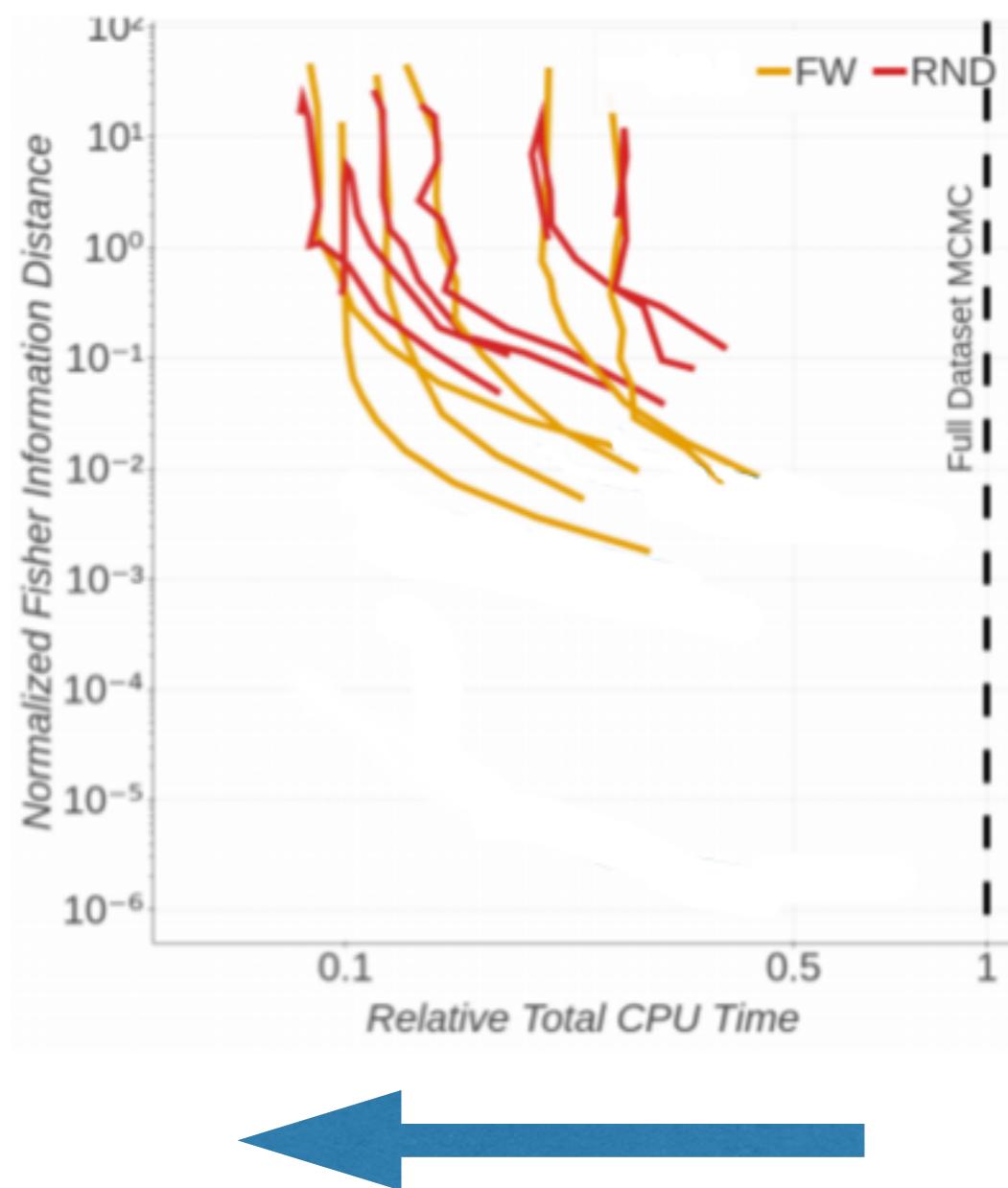
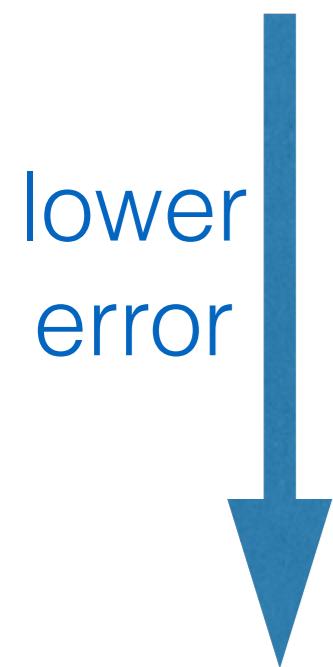
$M = 10$

