



# Estimating the Probability of Convexity of a Function Observed with Noise

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# Problem Statement

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- Consider a function  $g : \text{compact } S \subseteq \mathbb{R}^d \rightarrow \mathbb{R}$  that can only be evaluated with the presence of **noise** at  $r$  points  $\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_r) \in \mathbb{R}^d$ . Let the true values of the function  $g$  at  $\mathbf{x}$  be denoted  $\mathbf{g} = (g(\mathbf{x}_1), g(\mathbf{x}_2), \dots, g(\mathbf{x}_r))^T$ .
- We wish to determine the **convexity/non-convexity of  $g$**  with some probabilistic guarantee, using only estimates of its values obtained through simulation at the points  $\mathbf{x}$ .

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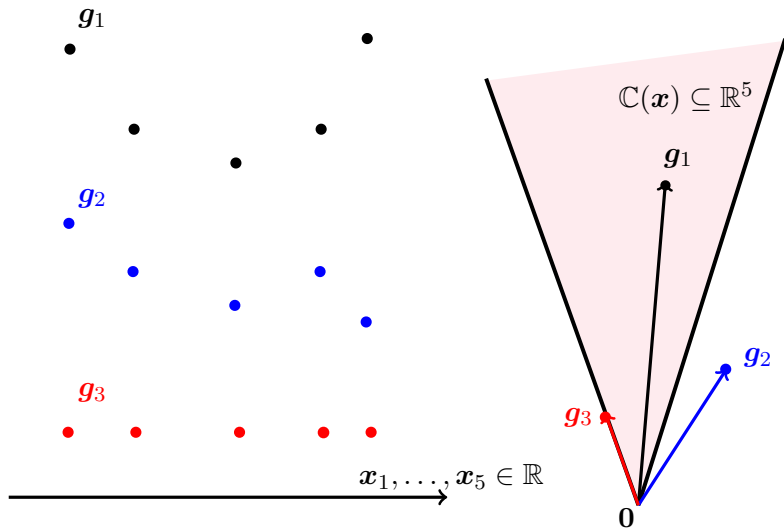
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3. More tractable

Not in this talk!

# Vector Convexity and Cone of $\mathbb{C}$



# Motivation

- Curiosity towards black-box functions



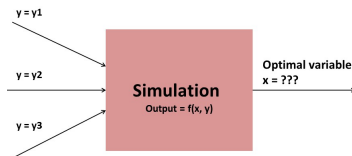
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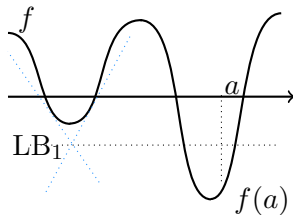
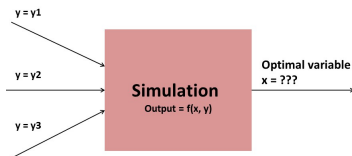


# Motivation

- Curiosity towards black-box functions
- Ease of Optimization
- Stopping rule for global (stochastic) optimization algorithms



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# Motivation

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Previous research: **One-shot frequentist** hypothesis test, with the number of samples predetermined [Jian, Henderson, and Hunter, 2014].

Dim	Distance	Regression parameters
1	Juditsky and Nemirovski [2002]	Baraud et al. [2005] Diack and Thomas-Agnan [1998] Meyer [2012] Wang and Meyer [2011]
$> 1$	Silvapulle and Sen [2001]	Lau [1978] Abrevaya and Jiang [2005]



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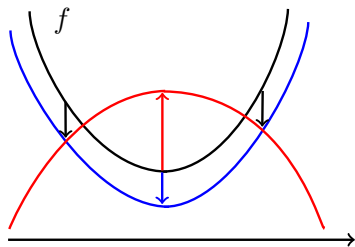
**Our Goal:** A **sequential** algorithm in the **Bayesian** setting with indefinite number of samples and can be stopped at any time.

