ISTA 421/521
Introduction to Machine Learning

Lecture 19: Estimation: Sampling, Metropolis-Hastings

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$$g(\mathbf{w};\mathbf{X},\mathbf{t},\sigma^2) = p(\mathbf{t}|\mathbf{X},\mathbf{w})p(\mathbf{w}|\sigma^2)$$

$$\boxed{p(\mathbf{w}|\mathbf{X},\mathbf{t},\sigma^2)} = Z^{-1}g(\mathbf{w};\mathbf{X},\mathbf{t},\sigma^2)$$

$$Z^{-1} = p(\mathbf{t}|\mathbf{X},\sigma^2) = \int p(\mathbf{t}|\mathbf{X},\mathbf{w})p(\mathbf{w}|\sigma^2)\ d\mathbf{w}$$

Our Options (when cannot compute ***posterior*** directly)

1. Find the single value of **w** that corresponds to the highest value of the posterior. As $g(\mathbf{w};\mathbf{X},\mathbf{t},\sigma^2)$ is proportional to the posterior, a maximum of *g* will also correspond to a maximum of the posterior. Z^{-1} is not a function of **w**. MAP
2. Approximate $p(\mathbf{w};\mathbf{X},\mathbf{t},\sigma^2)$ with some other density that we can compute analytically.
3. Sample directly from the posterior $p(\mathbf{w};\mathbf{X},\mathbf{t},\sigma^2)$, knowing only $g(\mathbf{w};\mathbf{X},\mathbf{t},\sigma^2)$

Method 1: MAP point estimate

- While we cannot derive a direct analytic posterior density that we can compute, we can computer something proportional to it:

$$g(\mathbf{w}; \mathbf{X}, \mathbf{t}, \sigma^2) = p(\mathbf{t}|\mathbf{X}, \mathbf{w})p(\mathbf{w}|\sigma^2)$$

- We will find the value of **w** that maximizes *g*
- This will correspond to the value at the maximum of the posterior.
- This will be the most likely value $\hat{\mathbf{w}}$ under the posterior.
- In cases like logistic regression, need to estimate $\hat{\mathbf{w}}$ though an approximation method; we introduced gradient methods (Woodrow-Hoff, Newton-Raphson)

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Using Newton-Raphson for MAP

$$\log g(\mathbf{w}; \mathbf{X}, \mathbf{t}) = \log p(\mathbf{t}|\mathbf{X}, \mathbf{w}) + \log p(\mathbf{w}|\sigma^2)$$

$$x_{n+1} = x_n - \frac{f'(x_n)}{f''(x_n)}$$

$$\mathbf{w}' = \mathbf{w} - \left(\frac{\partial^2 \log g(\mathbf{w}; \mathbf{X}, \mathbf{t})}{\partial \mathbf{w} \partial \mathbf{w}^\mathsf{T}}\right)^{-1} \frac{\partial \log g(\mathbf{w}; \mathbf{X}, \mathbf{t})}{\partial \mathbf{w}}$$

Point is guaranteed maximum if Hessian is negative definite
(as we showed for max likelihood)

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Method 2:
The Laplace* Approximation

- **The Idea**: *approximate* the density of interest with a Gaussian.
- (Recall that the Gaussian is used quite often in statistics to approximate other distributions!)
- However, **keep in mind**: our predictions will only be as good as our approximation – if the true posterior is not very Gaussian, then our predictions will be easy to compute but not very useful.

*Following the note in the book: the Machine Learning community has come to refer to the method this way, but this is elsewhere referred to as **saddle-point approx.**, and in statistics, the Laplace approx. is something different.

$$p(\mathbf{t}|\mathbf{X},\mathbf{w}) = \prod_{n=1}^{N}\left(\frac{1}{1+\exp(-\mathbf{w}^\top\mathbf{x}_n)}\right)^{t_n}\left(\frac{\exp(-\mathbf{w}^\top\mathbf{x}_n)}{1+\exp(-\mathbf{w}^\top\mathbf{x}_n)}\right)^{1-t_n} \qquad p(\mathbf{w}|\sigma^2) = \mathcal{N}(0,\sigma^2\mathbf{I})$$