$M = 100$

$M = 1000$

Real data experiments

lower error



less total time



Uniform
subsampling

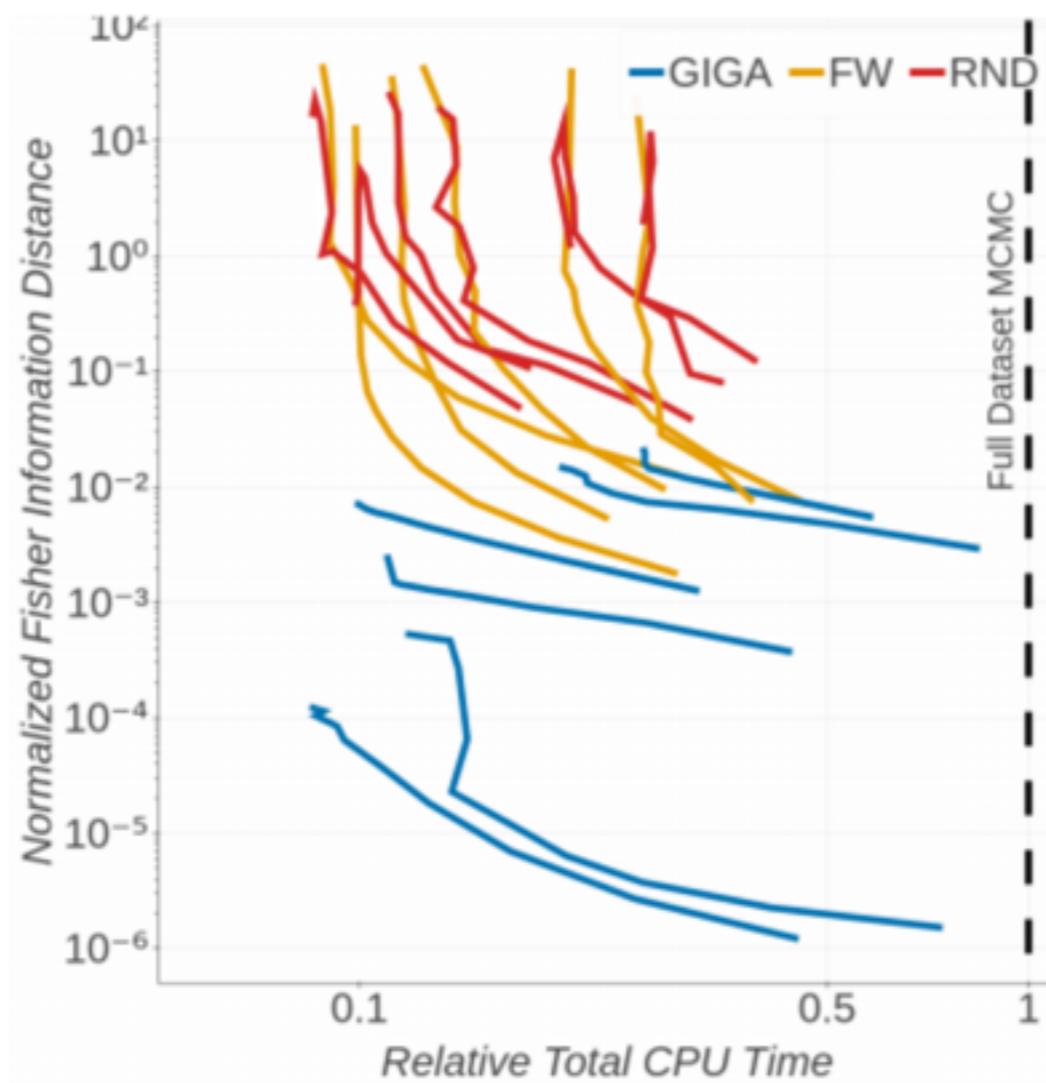
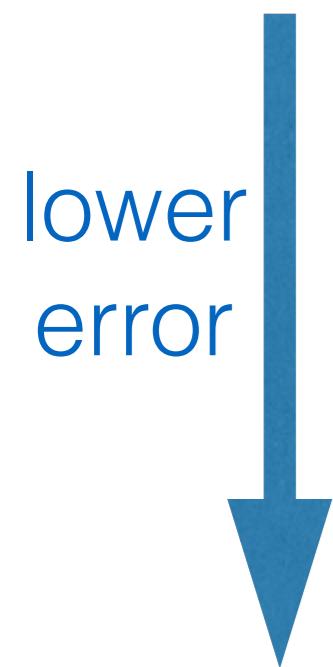
Frank Wolfe
coresets

Data sets include:

- Phishing
- Chemical reactivity
- Bicycle trips
- Airport delays

Real data experiments

lower error



less total time



Uniform
subsampling

Frank Wolfe
coresets

GIGA coresets

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Roadmap

- Approximate Bayes review
- The “core” of the data set
- Uniform data subsampling isn’t enough
- Importance sampling for “coresets”
- Optimization for “coresets”
- Approximate sufficient statistics

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Sufficient statistics

Data summarization

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- E.g. Bayesian logistic regression; GLMs; “deeper” models

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 - Likelihood $p(y_{1:N}|x_{1:N}, \theta) = \prod_{n=1}^N \frac{1}{1 + \exp(-y_n x_n \cdot \theta)}$
 - Our proposal: (polynomial) *approximate* sufficient statistics

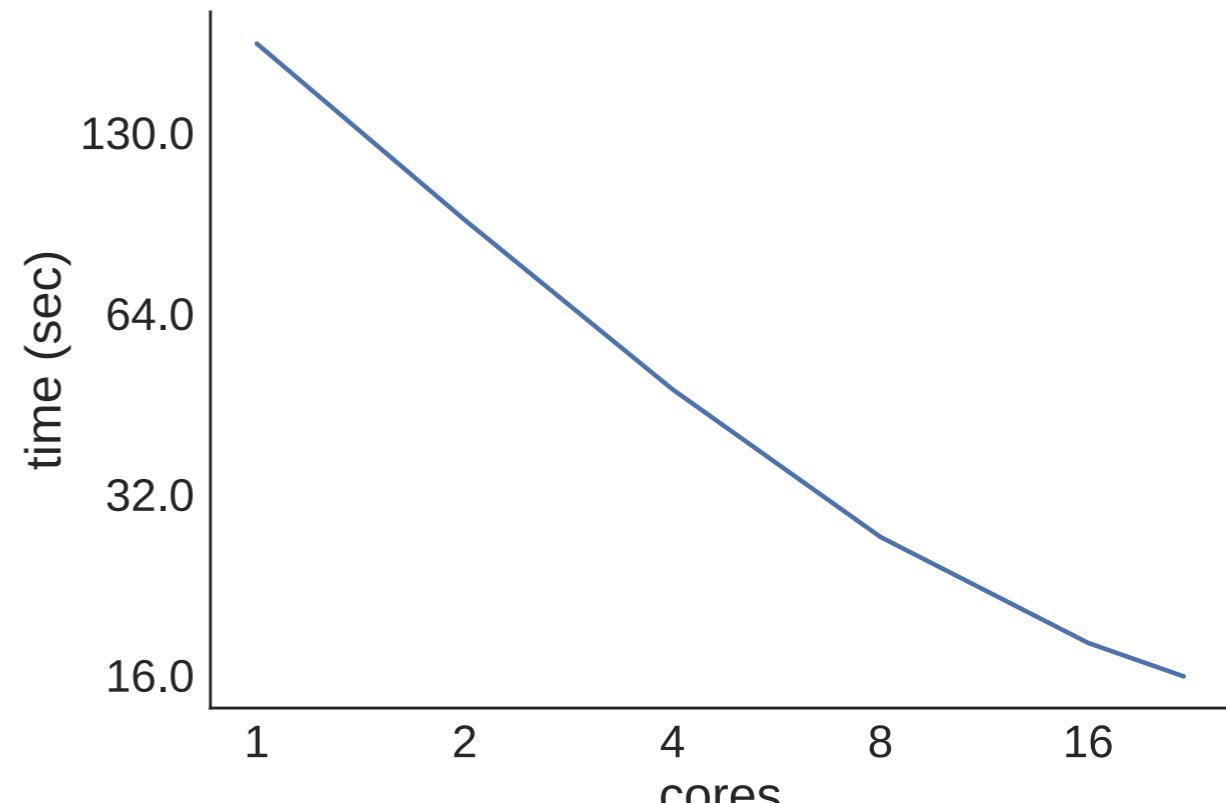
Data summarization

Criteo Labs > Algorithms > Criteo Releases its New Dataset

Criteo Releases its New Dataset

By: CriteoLabs / 31 Mar 2015

- 6M data points, 1000 features
- Streaming, distributed; minimal communication
- 22 cores, 16 sec
- Finite-data guarantees on Wasserstein distance to exact posterior



[Huggins, Adams, Broderick 2017]

Conclusions

- *Data summarization* for **scalable, automated** approx. Bayes algorithms with **error bounds on quality for finite data**
 - Get more accurate with more computation investment
 - Coresets
 - Approx. suff. stats