- 1 Algorithm
- 2 Monte Carlo
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# Assumptions

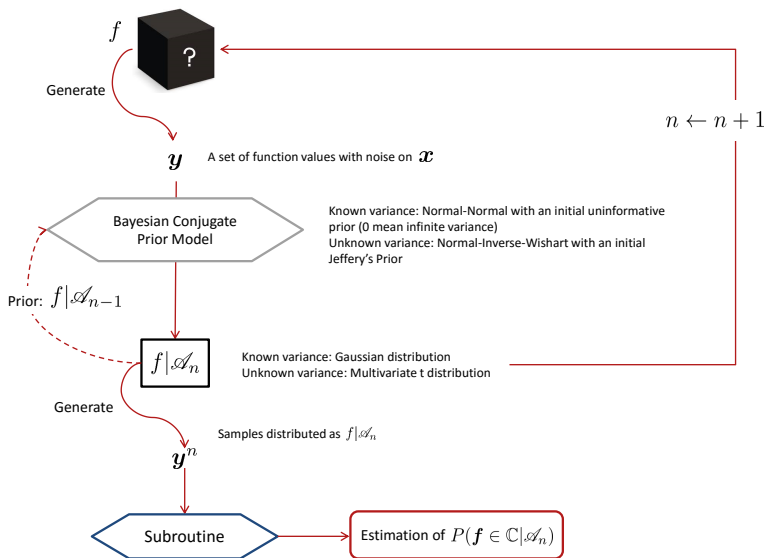
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1. We obtain realizations of a random vector  $\mathbf{Y} = \mathbf{f} + \boldsymbol{\xi}$ , where  $\boldsymbol{\xi} \sim N(\mathbf{0}, \Gamma) \in \mathbb{R}^r$ , with  $\Gamma$  positive-definite.
2. Conditional on  $\mathbf{f}$ , the samples  $(\mathbf{y}_n : n = 1, 2, \dots)$  in each iteration consists of i.i.d. random vectors.



Note that  $\Gamma$  is not necessarily diagonal because using **Common Random Numbers** can maintain the function structural properties (e.g. Chen et al. [2012]).

# Main Idea



# Convergence

## Theorem

Let  $p_n = P(\mathbf{f} \in \mathbb{C} | \mathcal{A}_n)$  be the  $n$ -iteration posterior probability that  $\mathbf{f}$  is convex. As  $n \rightarrow \infty$ ,  $p_n - \mathbb{1}\{\mathbf{f} \in \mathbb{C}\} \rightarrow 0$  a.s.

*Proof sketch (assume  $\Gamma$  known):*

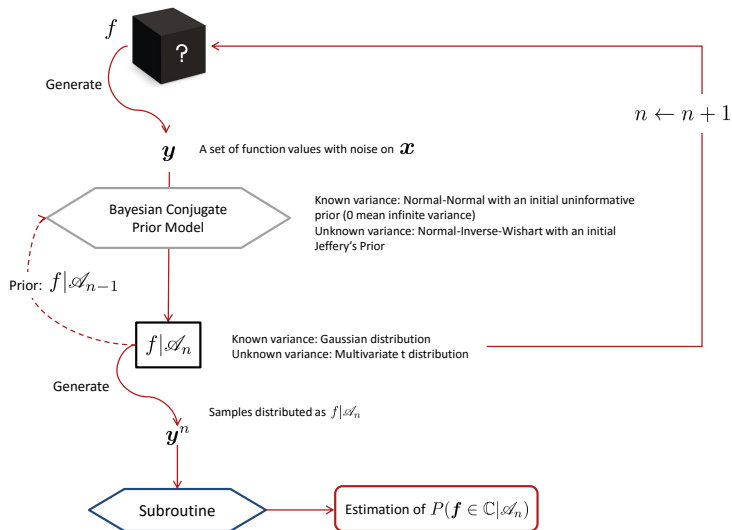
1.  $P(\mathbf{f} \in \partial\mathbb{C}) = 0$  leaves cases  $\mathbf{f} \notin \mathbb{C}$  and  $\mathbf{f} \in \mathbb{C}^\circ$ .
2.  $\mu_n - \mathbf{f} \rightarrow 0$  in probability and  $\Lambda_n \sim \Gamma/n \rightarrow \mathbf{0}$  as  $n \rightarrow \infty$  (CLT).
3. When  $\mathbf{f} \notin \mathbb{C}$ , define  $D_{\mathbf{f}} = \min_{\mathbf{h} \in \mathbb{C}} \|\mathbf{f} - \mathbf{h}\|$ , then
 
$$p_n - \mathbb{1}\{\mathbf{f} \in \mathbb{C}\} = P(\mu_n + \Lambda_n^{1/2} Z \in \mathbb{C} | \mathcal{A}_n) \leq$$

$$P(\|\mu_n + \Lambda_n^{1/2} Z - \mathbf{f}\| \geq D_{\mathbf{f}} | \mathcal{A}_n) \leq P(\|\mu_n - \mathbf{f}\| \geq$$

$$D_{\mathbf{f}}/2 | \mathcal{A}_n) + P(\|\Lambda_n^{1/2} Z\| \geq D_{\mathbf{f}}/2 | \mathcal{A}_n) \rightarrow_p 0$$
 by Markov's Inequality. A lower bound of 0 can be given when  $\mathbf{f} \in \mathbb{C}^\circ$ .
4.  $(p_n : n \geq 0)$  is a uniformly integrable martingale, so the convergence is almost surely.