Approximating *g* using the Taylor Expansion

$$g(\mathbf{w};\mathbf{X},\mathbf{t},\sigma^2) = p(\mathbf{t}|\mathbf{X},\mathbf{w})p(\mathbf{w}|\sigma^2)$$

$$\log g(\mathbf{w};\mathbf{X},\mathbf{t}) = \log p(\mathbf{t}|\mathbf{X},\mathbf{w}) + \log p(\mathbf{w}|\sigma^2)$$

$$\sum_{n=0}^{\infty}\frac{(\mathbf{w}-\hat{\mathbf{w}})^n}{n!}\left.\frac{\partial^n f(\mathbf{w})}{\partial \mathbf{w}^n}\right|_{\hat{\mathbf{w}}}$$

Recall, the univariate Gaussian:

$$\frac{1}{\sqrt{2\pi}\sigma}\exp\left\{-\frac{1}{2\sigma^2}(w-\mu)^2\right\}$$

The log of the univ. G
(K is the normalizing constant):

$$\log(K) - \frac{1}{2\sigma^2}(w-\mu)^2$$

This is the Laplace approximation!
We approximate the posterior with a Gaussian that has its
mean at the posterior **mode** ($\hat{w}$),
variance inversely proportional to the curvature of the posterior (g'') at its mode.

Univariate version:

$\mu = \widehat{w}$ $\quad \sigma^2 = 1/v$

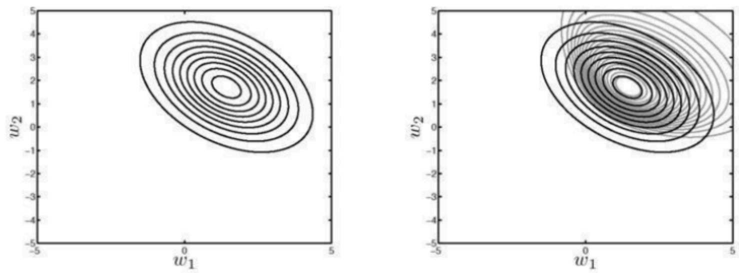
Multivariate version:

$$\mu = \hat{\mathbf{w}}, \quad \mathbf{\Sigma}^{-1} = -\left.\left(\frac{\partial^2 \log g(\mathbf{w};\mathbf{X},\mathbf{t})}{\partial\mathbf{w}\partial\mathbf{w}^\top}\right)\right|_{\hat{\mathbf{w}}}$$

similar form!

$$\log g(w;\mathbf{X},\mathbf{t},\sigma^2) \approx \log g(\widehat{w};\mathbf{X},\mathbf{t},\sigma^2) - \frac{v}{2}(w-\widehat{w})^2 \qquad v = -\left.\frac{\partial^2 \log g(w;\mathbf{X},\mathbf{t},\sigma^2)}{\partial w^2}\right|_{\widehat{w}}$$

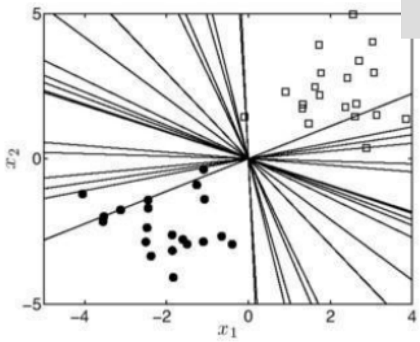
Laplace Approximation Example



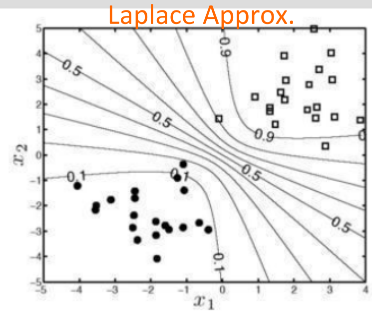
(a) Laplace approximation to the posterior

$$\mathbf{w}_s \leftarrow \mathcal{N}(\mu, \mathbf{\Sigma})$$

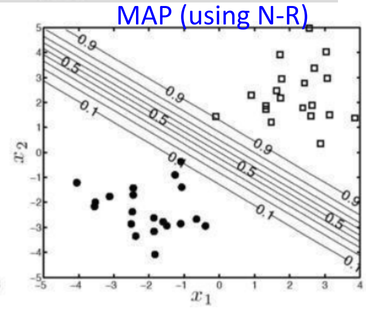
$$P(T_{\text{new}} = 1|\mathbf{x}_{\text{new}}, \mathbf{X}, \mathbf{t}, \sigma^2) = \frac{1}{N_s}\sum_{s=1}^{N_s} \frac{1}{1+\exp(-\mathbf{w}_s^{\mathsf{T}}\mathbf{x}_{\text{new}})}$$



Laplace Approx.