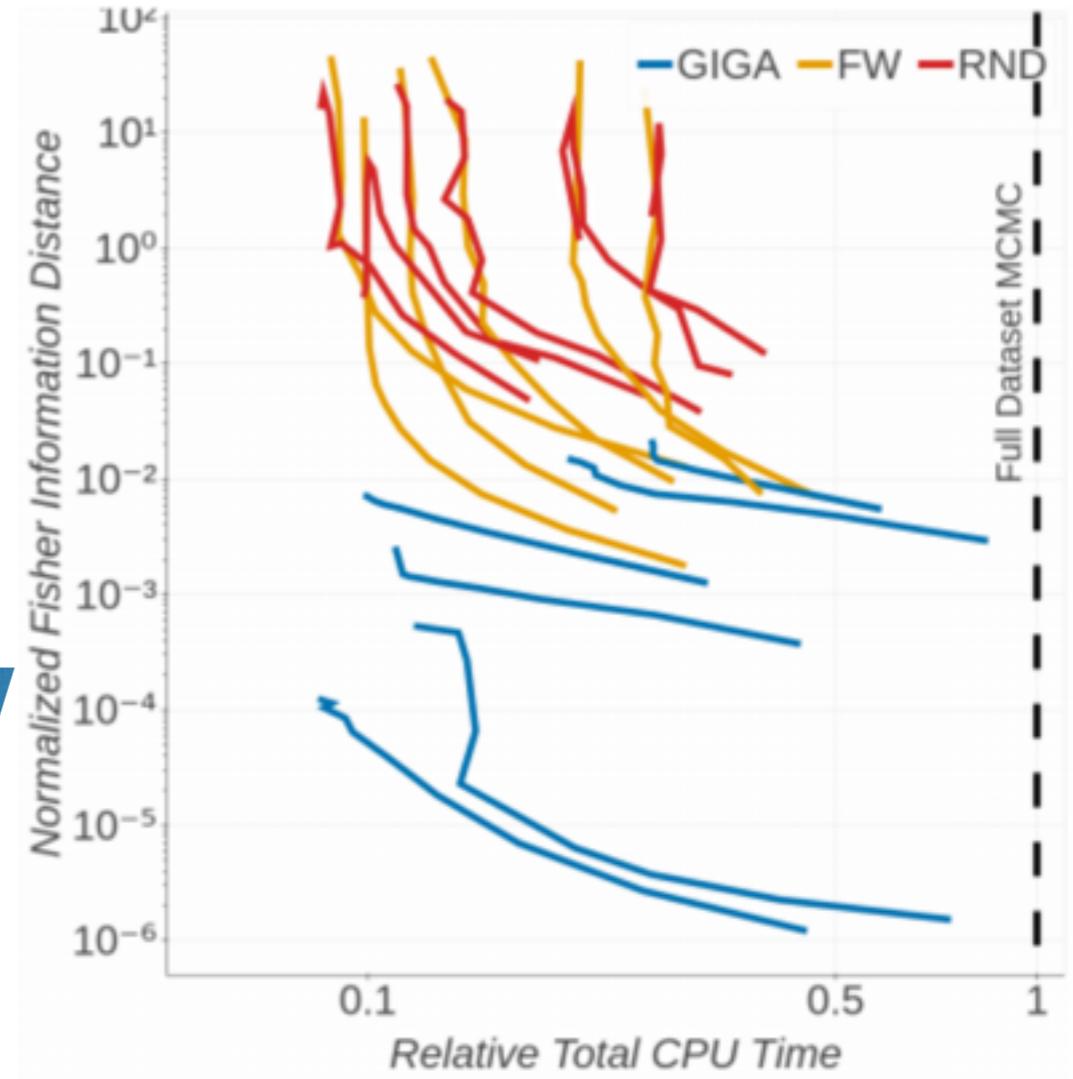
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lower
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[Campbell, Broderick 2018]

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T Campbell and T Broderick. Bayesian Coreset Construction via Greedy Iterative Geodesic Ascent. *ICML* 2018.

JH Huggins, T Campbell, and T Broderick. Coresets for scalable Bayesian logistic regression. *NIPS* 2016.

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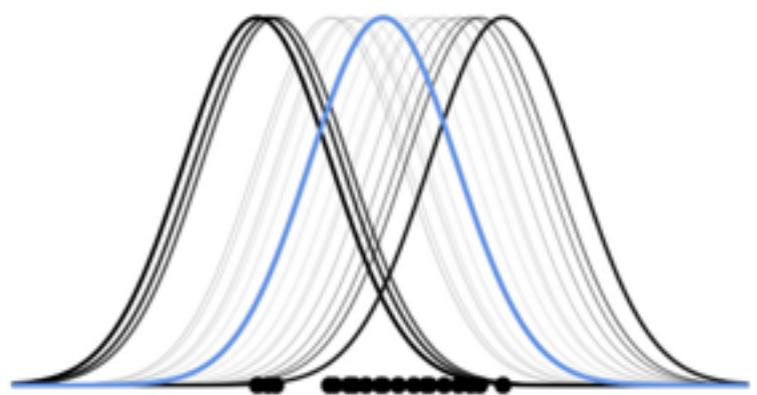
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Additional image references (5/5)

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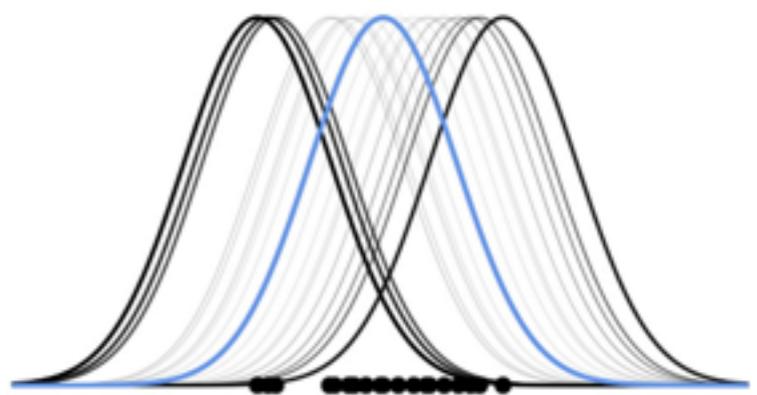
J. Herzog. 3 June 2016, 17:17:30. Obtained from: https://commons.wikimedia.org/wiki/File:Airbus_A350-941_F-WWCF_MSN002ILA_Berlin_2016_17.jpg (Creative Commons Attribution 4.0 International License)

