Toward Transparent and Parsimonious Methods for Automatic Performance Tuning

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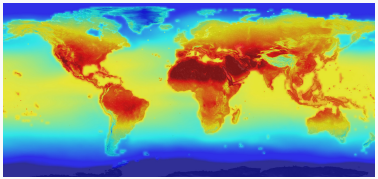
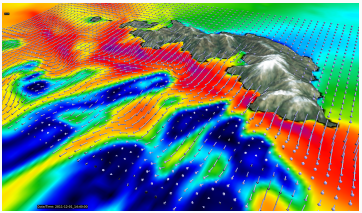
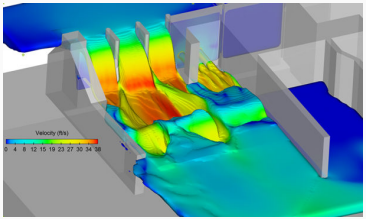
High Performance Computing is Needed at Multiple Scales, . . .

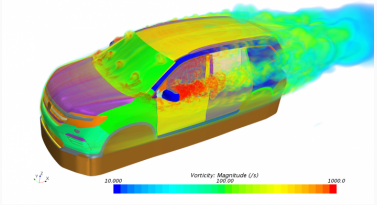
Climate simulation for policies to fight climate change



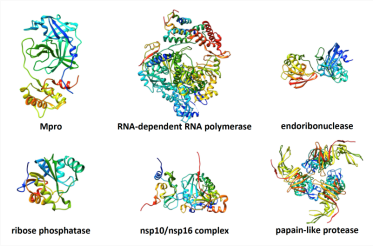


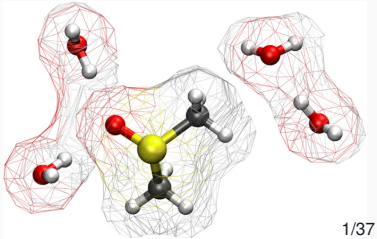
Fluid dynamics for stronger infrastructure and fuel efficiency