MAP (using N-R)



Method 3:
Sampling from Posterior

- Interest in Posterior density is to allow us to take *all* the uncertainty in **w** into account when making predictions.

Posterior density over the parameters

$$P(T_{\text{new}} = 1|\mathbf{x}_{\text{new}}, \mathbf{X}, \mathbf{t}, \sigma^2) = \mathbf{E}_{p(\mathbf{w}|\mathbf{X},\mathbf{t},\sigma^2)}\left\{P(T_{\text{new}} = 1|\mathbf{x}_{\text{new}}, \mathbf{w})\right\}$$

- Laplace method uses a *similar* density to provide an approximation of the posterior; still had to sample from it to estimate the integral.
- Now we'll look at sampling ***directly*** from the posterior.

The Intuition

$\mathbf{y}$: position of the dart

$\mathbf{\Delta}$: intended target

$p(\mathbf{y}|\mathbf{\Delta})$ Can be hard to model

$T = f(\mathbf{y})$ A new random variable:
T=1 : within 20
T=0 : outside of 20

$P(T = 1|\mathbf{\Delta})$

$$P(T = 1|\mathbf{\Delta}) = \mathbb{E}_{p(\mathbf{y}|\mathbf{\Delta})}\{f(\mathbf{y})\} = \int f(\mathbf{y})p(\mathbf{y}|\mathbf{\Delta})\mathrm{d}\mathbf{y}$$

OR: have your friend try to hit the 20, and find average hits!

$$\mathbf{y}_s \leftarrow p(\mathbf{y}|\mathbf{\Delta}) \qquad P(T = 1|\mathbf{\Delta}) \simeq \frac{1}{N_s}\sum_{s=1}^{N_s} f(\mathbf{y}_s)$$

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Expectation

$$\mathbb{E}_{p(z)}\{f(z)\} = \int f(z)p(z)\mathrm{d}z$$

Normalization

$$\int p(z)\mathrm{d}z = \mathbb{E}_{p(z)}\{\mathbf{1}_{\mathbb{R}}(z)\}$$

$$\mathbf{1}_S(x) = \begin{cases} 1 & \text{if } x \in S \\ 0 & \text{otherwise} \end{cases}$$

Probability

$$P(Z \leq z_0) = \int_{-\infty}^{z_0} p(z)\mathrm{d}z = \int_{-\infty}^{\infty} \mathbf{1}_{(-\infty,z_0]}(z)\mathrm{d}z = \mathbb{E}_{p(z)}\{\mathbf{1}_{(-\infty,z_0]}(z)\}$$

Marginalization

$$p(v) = \int p(v,z)\mathrm{d}z = \int p(v|z)p(z)\mathrm{d}z = \mathbb{E}_{p(z)}\{p(v|z)\}$$

The **predictive distribution** is a marginalization:

$$P(T_{new}=1|\mathbf{x}_{new},\mathbf{X},\mathbf{t},\sigma^2) = \int P(T_{new}=1|\mathbf{x}_{new},\mathbf{w})p(\mathbf{w}|\mathbf{X},\mathbf{t},\sigma^2)\mathrm{d}\mathbf{w}$$
$$= \mathbb{E}_{p(\mathbf{w}|\mathbf{X},\mathbf{t},\sigma^2)}\{P(T_{new}=1|\mathbf{x}_{new},\mathbf{w})\}$$

… put another way: it's the expectation of the likelihood function under the posterior distribution

$$P(T_{new}=1|\mathbf{x}_{new},\mathbf{X},\mathbf{t},\sigma^2) \simeq \frac{1}{N_s}\sum_{s=1}^{N_s} P(T_{new}=1|\mathbf{x}_{new},\mathbf{w}_s)$$
$$\mathbf{w}_s \leftarrow \underbrace{p(\mathbf{w}|\mathbf{X},\mathbf{t},\sigma^2)}$$

But how do we estimate this?