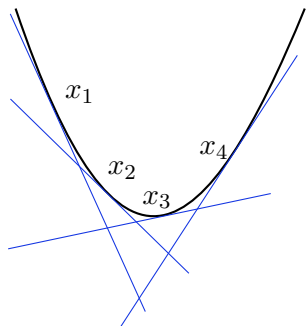
For the **unknown**  $\Gamma$  case, a similar proof can be constructed by conditioning on  $\Gamma$ .

# Main Idea



- 1 Algorithm
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# Convexity



$g \in \mathbb{C}$  if and only if each of the following linear system

$LS(i), i \in \{1, \dots, r\}$

$$\mathbf{a}_i^T \mathbf{x}_i + b_i = g(\mathbf{x}_i)$$

$$\mathbf{a}_i^T \mathbf{x}_j + b_i \leq g(\mathbf{x}_j), \forall j \in \{1, \dots, r\} \setminus \{i\}$$

is feasible in the variables  $\mathbf{a}_i \in \mathbb{R}^d$  and  $b_i \in \mathbb{R}$  (Murty [1988]).



# Vanilla Monte Carlo Method

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In each iteration of the main algorithm, after updating the hyper-parameters of the posterior distribution,

1. Simulate  $m$  i.i.d. samples  $\mathbf{y}_k^n$  from the predictive distribution  $\mathbf{f}|\mathcal{A}_n$ .

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2. For each sample  $\mathbf{y}_k^n$ , set  $\mathbf{g} = \mathbf{y}_k^n$  in LS( $i$ ),  $i = 1, \dots, r$ . Obtain an indicator  $\mathbb{1}\{\mathbf{y}_k^n \in \mathbb{C}\}$  that is 0 if any of LS( $i$ ),  $i = 1, \dots, r$  is infeasible and 1 otherwise.

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3. Output the estimator  $\hat{p}_n = \frac{1}{m} \sum_{k=1}^m \mathbb{1}\{\mathbf{y}_k^n \in \mathbb{C}\}$  as the average of all indicators.

## Challenge: Variance Reduction

Vanilla Monte Carlo estimation converges slowly with wide confidence interval width:

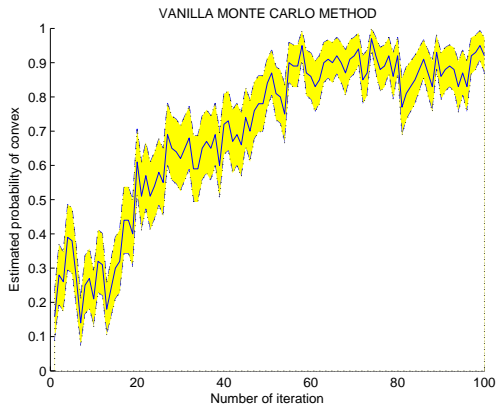
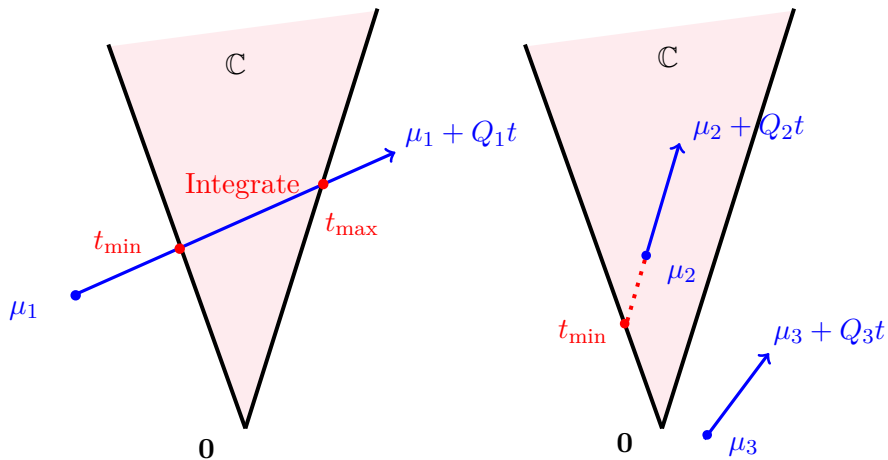


Figure: 3-d sphere function with 12 sample points.