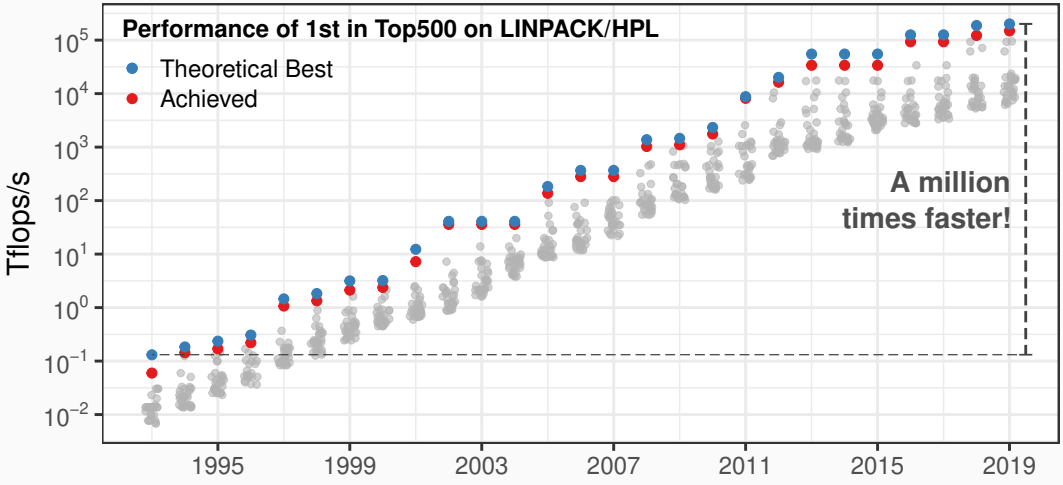


Molecular dynamics for virtual testing of drugs and vaccines

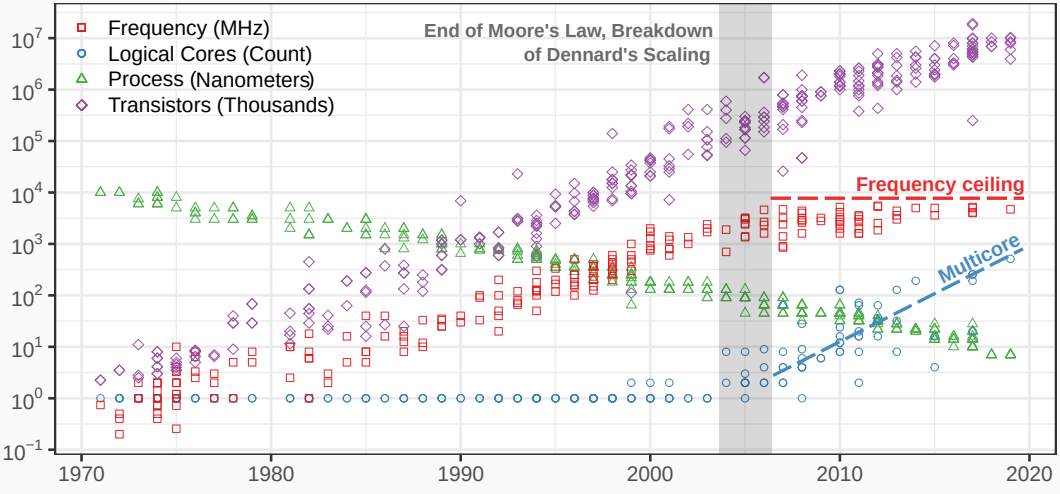




. . . and the Performance of Supercomputers has so far Improved Exponentially



Software must Improve to Leverage Complexity, and Autotuning can Help



An Autotuning Example: Loop *Blocking* and *Unrolling* for Matrix Multiplication

Optimizing Matrix Multiplication

How to restructure memory accesses in loops to increase throughput by leveraging cache locality?

```
int N = 256;

float A[N][N], B[N][N], C[N][N];
int i, j, k;
// Initialize A, B, C
for(i = 0; i < N; i++){ // Load A[i][]
  for(j = 0; j < N; j++){
    // Load C[i][j], B[][j] to fast memory
    for(k = 0; k < N; k++){




      C[i][j] += A[i][k] * B[k][j];
    }


    // Write C[i][j] to main memory
  }
}
```

An Autotuning Example: Loop *Blocking* and *Unrolling* for Matrix Multiplication

Optimizing Matrix Multiplication

How to restructure memory accesses in loops to increase throughput by leveraging cache locality?

```
int N = 256;
int B_size = 4;
float A[N][N], B[N][N], C[N][N];
int i, j, k, x, y;
// Initialize A, B, C
for(i = 0; i < N; i += B_size){
  for(j = 0; j < N; j += B_size){
    // Load block (i, j) of C to fast memory
    for(k = 0; k < N; k++){
      // Load block (i, k) of A to fast memory
      // Load block (k, y) of B to fast memory
      for(x = i; x < min(i + B_size, N); x++){
        for(y = j; y < min(j + B_size, N); y++){
          C[x][y] += A[x][k] * B[k][y];
        }
      }
    }
    // Write block (i, j) of C to main memory
  }
} // One parameter: B_size
```

An Autotuning Example: Loop *Blocking* and *Unrolling* for Matrix Multiplication

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How to restructure memory accesses in loops to increase throughput by leveraging cache locality?

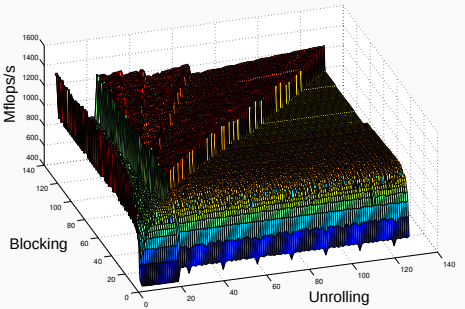
```
int N = 256;
int B_size = 4;
float A[N][N], B[N][N], C[N][N];
int i, j, k, x; // int U_size = 4;
// Initialize A, B, C
for(i = 0; i < N; i += B_size){
  for(j = 0; j < N; j += B_size){
    // Load block (i, j) of C to fast memory
    for(k = 0; k < N; k++){
      // Load block (i, k) of A to fast memory
      // Load block (k, y) of B to fast memory
      for(x = i; x < min(i + B_size, N); x++){
        C[i][j + 0] += A[i][k] * B[k][j + 0];
        C[i][j + 1] += A[i][k] * B[k][j + 1];
        C[i][j + 2] += A[i][k] * B[k][j + 2];
        C[i][j + 3] += A[i][k] * B[k][j + 3];
      }
    } // Write block (i, j) of C to main memory
  }
} // Two parameters: B_size and U_size
```

An Autotuning Example: Loop *Blocking* and *Unrolling* for Matrix Multiplication

Optimizing Matrix Multiplication

How to restructure memory accesses in loops to increase throughput by leveraging cache locality?