(A touch of theory on) **Markov Chains**

- A **Stochastic Process** is a collection of random variables indexed by a set T; i.e., $\{ X_t \mid t \in T \}$
  - Here, we only care about discrete-time stochastic processes, i.e., when T is a countable set.
  - For example, $T = \mathbf{Z}_+$ or $T = \{0,1,2,3,4,5\}$
- **Example**
  - The results of 100 coin tosses is a stochastic process, with random variables $C_1,\ldots,C_{100}$
  - The daily temperature is a stochastic process, represented by random variables T_1, T_2, …
- Stochastic processes are like any other sets of variables; we can talk about distributions:
  - $p_t(x_t)$, for any $t \in T$
  - $p(x_{t1},\ldots,x_{tn})$, for any $\{t_1, \ldots, t_n\} \subset T$

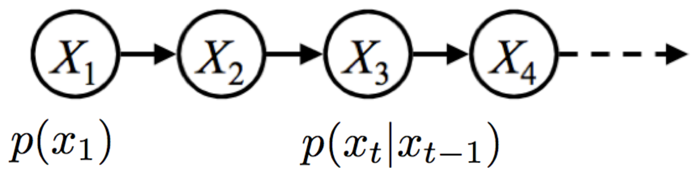
(A touch of theory on) **Markov Chains**

- A (first-order) **Markov chain** is a discrete-time stochastic process with the Markov Property:

$$p(x_t|x_{t-1}, x_{t-2}, ..., x_1) = p(x_t|x_{t-1})$$

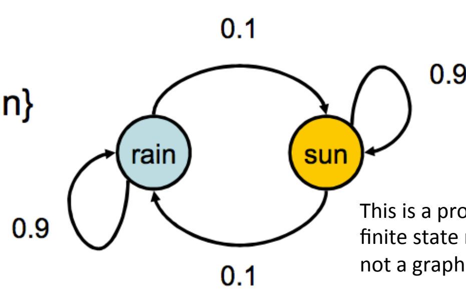
  – That is, the variable at time *t* only depends on the variable at time *t*–1.

  – Here, the conditional density p(x_t | $x_{t\text{-}1}$) (also called the transition kernel) is the same for all $t \in T$



Example Markov Chain

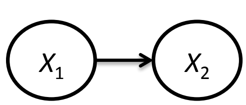
- Weather:
  - States: X = {rain, sun}
  - Transitions:



This is a probabilistic finite state machine, not a graphical model!

  - Initial distribution: 1.0 sun
  - What's the probability distribution after one step?

$$P(X_2 = \text{sun}) = P(X_2 = \text{sun}|X_1 = \text{sun})P(X_1 = \text{sun}) + P(X_2 = \text{sun}|X_1 = \text{rain})P(X_1 = \text{rain})$$



$$0.9 \cdot 1.0 + 0.1 \cdot 0.0 = 0.9$$

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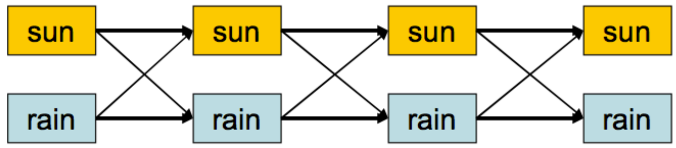
Join (product) of X_1 and X_2, followed by sum (marginalization) of X_1

Mini "Forward" Algorithm

- Question: What's P(X) on some day t?
  - An instance of variable elimination!



$$P(x_t) = \sum_{x_{t-1}} P(x_t|x_{t-1})P(x_{t-1})$$

$$P(x_1) = \text{known}$$

Forward simulation

Example Markov Chains

- From initial observation of sun

$$\underset{P(X_1)}{\begin{pmatrix} 1.0 \\ 0.0 \end{pmatrix}} \quad \underset{P(X_2)}{\begin{pmatrix} 0.9 \\ 0.1 \end{pmatrix}} \quad \underset{P(X_3)}{\begin{pmatrix} 0.82 \\ 0.18 \end{pmatrix}} \quad \Rightarrow \quad \underset{P(X_\infty)}{\begin{pmatrix} 0.5 \\ 0.5 \end{pmatrix}}$$