Practicalities



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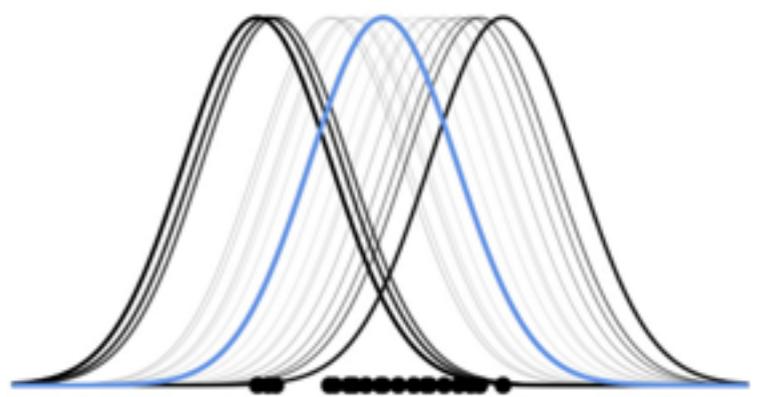
- Choice of norm



Practicalities

- Choice of norm
 - E.g. (weighted) Fisher information distance

$$\|\mathcal{L}(w) - \mathcal{L}\|_{\hat{\pi}, F}^2 := \mathbb{E}_{\hat{\pi}} [\|\nabla \mathcal{L}(\theta) - \nabla \mathcal{L}(w, \theta)\|_2^2]$$



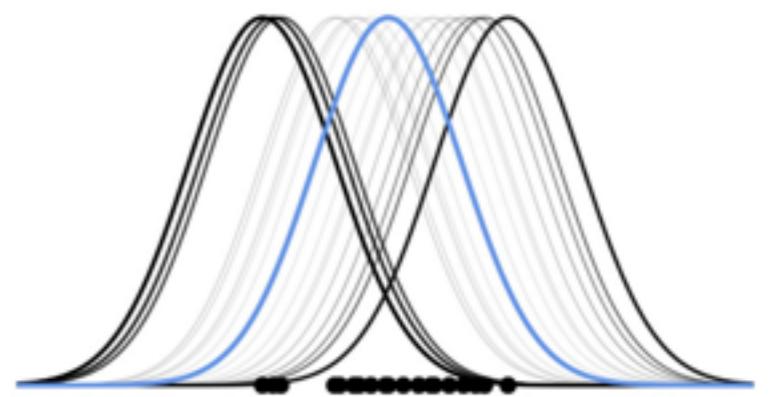
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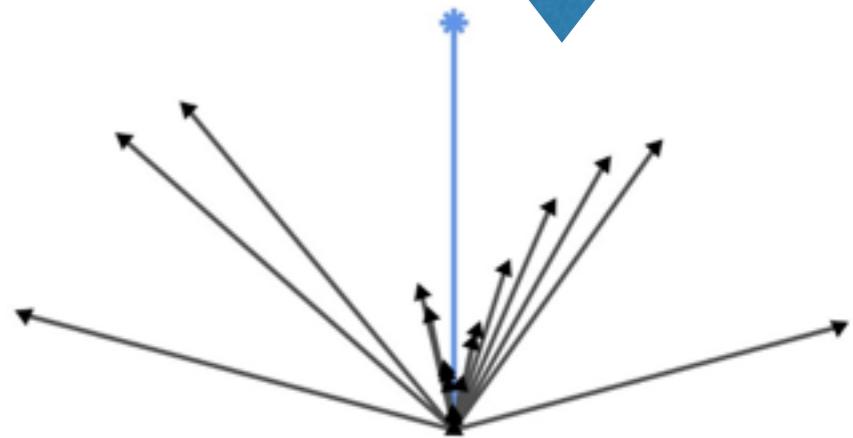
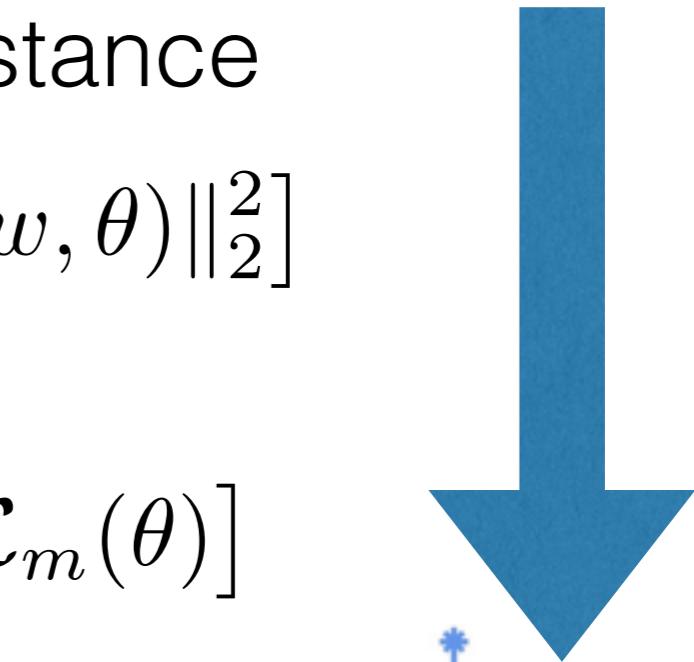
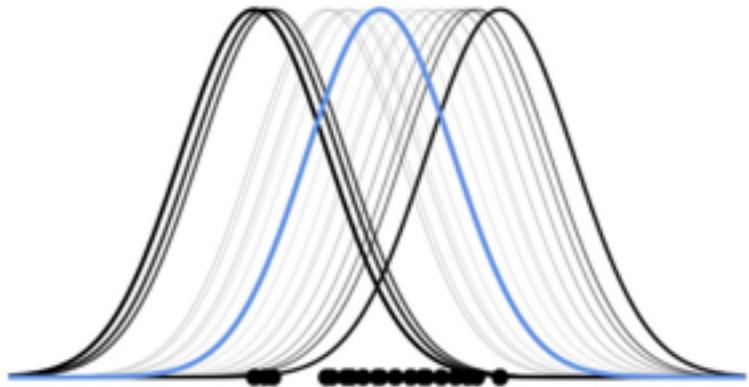
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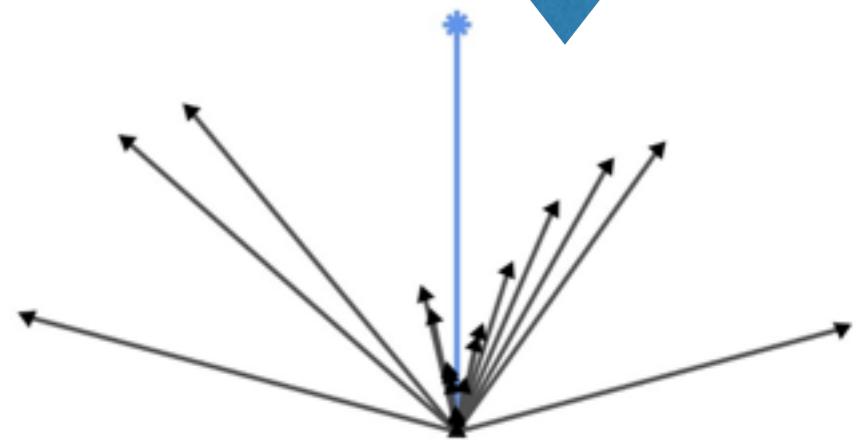
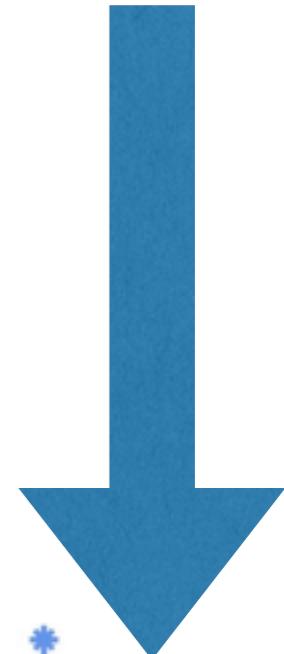
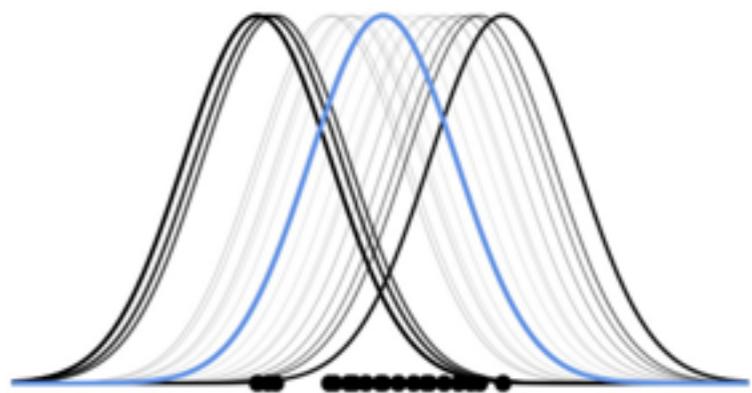