Resulting Search Space

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for(i = 0; i < N; i += B_size){
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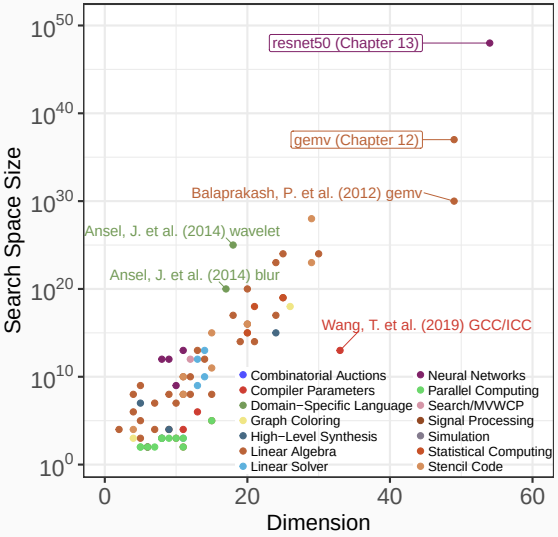
```

Autotuning Problems in Other Domains: Dimension Becomes an Issue



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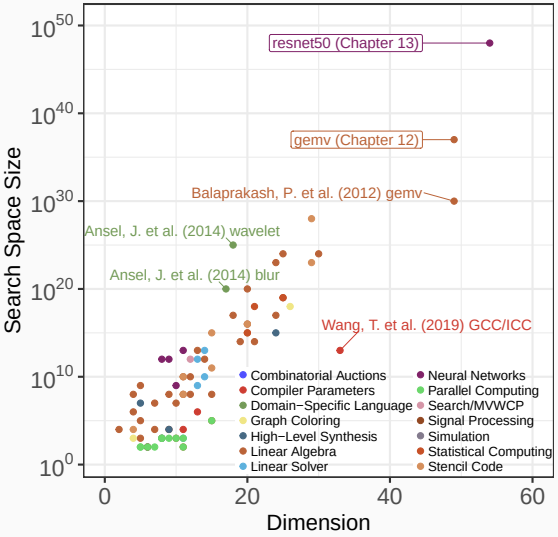
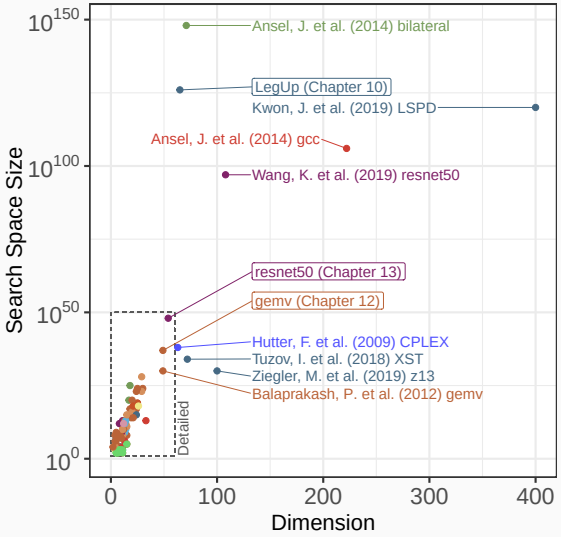




Autotuning as an *Optimization* or *Learning* Problem

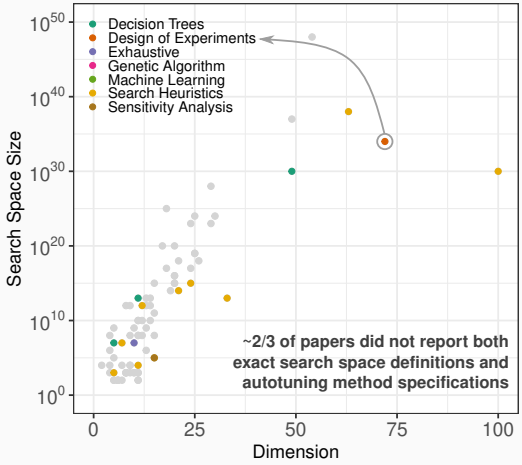
Performance as a Function

Performance: $f : \mathcal{X} \to \mathbb{R}$

- Parameters: $\mathbf{x} = [x_1 \ \ldots \ x_n]^\mathsf{T} \in \mathcal{X}$
- Performance metric: $y = f(\mathbf{x})$

To minimize f, we can adapt proven methods from other domains:

- **Function minimization**, **Learning**: not necessarily parsimonious and transparent
- **Design of Experiments**: can help, but not widely used for autotuning



Toward Transparent and Parsimonious Autotuning

Contributions of this Thesis

- Developing transparent and parsimonious autotuning methods based on the Design of Experiments
- Evaluating different autotuning methods in different HPC domains

Transparent

- Use statistics to justify code optimization choices
- Learn about the search space

Parsimonious

- Carefully choose which experiments to run
- Minimize f using as few measurements as possible

Domain	Method