- From initial observation of rain

$$\underset{P(X_1)}{\begin{pmatrix} 0.0 \\ 1.0 \end{pmatrix}} \quad \underset{P(X_2)}{\begin{pmatrix} 0.1 \\ 0.9 \end{pmatrix}} \quad \underset{P(X_3)}{\begin{pmatrix} 0.18 \\ 0.82 \end{pmatrix}} \quad \Rightarrow \quad \underset{P(X_\infty)}{\begin{pmatrix} 0.5 \\ 0.5 \end{pmatrix}}$$

Example Markov Chains

- What if we had a different transition probability ?

$$\begin{array}{cc} & & t+1 & \\ & & \text{sunny} & \text{rainy} \\ t & \begin{array}{c}\text{sunny} \\ \text{rainy}\end{array} & \multicolumn{2}{c}{\begin{bmatrix} 0.9 & 0.1 \\ 0.5 & 0.5 \end{bmatrix}} \end{array}$$

- If we set $\boldsymbol{\pi}_0 = [1, 0]^\top$, i.e., today is sunny:
  - $\boldsymbol{\pi}_2 = [0.844, 0.156]^\top$
  - $\boldsymbol{\pi}_5 = [0.834, 0.166]^\top$
  - $\boldsymbol{\pi}_{20} = [0.83333, 0.16667]^\top$
  - $\boldsymbol{\pi}_{50} = [0.83333, 0.16667]^\top$
  - See a pattern?

Stationary Distribution

- A distribution π is **stationary** for a Markov chain if the transition kernel for the chain preserves π; i.e., if for all $x_t \in R^d$

$$\int p(x_t|x_{t-1})\pi(x_{t-1})\mathrm{d}x_{t-1} = \pi(x_t)$$

- Implication: if at any time t, $p_t(x_t) = \pi(x_t)$, then the marginals from that point on will be $\pi(x_t)$, since

$$\begin{aligned} \int p_{t+1}(x_{t+1}) &= \int p(x_{t+1}|x_t)p_t(x_t)\mathrm{d}x_t \\ &= \int p(x_{t+1}|x_t)\pi(x_t)\mathrm{d}x_t \\ &= \pi(x_{t+1}) \end{aligned}$$

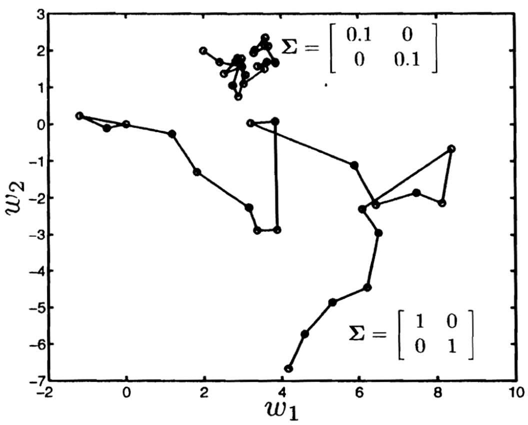
- **Ergodicity**: guarantees a stationary distribution exists and is unique
  - **Aperiodic**: can always transition back to state *a* having just transition from *a* to *b* (a state *x* has a period *k* if, starting from that state, it is only possible to return to it in multiples of *k*; in that case, the x is said to be periodic.)
  - **Irreducible**: It is possible to get to any state from any state (i.e., does not end up in a sink)
- **Theorem**: If a Markov chain is irreducible and aperiodic, then it will have a unique stationary distribution
- So, how do we construct one for our posterior distribution of interest?