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# Conditional Monte Carlo Method

Let  $Q = \Lambda_n^{1/2} Z$  where  $Z \sim \text{Uniform}(S^{r-1})$ . Instead of obtaining a 0 – 1 estimator...



# Conditional Monte Carlo Method

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How does this work?

$$\begin{aligned}
 & P(\mathbf{f} \in \mathbb{C} | \mathcal{A}_n) \\
 &= E_n \left( \mathbb{1} \left\{ \Lambda_n^{1/2} X + \mu_n \in \mathbb{C} \right\} \right), \text{ for } X \sim N(0, I) \text{ or } t_{\nu_n}(0, I) \\
 &= E_n \left( \mathbb{1} \left\{ T \Lambda_n^{1/2} Z + \mu_n \in \mathbb{C} \right\} \right), \text{ for } Z \text{ uniform on } S^{r-1} \\
 &= E_n \left( E \left( \mathbb{1} \left\{ T \Lambda_n^{1/2} Z + \mu_n \in \mathbb{C} \right\} \mid Z \right) \right) \\
 &= E_n \left( P(T \in [t_{\min}(Z), t_{\max}(Z)] \mid Z) \right) \\
 &= E_n \left( F_{T|Z}(t_{\max}(Z)) - F_{T|Z}(t_{\min}(Z)) \right)
 \end{aligned}$$

# Distribution of $T|Z$

## Distribution of $T|Z$

Known variance:  $F_{T|Z}(t) = \frac{1}{2} + \text{sign}(t)F_{\chi_r^2}(t^2)$ .

Unknown variance:  $F_{T|Z}(t) = \frac{1}{2} + \text{sign}(t)F_{F(r, \nu_n)}(t^2/r)$ .

*Proof sketch:*

$$\begin{aligned} F_{T|Z}(t) &= P(T \leq t|Z) \\ &= P(T \leq 0|Z) + P(0 \leq T \leq t|Z), \text{ when } t > 0 \\ &= 1/2 + 1/2P(\|X\|^2 \leq t^2|Z), \text{ for } X = TZ \end{aligned}$$

Known variance:  $X \sim N(0, I)$ , so  $\|X\|^2 \sim \chi_r^2$ .

Unknown variance:  $X \sim t_{\nu_n}(0, I) = \frac{N}{\sqrt{Y/\nu_n}}$  for  $N \sim N(0, I)$  and

$Y \sim \chi_{\nu_n}^2$ . Therefore  $\|X\|^2 = \frac{N^T N}{Y/\nu_n}$  where  $N^T N \sim \chi_r^2$ , so  $\|X\|^2/r \sim F(r, \nu_n)$ .



# Finding $t_{\min}$ and $t_{\max}$

LP for  $t_{\min}$  and  $t_{\max}$

$$\begin{aligned}
 & t_{\min} = \min t \quad (t_{\max} = \max t) \\
 \text{s.t.} \quad & \mathbf{a}_i^T \mathbf{x} + \mathbf{b}_i = \mu_i + (\Lambda^{1/2} Z)_i t, \quad \forall i \\
 & \mathbf{a}_i^T \mathbf{x}_j + \mathbf{b}_i \leq \mu_j + (\Lambda^{1/2} Z)_j t, \quad \forall i, \forall j \neq i \\
 & \mathbf{a}_i \in \mathbb{R}^r, \mathbf{b}_i \in \mathbb{R}, t \in \mathbb{R}, \quad \forall i
 \end{aligned}$$

Similarly, this can be decomposed into  $r$  subproblems:

$$\begin{aligned}
 & t_{\min}^i = \min t^i && \text{and} \\
 & (t_{\max}^i = \max t^i) && t_{\min} = \max_{i=1,2,\dots,r} t_{\min}^i, \\
 \text{s.t.} \quad & \mathbf{a}_i^T \mathbf{x}_i + b_i = \mu_i + (\Lambda^{1/2} Z)_i t^i && t_{\max} = \min_{i=1,2,\dots,r} t_{\max}^i. \\
 & \mathbf{a}_i^T \mathbf{x}_j + b_i \leq \mu_j + (\Lambda^{1/2} Z)_j t^i, \\
 & \forall j \neq i,
 \end{aligned}$$

# Conditional Monte Carlo Method

---

At each iteration  $n$ , to estimate

$$p_n = E_n(F_{T|Z}(t_{\max}(Z)) - F_{T|Z}(t_{\min}(Z))),$$

1. Simulate  $m$  i.i.d. samples  $z_k$  uniformly on the unit shell  $S^{r-1}$ .

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4. Output the estimator  $\hat{p}_n$  as a sample average of such integrations obtained from  $m$  samples.