CUDA compiler parameters	**F**, **D**
FPGA compiler parameters	**F**
OpenCL Laplacian Kernel	**F**, **L**, **D**
SPAPT Kernels	**L**, **D**
CNN Quantization	**L**, **D**

F: Function Minimization, **L**: Learning, **D**: Design of Experiments

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F: Function Minimization, L: Learning,
D: Design of Experiments
: In this presentation

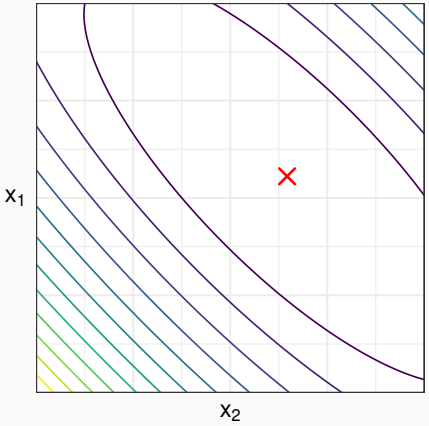
Autotuning with Methods for Function Minimization

Minimizing Functions using Derivatives and Heuristics

We know or can compute information about f

- Directly measure new $\mathbf{x}_1, \ldots, \mathbf{x}_k, \ldots, \mathbf{x}_n$
- Search for the global optimum

$$f(\mathbf{x}) = (x_1 + 2x_2 - 7)^2 + (2x_1 + x_2 - 5)^2 \quad ,$$
$$x_1, x_2 \in [-10, 10]$$



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$$f(\mathbf{x}) = (x_1 + 2x_2 - 7)^2 + (2x_1 + x_2 - 5)^2 + \varepsilon,$$

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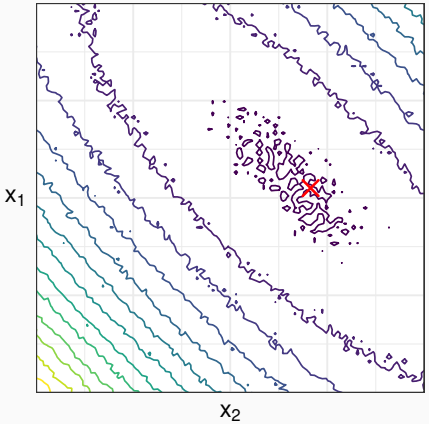

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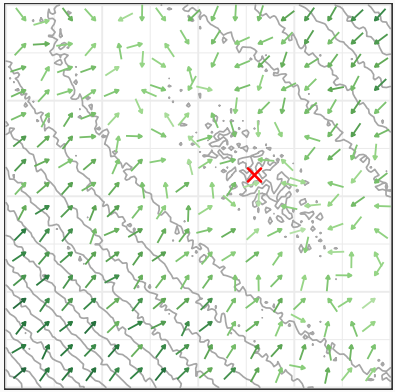

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- $\mathbf{x}_k = \mathbf{x}_{k-1} - \mathbf{H}f(\mathbf{x}_{k-1})\nabla f(\mathbf{x}_{k-1})$
- Move to best point in a neighborhood

$$f(\mathbf{x}) = (x_1 + 2x_2 - 7)^2 + (2x_1 + x_2 - 5)^2 + \varepsilon,$$