Named in the list of Top 10 Algorithms of the 20th Century (*SIAM News*, Vol 33, No 4, 2000)

Nicholas Metropolis-W. Keith Hastings Algorithm

physicist 1953 *statistician* 1970

Random Walk



Two desirable criteria for proposal distribution:
- (a) Easy to sample from
- (b) Symmetric:

$$p(\widetilde{\mathbf{w}}_s|\mathbf{w}_{s-1},\mathbf{\Sigma}) = p(\mathbf{w}_{s-1}|\widetilde{\mathbf{w}}_s,\mathbf{\Sigma})$$

$\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_{s-1}, \mathbf{w}_s, \ldots, \mathbf{w}_{N_s}$

(0) Getting started: choosing $\mathbf{w}_1$

Turns out it doesn't matter: in theory, sample long enough and guaranteed to converge

Generating $\mathbf{w}_s$ takes 2 steps:

(1) Propose a new sample (based on previous)

$$\widetilde{\mathbf{w}}_s \leftarrow p(\widetilde{\mathbf{w}}_s|\mathbf{w}_{s-1}) \quad \text{proposal distribution}$$

Does **not** have to be related to target distribution!
Popular to use Gaussian centered on $\mathbf{w}_{s-1}$

$$p(\widetilde{\mathbf{w}}_s|\mathbf{w}_{s-1},\mathbf{\Sigma}) = \mathcal{N}(\mathbf{w}_{s-1},\mathbf{\Sigma})$$

(2) Test whether to accept or reject $\widetilde{\mathbf{w}}_s$

posterior at proposed sample

$$r = \frac{p(\widetilde{\mathbf{w}}_s|\mathbf{X},\mathbf{t},\sigma^2)}{p(\mathbf{w}_{s-1}|\mathbf{X},\mathbf{t},\sigma^2)} \frac{p(\mathbf{w}_{s-1}|\widetilde{\mathbf{w}}_s,\mathbf{\Sigma})}{p(\widetilde{\mathbf{w}}_s|\mathbf{w}_{s-1},\mathbf{\Sigma})} \rightarrow 1$$

posterior at old sample

ratio of Proposal densities

Problem?: Cannot directly compute posteriors!

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physicist 1953 *statistician* 1970

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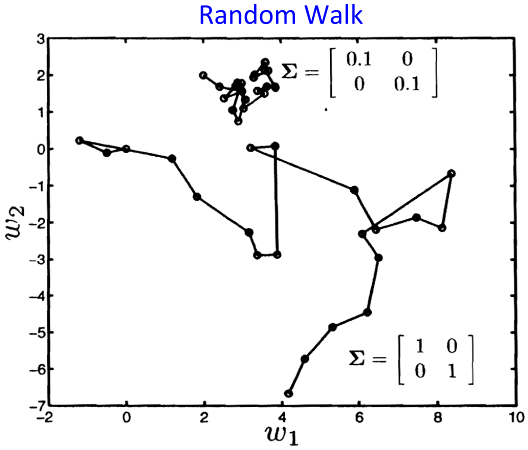

Two desirable criteria for proposal distribution:
- (a) Easy to sample from
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$$p(\widetilde{\mathbf{w}}_s|\mathbf{w}_{s-1},\mathbf{\Sigma}) = p(\mathbf{w}_{s-1}|\widetilde{\mathbf{w}}_s,\mathbf{\Sigma})$$

$\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_{s-1}, \mathbf{w}_s, \ldots, \mathbf{w}_{N_s}$

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$$p(\widetilde{\mathbf{w}}_s|\mathbf{w}_{s-1},\mathbf{\Sigma}) = \mathcal{N}(\mathbf{w}_{s-1},\mathbf{\Sigma})$$

(2) Test whether to accept or reject $\widetilde{\mathbf{w}}_s$

$$r = \frac{g(\widetilde{\mathbf{w}}_s;\mathbf{X},\mathbf{t},\sigma^2)}{g(\mathbf{w}_{s-1};\mathbf{X},\mathbf{t},\sigma^2)} = \frac{p(\widetilde{\mathbf{w}}_s|\sigma^2)}{p(\mathbf{w}_{s-1}|\sigma^2)} \frac{p(\mathbf{t}|\widetilde{\mathbf{w}}_s,\mathbf{X})}{p(\mathbf{t}|\mathbf{w}_{s-1},\mathbf{X})}$$

Don't need to calculate posteriors directly because the Marginal Likelihoods cancel in the ratio!