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This method achieves **variance reduction** compared to the vanilla Monte Carlo estimator.

# Reduced Variance and New Challenge

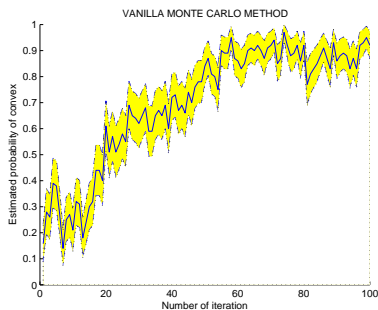


Figure: Vanilla Monte Carlo method.

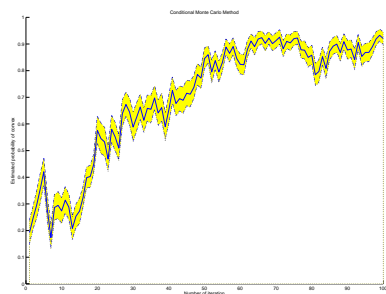
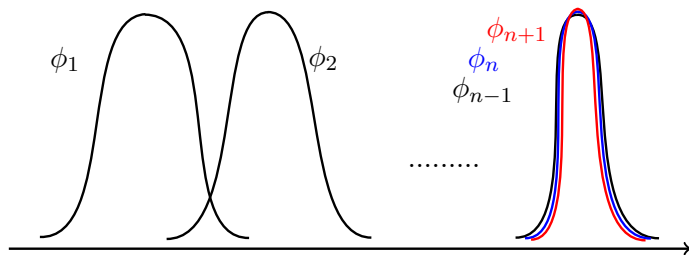


Figure: Conditional Monte Carlo method.

... but doubled the **computational time** to check the convexity for each sample!

# Can we reuse samples?



Maybe yes: as  $n$  grows large, we might expect  $\frac{\phi_{n+1}}{\phi_n}$  to become close to 1, where  $\phi_n$  is the density of  $\mathbf{f}|\mathcal{A}_n$ . Thus  $p_{n+1}$  may be estimated by  $\mathbf{y}_k^n, k = 1, \dots, m$ , for which  $\mathbb{1}\{\mathbf{y}_k^n \in \mathbb{C}\}$  has been calculated in iteration  $n$ .



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# LR Based Methods

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At iteration  $n$ , calculate  $\hat{p}_n$  using the vanilla Monte Carlo method with samples  $\mathbf{y}_k^n, k = 1, \dots, m$ . In iteration  $n + \ell$ ,

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**Change of Measure:** Reuse **all** the samples  $\mathbf{y}_k^n$  in the  $n$ -th iteration. Output  $p_{n+\ell}^{\hat{}} = \frac{1}{m} \sum_{k=1}^m \mathbb{1} \{ \mathbf{y}_k^n \in \mathbb{C} \} \frac{\phi_{n+\ell}(\mathbf{y}_k^n)}{\phi_n(\mathbf{y}_k^n)}$ .

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**Generalized Acceptance/Rejection:** Reuse **part of** the samples by accepting  $\mathbf{y}_k^n$  with probability  $\frac{\phi_{n+\ell}(\mathbf{y}_k^n)}{c\phi_n(\mathbf{y}_k^n)}$ , then generate new samples as needed:

$$p_{n+\ell}^{\hat{}} = \frac{1}{m} \left( \sum_{k \in S} \mathbb{1} \{ \mathbf{y}_k^n \in \mathbb{C} \} + \sum_{k=1}^{m-|S|} \mathbb{1} \{ \mathbf{y}_k^{n+\ell} \in \mathbb{C} \} \right)$$

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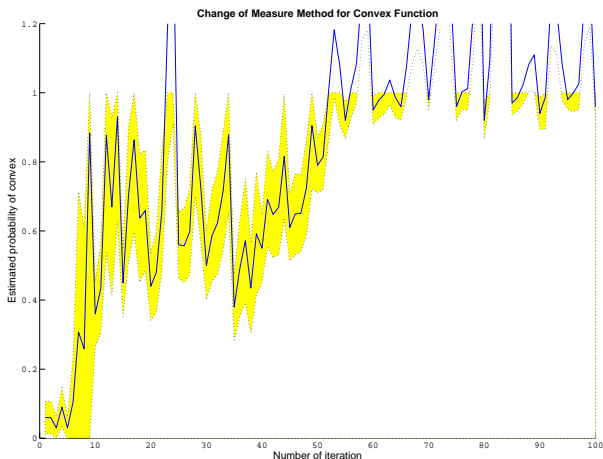
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By utilizing the samples and results in an earlier iteration, these two methods saves **computational time**.

