Meeting Update

Gaussian Process Covariance Function Selection Using Minimum Energy Designs, For Real This Time

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Outline

Last Time

Sequentially Chosen Candidates in One-at-a-Time Algorithm

- Expected posterior probabilities of hypotheses
- Another metric, using distances in both x and y

Timing Things

Comments

Last Time

Last Time

What happened last time

1. Started Gaussian Process Model Selection
2. Saw results for large K

Things to do:

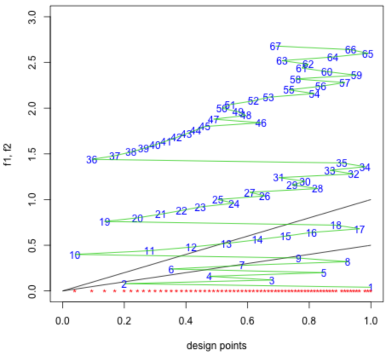
1. Some statistics/numbers for evaluating the criterion, for the purpose of doing comparisons with other designs. Basically a way to show that the design is better!
2. Time things!
3. Clean up code, address pull request comments.

Sequentially Chosen Candidates in One-at-a-Time Algorithm

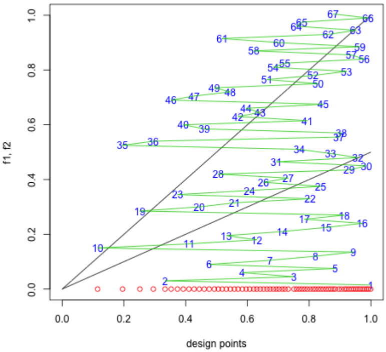
Uniformly vs. Sequentially Chosen Candidates for One-at-a-Time Algorithm

Here, *numCandidates* = 1500 in One-at-a-Time Algorithm, with candidates picked uniformly.
(Even when sorting uniformly-selected candidates)

Fast Algorithm K=100



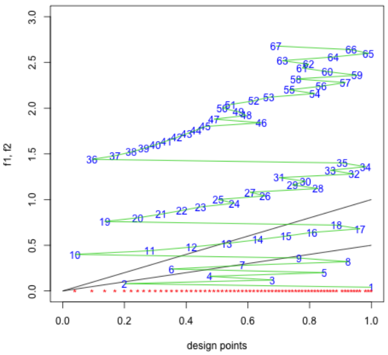
One-at-a-Time Uniform



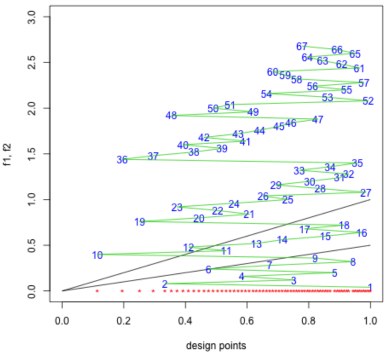
Uniformly vs. Sequentially Chosen Candidates for One-at-a-Time Algorithm

When we choose candidates along a sequence instead of uniformly, the two designs are closer. (Why? Rui Tui's seminar talk, when he mentioned difference in sphere packing)

Fast Algorithm K=100



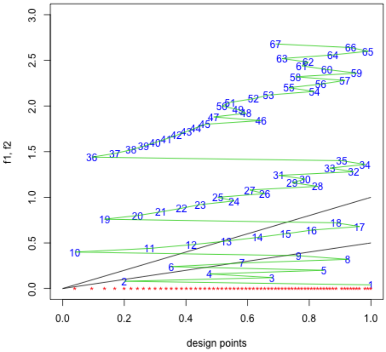
One-at-a-Time Sequential



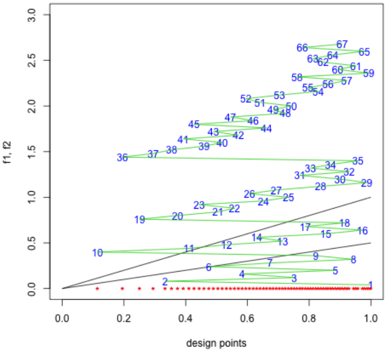
Uniformly vs. Sequentially Chosen Candidates for One-at-a-Time Algorithm

Here, *numCandidates* $= 10^5$ in One-at-a-Time Algorithm. They're even closer!