$r \geq 1$? If **yes**: always choose best: $\mathbf{w}_s = \widetilde{\mathbf{w}}_s$

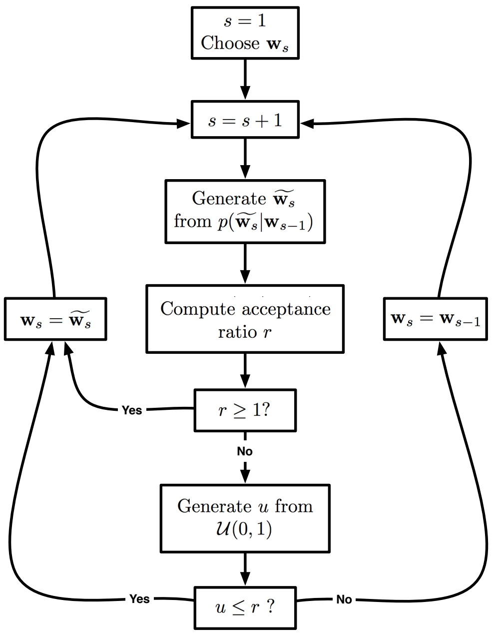
If **no**: possibly accept anyway

$u \leftarrow \mathcal{U}(0,1)$, $u \leq r$? **yes** $\rightarrow \mathbf{w}_s = \widetilde{\mathbf{w}}_s$; **no** $\rightarrow \mathbf{w}_s = \mathbf{w}_{s-1}$

Named in the list of Top 10 Algorithms of the 20th Century (*SIAM News*, Vol 33, No 4, 2000)

Metropolis-Hastings Algorithm

Nicholas Metropolis, *physicist*, 1953 — W. Keith Hastings, *statistician*, 1970



$\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_{s-1}, \mathbf{w}_s, \ldots, \mathbf{w}_{N_s}$

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$$p(\widetilde{\mathbf{w}}_s|\mathbf{w}_{s-1}, \boldsymbol{\Sigma}) = \mathcal{N}(\mathbf{w}_{s-1}, \boldsymbol{\Sigma})$$

(2) Test whether to accept or reject $\widetilde{\mathbf{w}}_s$

$$r = \frac{g(\widetilde{\mathbf{w}}_s; \mathbf{X}, \mathbf{t}, \sigma^2)}{g(\mathbf{w}_{s-1}; \mathbf{X}, \mathbf{t}, \sigma^2)} = \frac{p(\widetilde{\mathbf{w}}_s|\sigma^2)}{p(\mathbf{w}_{s-1}|\sigma^2)} \frac{p(\mathbf{t}|\widetilde{\mathbf{w}}_s, \mathbf{X})}{p(\mathbf{t}|\mathbf{w}_{s-1}, \mathbf{X})}$$

Don't need to calculate posteriors directly because the Marginal Likelihoods cancel in the ratio!

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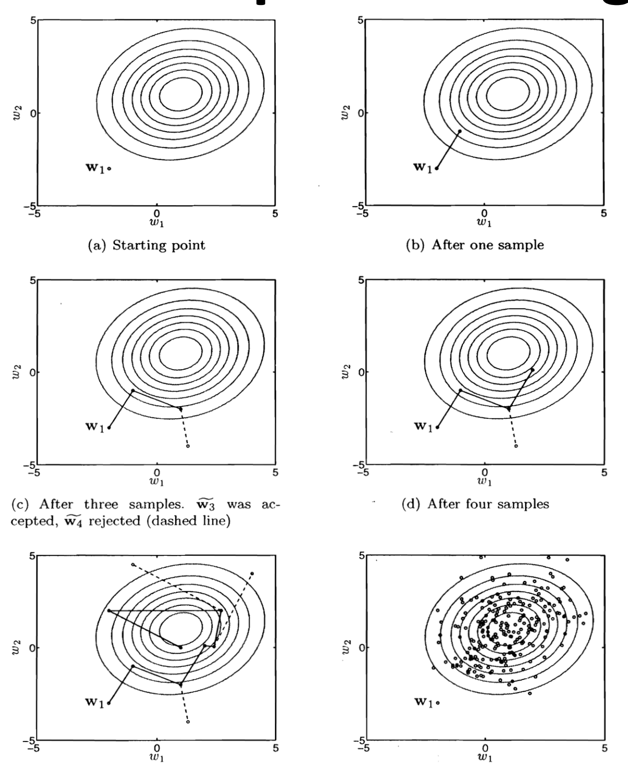
If **no**: possibly accept anyway