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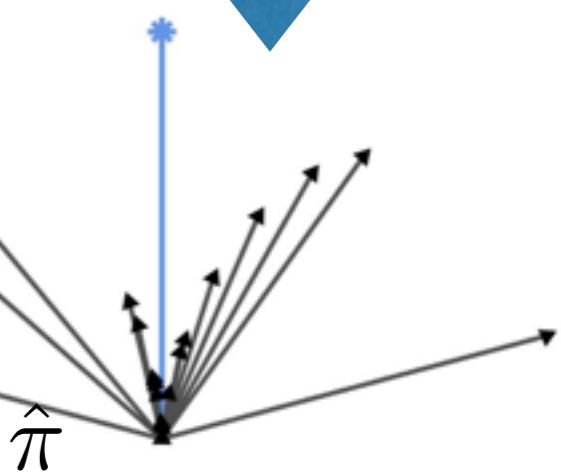
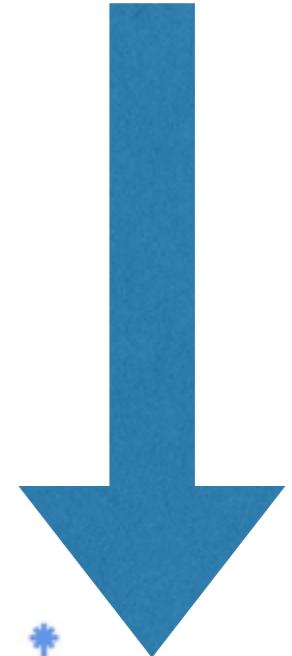
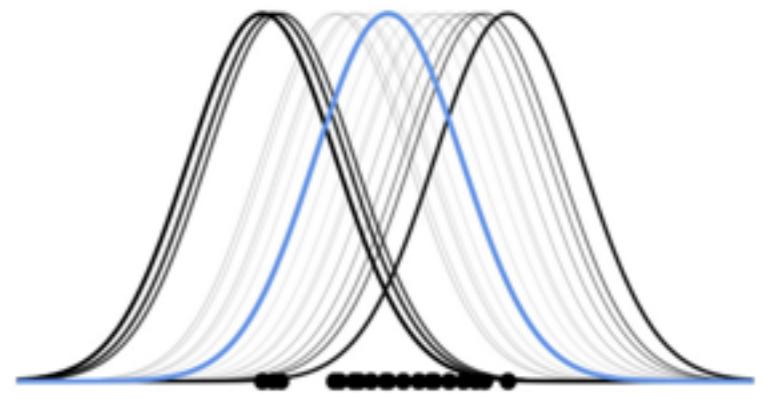
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$$\langle \mathcal{L}_n, \mathcal{L}_m \rangle_{\hat{\pi}, F} \approx \frac{D}{J} \sum_{j=1}^J (\nabla \mathcal{L}_n(\theta_j))_{d_j} (\nabla \mathcal{L}_m(\theta_j))_{d_j},$$

$d_j \stackrel{iid}{\sim} \text{Unif}\{1, \dots, D\}, \theta_j \stackrel{iid}{\sim} \hat{\pi}$