# Theory vs. Reality



**Figure:** The probability of convex is estimated to be over 1.

# Theory vs. Reality

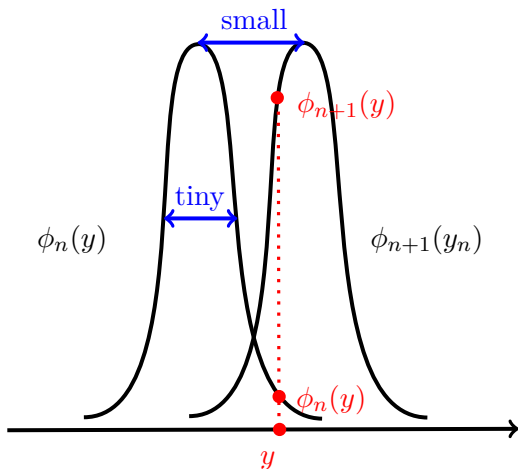


Figure: When  $\frac{\phi_{n+1}(y)}{\phi_n(y)}$  is huge.

# How likely does this happen?

It can be shown that  $\hat{p}_{n+l}$  is **unbiased** and has **finite variance** [Jian et al., 2014]. However, when  $n$  becomes large,  $\max_{y^n} \frac{\phi_{n+1}(y^n)}{\phi_n(y^n)} = c$  has **infinite expectation**.

*Proof sketch:* For example, assume  $r = 1$ , and  $\Gamma = \lambda^{-2}$  is known, so the  $n$ -iteration posterior precision is  $\sigma_n^{-2} = \sigma_0^{-2} + n\lambda^2$ . Let  $y \sim N(0, \lambda^{-2})$ , and  $y^n \sim N(\mu_n, \sigma_n^2)$ .

$$\max_{y^n} 2 \ln \frac{\phi_{n+1}(y^n)}{\phi_n(y^n)} = (\mu_n - \mu_{n+1})^2 (\sigma_{n+1}^{-2} + \frac{1}{\lambda^2} (\sigma_{n+1}^{-4})) + \ln \frac{\sigma_n}{\sigma_{n+1}},$$

$$(\mu_n - \mu_{n+1})^2 = ((1 - \frac{\sigma_{n+1}^2}{\sigma_n^2}) \mu_n - \sigma_{n+1}^2 \lambda^2 y)^2 \rightarrow (\sigma_{n+1}^2 \lambda^2 y)^2 \text{ and}$$

$$\sigma_n / \sigma_{n+1} \rightarrow 1. \text{ So } \max_{y^n} 2 \ln \frac{\phi_{n+1}(y^n)}{\phi_n(y^n)} \rightarrow \lambda^2 y^2 \sim \chi_1^2.$$

Thus  $c \geq \exp \frac{\lambda^2 y^2}{2} \sim \exp \frac{\chi_1^2}{2}$  with expectation  $\infty$ .



# The Combination of Methods

---

Combining the Conditional Monte Carlo method with the Change of Measure method, we get an hybrid algorithm:

1. At every iteration  $n$ , simulate  $m$  i.i.d. samples  $z_k$  uniformly on the unit shell  $S^{r-1}$ . Solve for  $t_{\min}(z_k)$  and  $t_{\max}(z_k)$  and output the Conditional Monte Carlo estimator  $\hat{p}_n$ .

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1. At every iteration  $n$ , simulate  $m$  i.i.d. samples  $z_k$  uniformly on the unit shell  $S^{r-1}$ . Solve for  $t_{\min}(z_k)$  and  $t_{\max}(z_k)$  and output the Conditional Monte Carlo estimator  $\hat{p}_n$ .
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3. In the next  $\ell$  iterations, output

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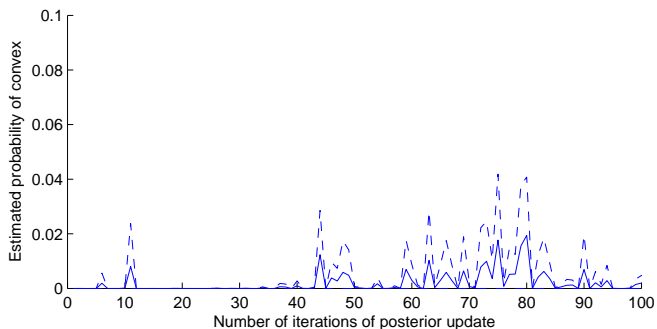
$$\hat{p}_{n+\ell} = \frac{1}{m} \sum_{k=1}^m \mathbb{1}\{\mathbf{y}_k^n \in \mathbb{C}\} \frac{\phi_{n+\ell}(\mathbf{y}_k^n)}{\phi_n(\mathbf{y}_k^n)}.$$

(Careful!  $\frac{\phi_{n+\ell}(\mathbf{y}_k^n)}{\phi_n(\mathbf{y}_k^n)} \gg 1$  may happen.)