Fast Algorithm K=100



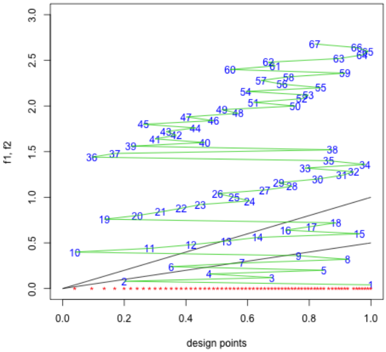
One-at-a-Time Sequential



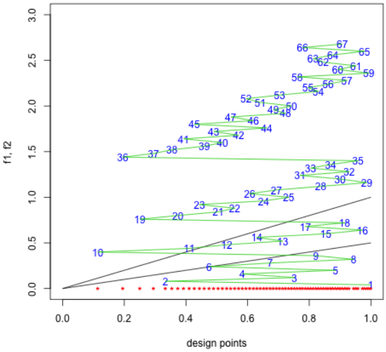
Uniformly vs. Sequentially Chosen Candidates for One-at-a-Time Algorithm

Compare Fast with $K = 20$ and One-at-a-Time with $numCandidates = 10^5$ in One-at-a-Time Algorithm.

Fast Algorithm K=100



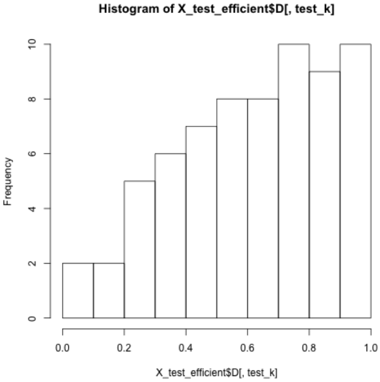
One-at-a-Time Sequential



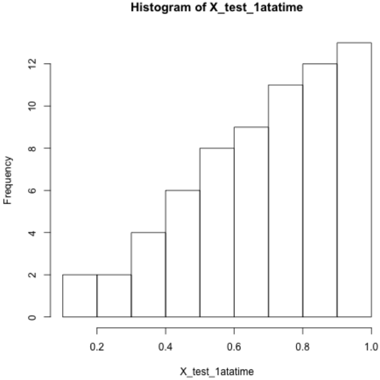
Histograms for Designs

Comparing designs in Fast ($K = 100$) and One-at-a-Time with candidates along sequence ($numCandidates = 10^5$)

Fast



One-at-a-Time Seq



Summary Stats on Designs

Comparing designs in Fast ($K = 100$) and One-at-a-Time with candidates along sequence ($numCandidates = 10^5$)

Fast

1. mean, sd of design points = 0.6129598, 0.2540533
2. sum, mean, sd of differences between consecutive sorted points = 0.9599863, 0.01454525, 0.00766221
3. sum, mean, sd of differences between f_0 and f_1 = 20.53415, 0.3064799, 0.1270267

One-at-a-Time

1. mean, sd of design points = 0.6882634, 0.2182556
2. sum, mean, sd of differences between consecutive sorted points = 0.8859489, 0.01342347, 0.01187598
3. sum, mean, sd of differences between f_0 and f_1 = 23.05683, 0.3441317, 0.1091278

Thoughts

Comparing designs in Fast ($K = 100$) and One-at-a-Time with candidates along sequence ($numCandidates = 10^5$), it seems....

1. The fast algorithm is more space-filling
2. Its mean is smaller... not sure what this implies. Not as focused on distinguishing the models? More for prediction/parameter estimation?
3. ...