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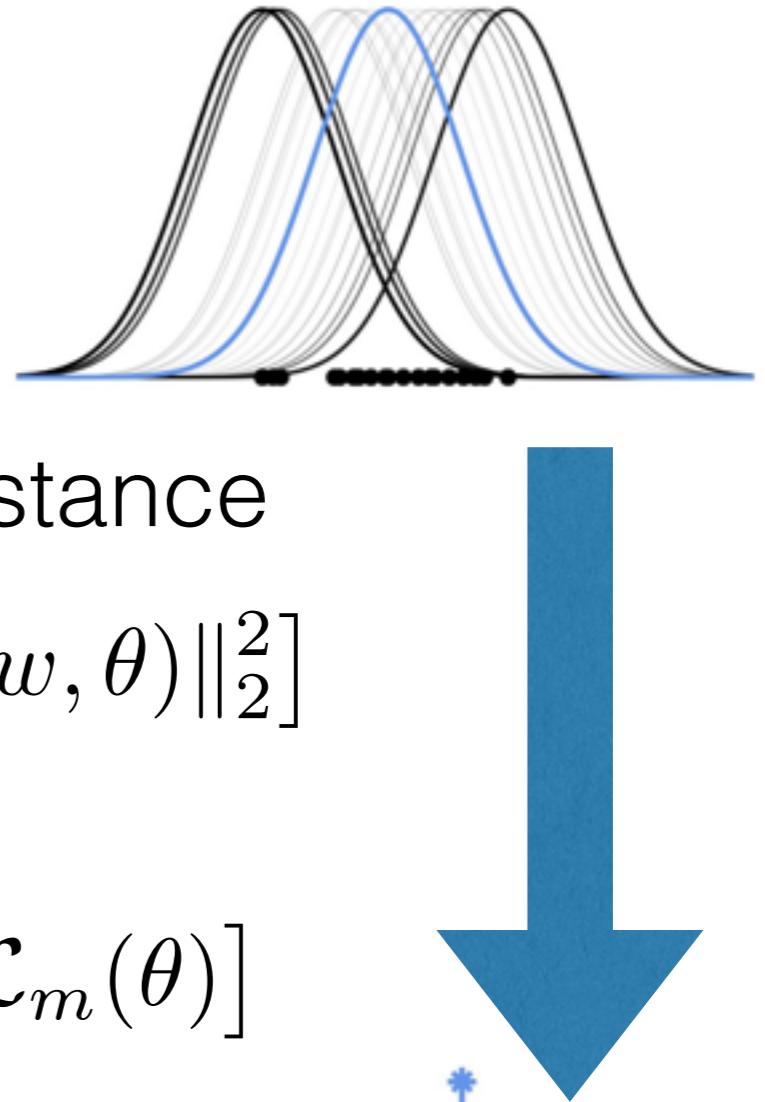
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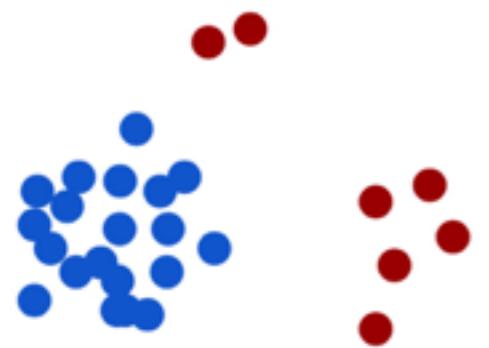
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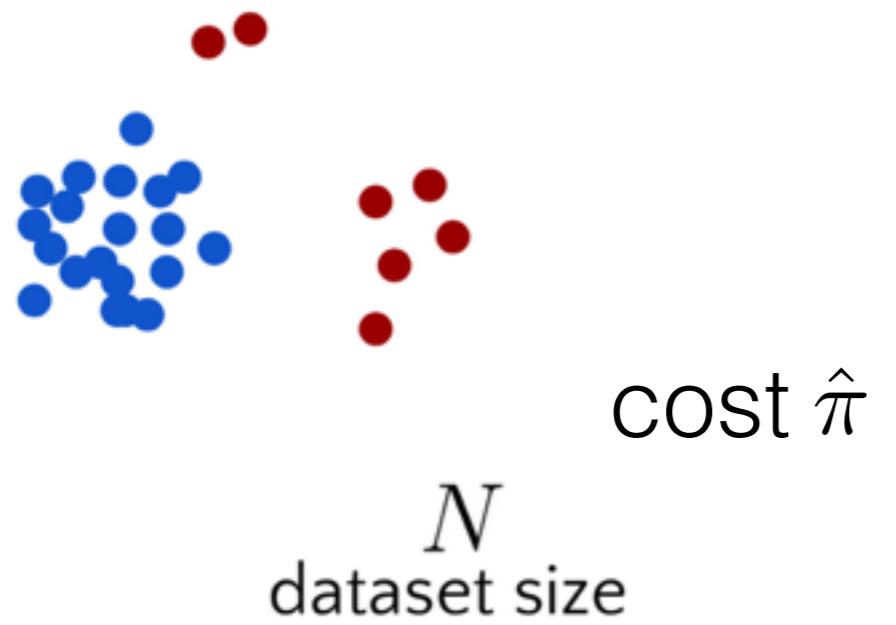
Thm sketch (CB). With high probability and large enough J , a good coresset after random feat. proj. is a good coresset for $(\mathcal{L}_n)_{n=1}^N$