- 1 Algorithm
- 2 Monte Carlo
- 3 Conditional MC
- 4 LR Based Methods
- 5 Implementations**
- 6 Conclusion

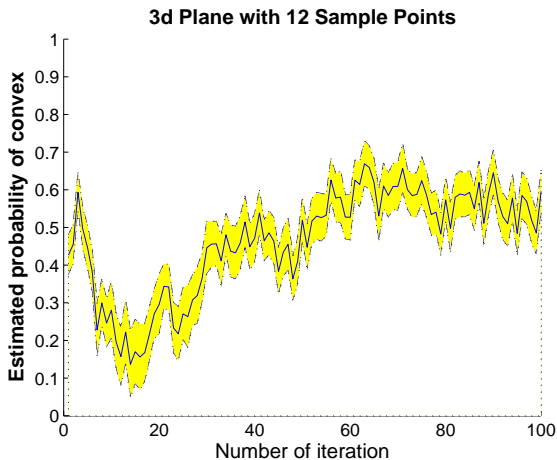
# Inverted Bowl

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**Figure:**  $\hat{p}_n$  for  $g = -\|\mathbf{x}\|^2$ ,  $\mathbf{x} \in [-1, 1]^{30}$ ,  $r = 61$ ,  $\Gamma$  has  $10^4$  on the diagonal.

# Plane



**Figure:**  $\hat{p}_n$  for  $g = 0$ ,  $\mathbf{x} \in [-1, 1]^2$ ,  $r = 6$ ,  $\Gamma$  has  $1e - 18$  on the diagonal.

# Ambulances in a Square

A "real" example from SimOpt.org: What does the long run average response time behave like as a function of the ambulance base location?

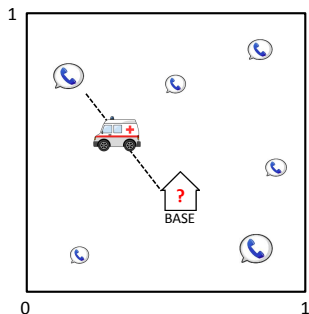
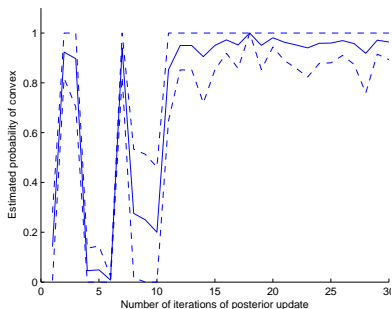


Figure: Problem illustration.

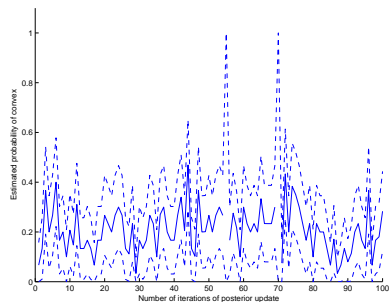




# One Base, Two Bases



**Figure:**  $\hat{p}_n$  for one ambulance base ( $d = 2$ ).



**Figure:**  $\hat{p}_n$  for two ambulance bases ( $d = 4$ ).

- 1 Algorithm
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# Conclusion

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In this talk:

- a sequential Bayesian method for estimating the probability of convex utilizing Monte Carlo simulation
- a Conditional Monte Carlo variance reduction method
- two likelihood-ratio-based variance reduction methods with limitation

# Conclusion

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In this talk:

- a sequential Bayesian method for estimating the probability of convex utilizing Monte Carlo simulation
- a Conditional Monte Carlo variance reduction method
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On-going research:

- The asymptotic behavior of the probability that a function is convex using a kriging model as the number of samples goes to infinity.

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Jianqiang C. Wang and Mary C. Meyer. Testing the monotonicity or convexity of a function using regression splines. *Canadian Journal of Statistics*, 39(1):89–107, 2011. ISSN 1708-945X. doi: 10.1002/cjs.10094. URL <http://dx.doi.org/10.1002/cjs.10094>.