Sequentially Chosen Candidates in One-at-a-Time Algorithm

Expected posterior probabilities of hypotheses

Expected Posterior Probability of Model

- Posterior probability of a model given by $H_\ell, \ell = 1, ..., M$ to see which model is more likely to be the correct one.
- Posterior Probability is

$$P(H_\ell|Y) = \frac{\pi_\ell P(Y|H_\ell)}{\sum_{m=1}^{M} \pi_m P(Y|H_m)} \tag{1}$$

  where π_m is the prior on the model given by H_m, and $P(Y|H_m)$ is the model evidence.
- Consider the linear model,

$$\begin{aligned} y &= f(\mathbf{x}) + \epsilon \\ f(x) &= \mathbf{x}\beta \end{aligned}$$

  where $\epsilon \sim N(0, \sigma_\epsilon^2)$ and $\beta \sim N(\tilde{\beta}, \sigma_\beta^2)$.
- For model H_ℓ with $\epsilon_\ell \sim N(0, \sigma_{\epsilon_\ell}^2)$ and $\beta_\ell \sim N(\tilde{\beta}_\ell, \sigma_{\beta_\ell}^2)$, we have $y|H_\ell \sim N(\tilde{\beta}_\ell \mathbf{x}, \sigma_{\epsilon_\ell}^2 + \mathbf{x}^2 \sigma_{\beta_\ell}^2)$ where the mean and variance are computed by iterated expectation and variance.
- Since we don't have Y to calculate the model evidence, instead calculate the expected model evidence $E_Y[P(Y|H_m)]$

Estimate Expected Posterior Probability of Model

1. Obtain design $\mathbf{D} = \{x_1, ..., x_N\}$ from the Fast Algorithm for Linear Model Selection.
2. Draw $y_i^{(j)} \sim N(\tilde{\beta}_\ell \mathbf{x}, \sigma^2_{\epsilon_\ell} + \mathbf{x}^2 \sigma^2_{\beta_\ell}), \forall \mathbf{x}_i \in \mathbf{D}, j = 1, ..., J$ to obtain J simulations of $Y = \{y_1, ..., y_N\}$ for model H_ℓ, which gives the linear model:

$$
\begin{aligned}
y &= f(\mathbf{x}) + \epsilon \\
f(x) &= \mathbf{x}\beta_\ell
\end{aligned}
$$

   where $\epsilon \sim N(0, \sigma^2_{\epsilon_\ell})$ and $\beta_\ell \sim N(\tilde{\beta}_\ell, \sigma^2_{\beta_\ell})$.
3. Estimate $E_y[P(Y|H_m)] \approx \frac{1}{J} \sum_{j=1}^{J} P(Y|H_m), \forall m \in \{1, ..., M\}$, where $P(Y|H_m)$ is the pdf of the distribution $N(\tilde{\beta_m}\mathbf{x}, \sigma^2_{\epsilon_m} + \mathbf{x}^2 \sigma^2_{\beta_m})$.
4. Then estimate $E_Y[P(H_\ell|Y)]$ by

$$
E_Y[P(H_\ell|Y)] = \frac{\pi_\ell E_Y[P(Y|H_\ell)]}{\sum_{m=1}^{M} \pi_m E_Y[P(Y|H_m)]} \tag{2}
$$

Questions about Step 3

- How to get a single number out of this computation?
- Where to put the design points $\mathbf{D} = \{x_1, ..., x_N\}$?
- What do we do we do with $y_i^{(j)}$ from simulations?
- Is there some kind of likelihood for linear regression? Some sources talk about Laplace approximation to marginal Y... did I compute that wrong? I averaged over β, am I supposed to somehow average over $\mathbf{D}$ as well?
- Need to get rid of $\mathbf{x}$'s somehow...