Full pipeline

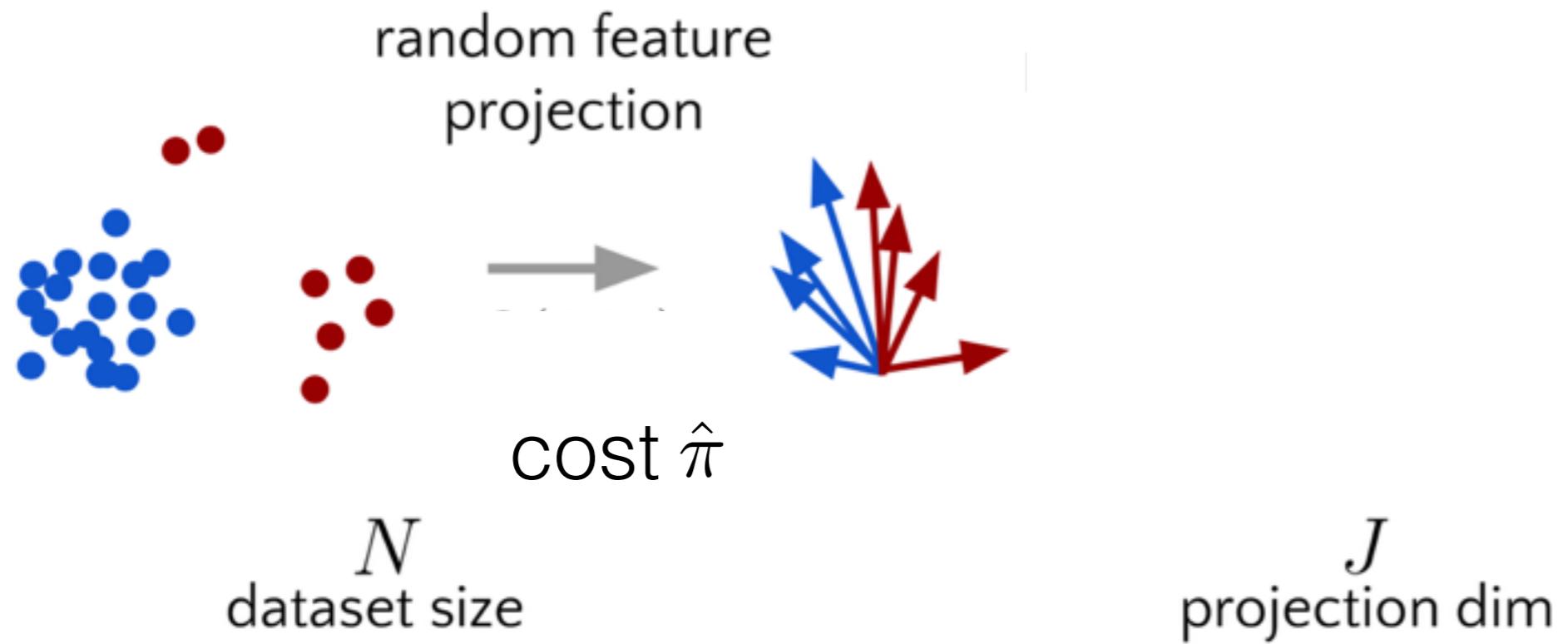


N
dataset size

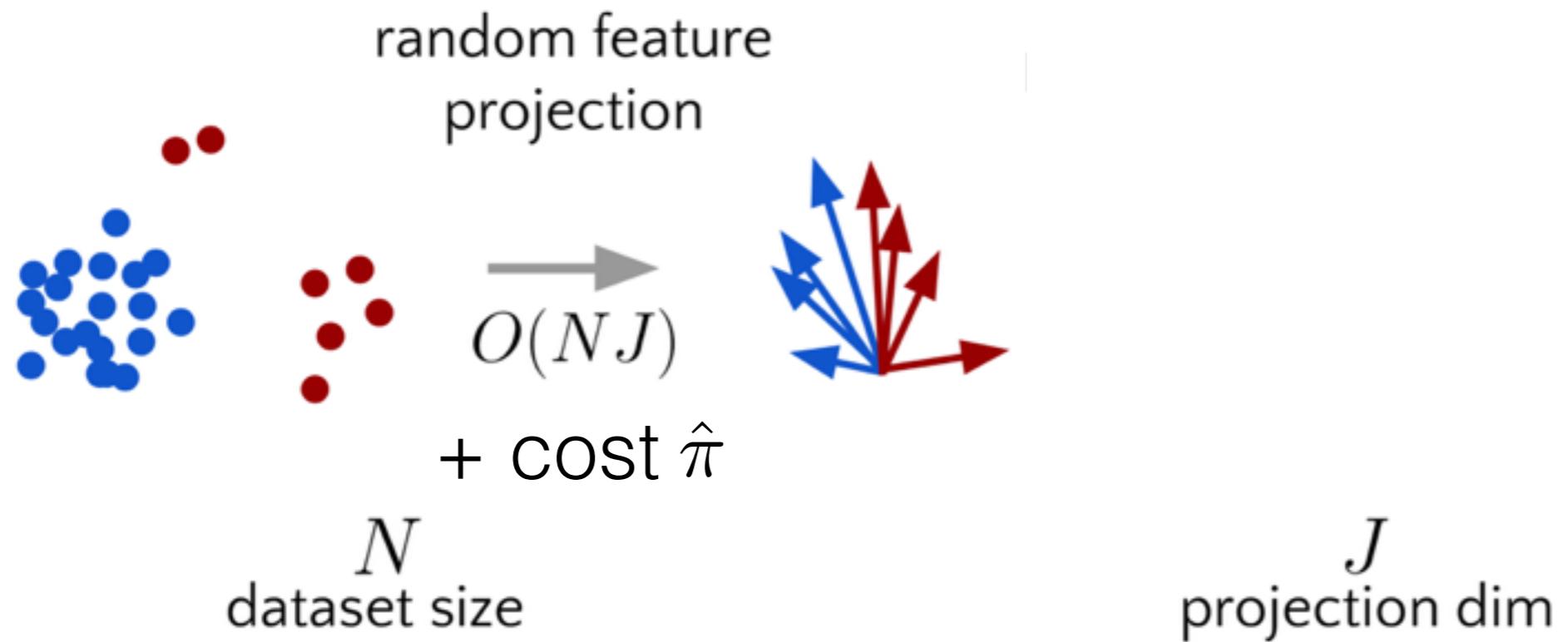
Full pipeline



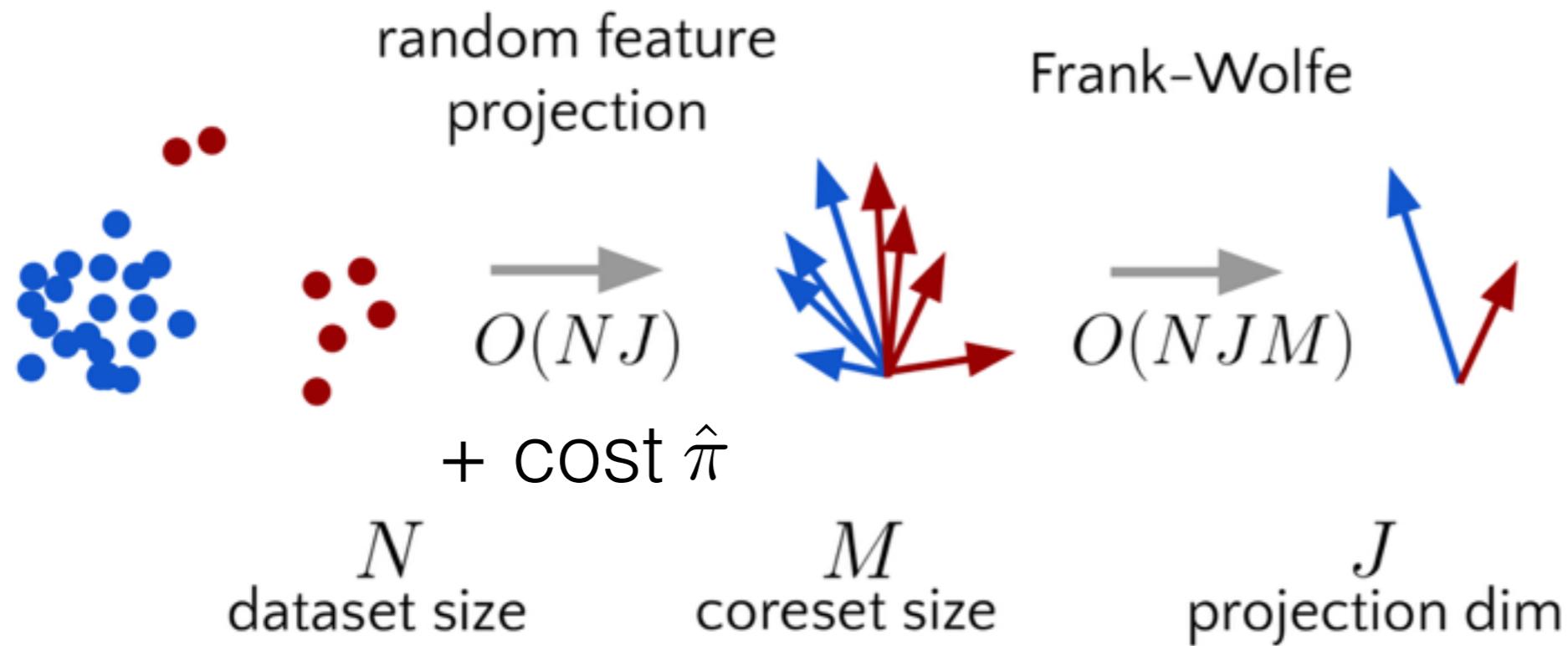
Full pipeline



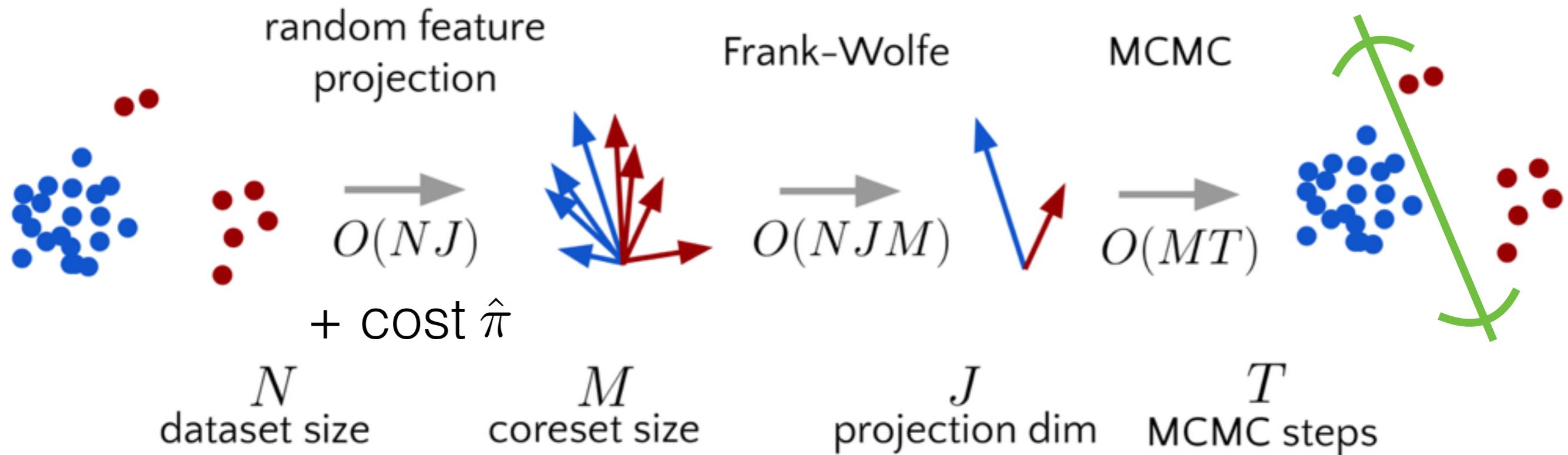