# Constant for the Generalized A/R

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How to find  $c$  in the generalized acceptance/rejection method,  
so that  $c \geq \frac{\phi_{n+\ell}(\mathbf{y})}{\phi_n(\mathbf{y})}$  for all  $\mathbf{y}$ ?

**Known variance:**  $c \geq$

$$\left\{ \frac{|\Lambda_{n+\ell}|}{|\Lambda_n|} \exp \frac{1}{\ell} (\Lambda_{n+\ell}^{-1} \mu_{n+\ell} - \Lambda_n^{-1} \mu_n)^T \Gamma (\Lambda_{n+\ell}^{-1} \mu_{n+\ell} - \Lambda_n^{-1} \mu_n) + \mu_n^T \Lambda_n^{-1} \mu_n - \mu_{n+\ell}^T \Lambda_{n+\ell}^{-1} \mu_{n+\ell} \right\}^{1/2}.$$

**Unknown variance:** Intractable and needs numerical estimation.



# The Dual

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$$Q = \Lambda^{1/2} Z.$$

**Primal:**  $t_{\min} = \min t$

$$\text{s.t. } \mathbf{a}_i^T \mathbf{x} + \mathbf{b}_i = \mu_i + Q_i t, \quad \forall i$$

$$\mathbf{a}_i^T \mathbf{x}_j + \mathbf{b}_i \leq \mu_j + Q_j t,$$

$$\forall i, \forall j \neq i$$

$$\mathbf{a}_i \in \mathbb{R}^r, \mathbf{b}_i \in \mathbb{R}, t \in \mathbb{R}, \quad \forall i$$

**Dual:**  $t_{\min} = -\min \sum_i \sum_j v_{ij} \mu_j$

$$\text{s.t. } \sum_i \sum_j v_{ij} Q_j = \mathbf{1}, \quad (1)$$

$$\sum_j \mathbf{x}_j v_{ij} = \mathbf{0}^d, \quad \forall i, \quad (2)$$

$$\sum_j v_{ij} = \mathbf{0}^r, \quad \forall i, \quad (3)$$

$$v_{ij} \geq 0, \quad \forall i, \forall j \neq i, \quad (4)$$

## Meaning

min distance from  $\mu$  to  $\mathbb{C}$

$(vQ)_i \neq 0$  for the nearest face of  $\mathbb{C}$

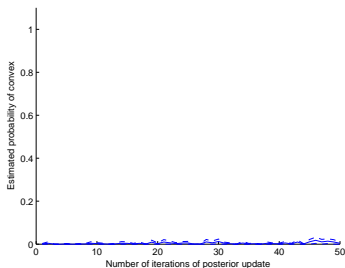
$$\sum_j \mathbf{x}_j \frac{v_{ij}}{-v_{ii}} = \mathbf{0}^d, \quad \forall i$$

$$\frac{v_{ij}}{-v_{ii}} \geq 0, \quad \sum_j \frac{v_{ij}}{-v_{ii}} = 1$$

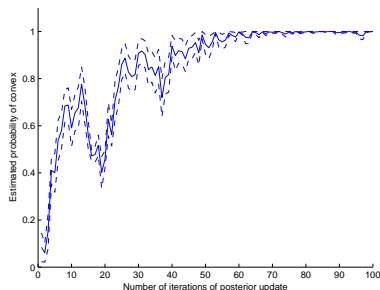
$v_{i \cdot}$  characterizes faces of  $\mathbb{C}$

## Where to sample?

An interesting example for  $g = \|\mathbf{x}\|^2$ ,  $\mathbf{x} \in [-1, 1]^{30}$ ,  $r = 60$ , and  $\Gamma$  has  $10^4$  on the diagonal.



**Figure:** Sampling the 60 points uniformly at random in space.

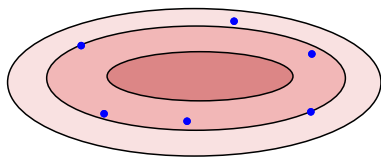


**Figure:** Sampling along 20 random lines with 3 points on each.

# Where to sample?

Consider a 2-dimensional concave function with the following level sets (higher values in darker shades):

Convex?



Not convex!

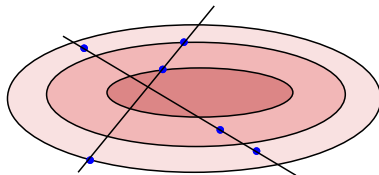


Figure: Sampling uniformly vs. Sampling along random lines.