$u \leftarrow \mathcal{U}(0,1), \quad u \leq r$? **yes** → $\mathbf{w}_s = \widetilde{\mathbf{w}}_s$; **no** → $\mathbf{w}_s = \mathbf{w}_{s-1}$

Metropolis-Hastings Example 1



(a) Starting point

(b) After one sample

(c) After three samples. $\widetilde{\mathbf{w}}_3$ was accepted, $\widetilde{\mathbf{w}}_4$ rejected (dashed line)

(d) After four samples

(e) After 10 samples

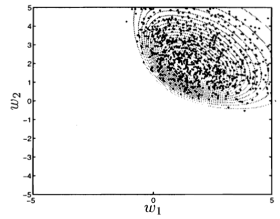
(f) The first 300 samples

$$\boldsymbol{\mu} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \mathbf{S} = \begin{bmatrix} 3 & 0.4 \\ 0.4 & 3 \end{bmatrix}$$

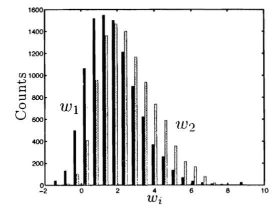
$$\boldsymbol{\mu}' = \frac{1}{N_s}\sum_{s=1}^{N_s} \mathbf{w}_s, \quad \mathbf{S}' = \frac{1}{N_s}\sum_{s=1}^{N_s} (\mathbf{w}_s - \boldsymbol{\mu}')(\mathbf{w}_s - \boldsymbol{\mu}')^{\mathsf{T}}$$

$$\boldsymbol{\mu}' = \begin{bmatrix} 0.9770 \\ 1.0928 \end{bmatrix}, \quad \mathbf{S}' = \begin{bmatrix} 3.0777 & 0.4405 \\ 0.4405 & 2.8983 \end{bmatrix}$$

Metropolis-Hastings Example 2



(a) 1000 of the MH samples along with the posterior contours



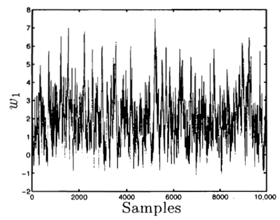
(b) Histograms of the samples for both w_1 (black) and w_2 (grey)

Burn In

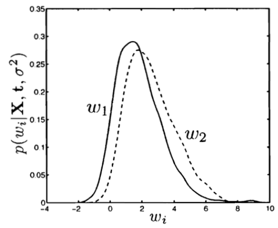
Convergence

Estimating predictions from samples $\mathbf{w}_s$

$$P(T_{\text{new}} = 1 | \mathbf{x}_{\text{new}}, \mathbf{X}, \mathbf{t}, \sigma^2) = \frac{1}{N_s} \sum_{s=1}^{N_s} \frac{1}{1 + \exp(-\mathbf{w}_s^{\mathsf{T}} \mathbf{x}_{\text{new}})}$$

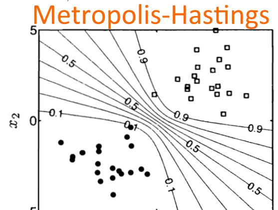


(c) All of the w_1 samples plotted against iteration, s



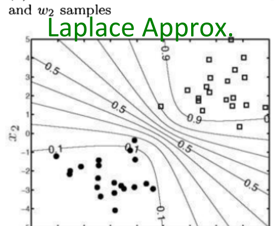
(d) Continuous densities fitted to the w_1 and w_2 samples

Metropolis-Hastings



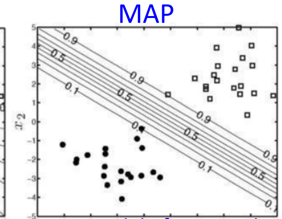
Accurate estimate of variance!

Laplace Approx.



Note how Laplace Gaussian overestimates variance

MAP



No model of variance!