Full pipeline



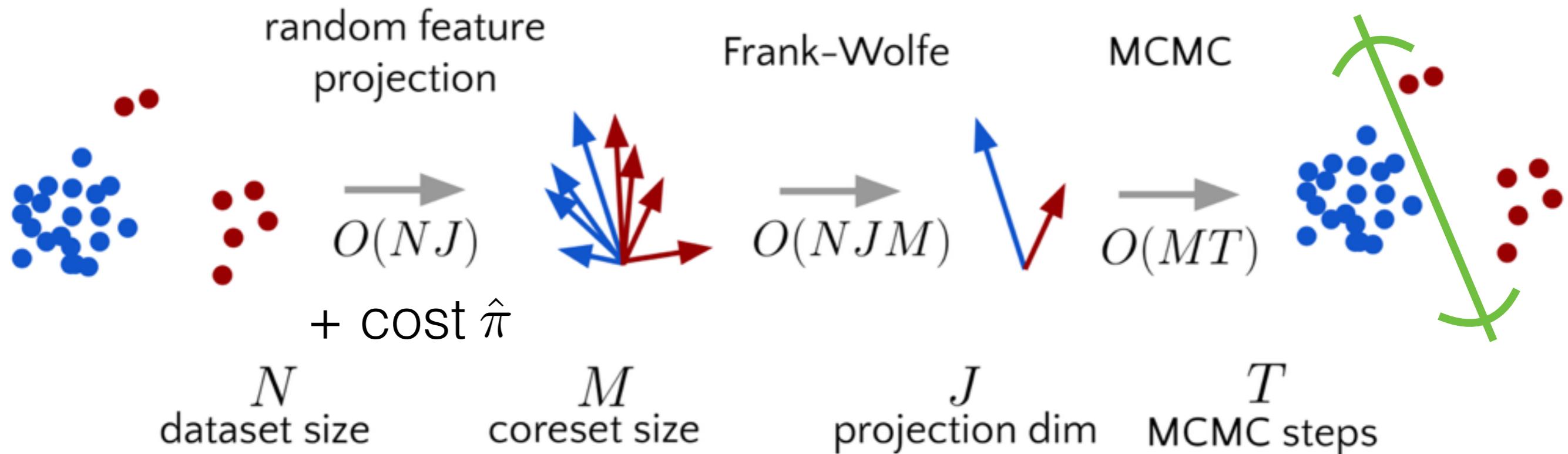
Full pipeline



Full pipeline

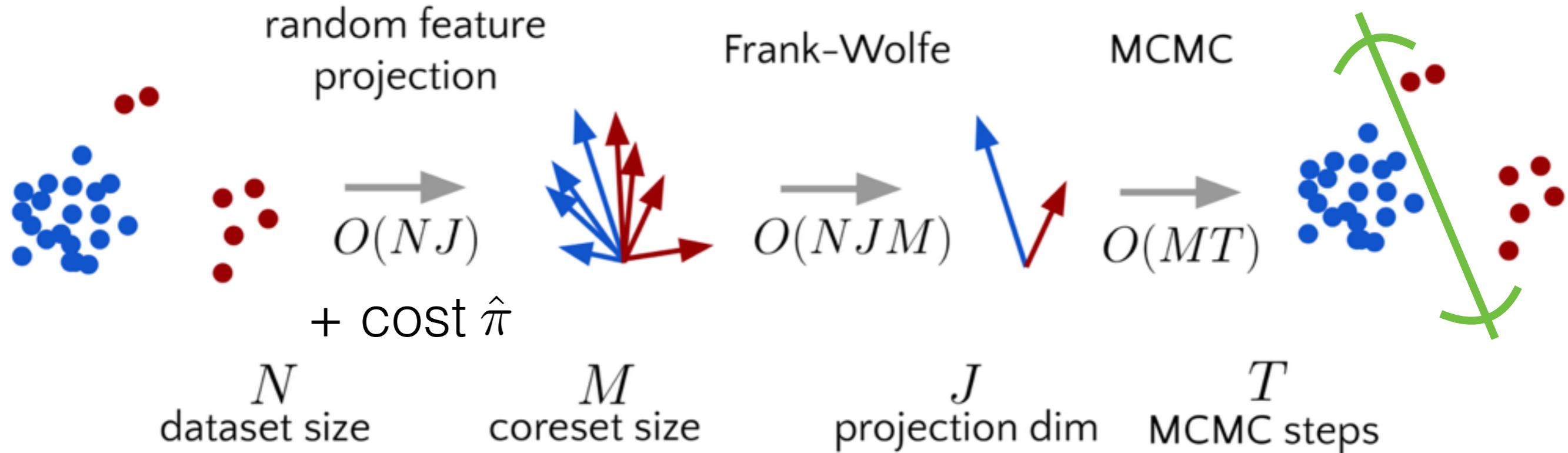


Full pipeline



- vs. $O(NT)$

Full pipeline



- vs. $O(NT)$
- Can make streaming, distributed