What I Ended Up Doing

1. Obtain design $\mathbf{D}$ from the Fast Algorithm for Linear Model Selection.
2. Draw $y_i^{(j)} \sim N(\tilde{\beta}_\ell \mathbf{x}, \sigma^2_{\epsilon_\ell} + \mathbf{x}^2 \sigma^2_{\beta_\ell}), \forall \mathbf{x}_i \in \mathbf{D}, j = 1, ..., J$ for model H_ℓ. For now, $M = 2$.
3. Estimate $E_y[P(Y|H_m)] \approx \frac{1}{JN} \sum_{j=1}^{J} \sum_{i=1}^{N} P(y_i|H_m, \mathbf{x}_i)$, $\forall m \in \{1, ..., M\}$, where $P(y_i|H_m, \mathbf{x}_i)$ is the pdf of $N(\tilde{\beta}_m \mathbf{x}, \sigma^2_{\epsilon_m} + \mathbf{x}^2 \sigma^2_{\beta_m})$.
4. Assume $\pi_m = \frac{1}{M}, \forall m = 1, ..., M$ and estimate $E_Y[P(H_\ell|Y)]$ by

$$E_Y[P(H_\ell|Y)] \approx \frac{E_Y[P(Y|H_\ell)]}{\sum_{m=1}^{M} \pi_m E_Y[P(Y|H_m)]} \tag{3}$$

5. Since $M = 2$, can also compute the Bayes Factor,

$$BF_{01} \approx \frac{E_Y[P(Y|H_0)]}{E_Y[P(Y|H_1)]} \tag{4}$$

New Results

For both H_0, H_1, $\sigma_\epsilon = 0.01, \sigma_\beta = 0.001, N = 51$.
$\tilde{\beta}_0 = 1, \tilde{\beta}_0 = 1/2$.

For generating Y under the null model given by H_0,

- $E_Y[P(H_0|Y)] \approx 0.8196135$
- $E_Y[P(H_1|Y)] \approx 0.1803865$
- $BF_{01} \approx 4.543653$: supports H_0

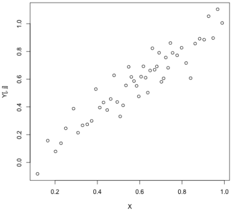
For generating Y under the alternative model given by H_1,

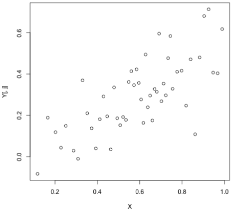
- $E_Y[P(H_0|Y)] \approx 0.1818883$
- $E_Y[P(H_1|Y)] \approx 0.8181117$
- $BF_{01} \approx 0.222327$: supports H_1

Results, continued...

For both H_0, H_1, $\sigma_\epsilon = 0.01, \sigma_\beta = 0.001, N = 51$.
$\tilde{\beta}_0 = 1, \tilde{\beta}_0 = 1/2$.

Example Simulation from H_0 Model,





Interpreting Bayes Factors (Kass & Raftery 1995):

BF_{01}	Evidence for H_0
< 1	Supports H_1
1 to 3	not worth mentioning
3 to 20	positive
20 to 150	Strong
> 150	v strong

Sequentially Chosen Candidates in One-at-a-Time Algorithm

Another metric, using distances in both x and y

Summary Stats on Designs

How do we use these to evaluate the design?

Fast

1. mean, sd of design points = 0.6129598, 0.2540533
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Timing Things

Times

1. Fast Algorithm with $K = 20$: 2.77915 minutes
2. Fast Algorithm with $K = 100$: 58.4566 minutes
3. One-at-a-Time Sequential with $numCandidates = 10^5$: 17.37015 minutes
4. The "Fast" Algorithm is probably slower since K is so large... but it has to be.

Comments

Some Things.

1. Candidate set: $N/2$ from space filling design in L_{jk}, and other $N/2$ some linear combination of nearby points (Nesterov?) - get a total of N additional candidates in each new design $k = 1, \ldots, K$
2. So I suppose that would be the next step? Will hopefully see faster convergence.
3. Maybe choose a different power than $2p = 2$ for $d(.,.)$ to see if it makes the designs even more similar?
4. $gamma_{k+1} = \frac{k}{K-1}$ since we're indexing from $k = 1, \ldots, K-1$ to create the next design $k = 2, \ldots, K$, resp.
5. Still thinking about asymptotic properties / limiting distribution (if it exists) for the fact that we're using Wasserstein distance instead of a density now.