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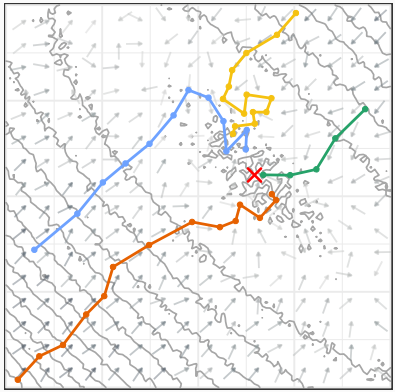

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Hard to State Hypotheses: Search Heuristics

- Random Walk, Simulated Annealing, Genetic Algorithms, and many others

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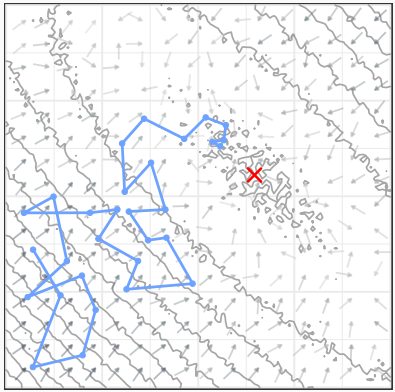

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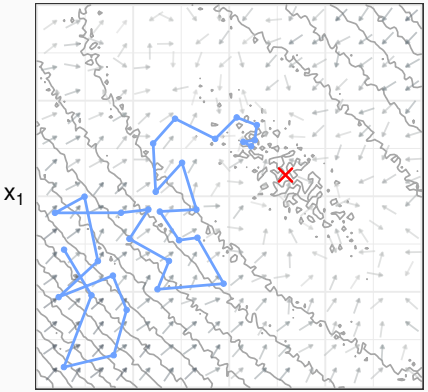
How to choose a method?

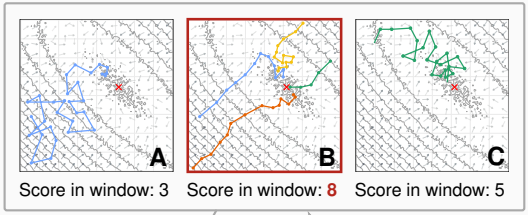
$$f(\mathbf{x}) = (x_1 + 2x_2 - 7)^2 + (2x_1 + x_2 - 5)^2 + \varepsilon,$$

$x_1, x_2 \in [-10, 10]$, and $\varepsilon \sim \mathcal{N}(0, \sigma^2)$



Choosing Methods from an Ensemble

Example of an Ensemble of Methods



Methods in this Ensemble

- **A**, **C**: Simulated Annealing with different temperature, **B**: Gradient Descent

Minimization of f using OpenTuner

- Coordinated by a Multi-Armed Bandit (MAB) algorithm
- Methods perform measurements proportionally to their score
- Score: the number of times a method found the best $\mathbf{x}$ in a time window
- The best $\mathbf{x}$ over all methods is reported

Application: High-Level Synthesis for FPGAs

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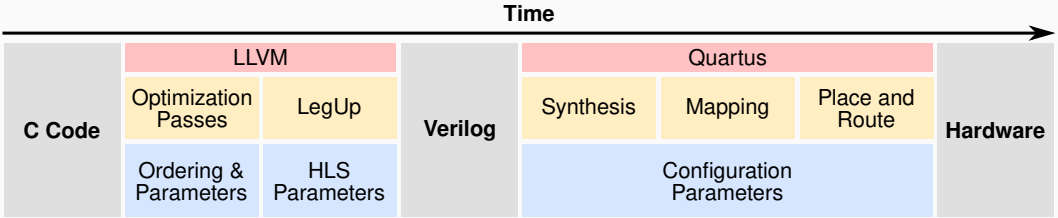
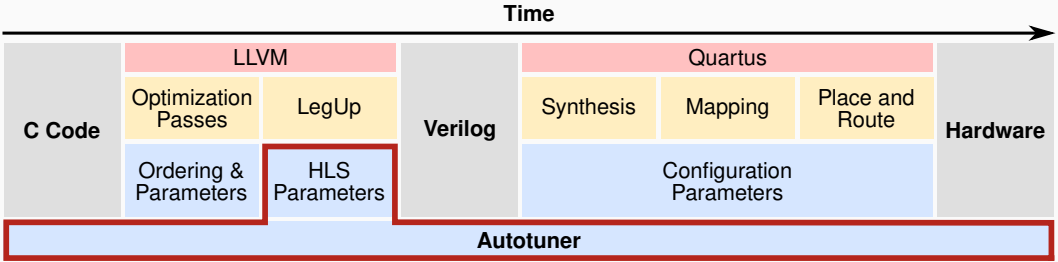


Application: High-Level Synthesis for FPGAs



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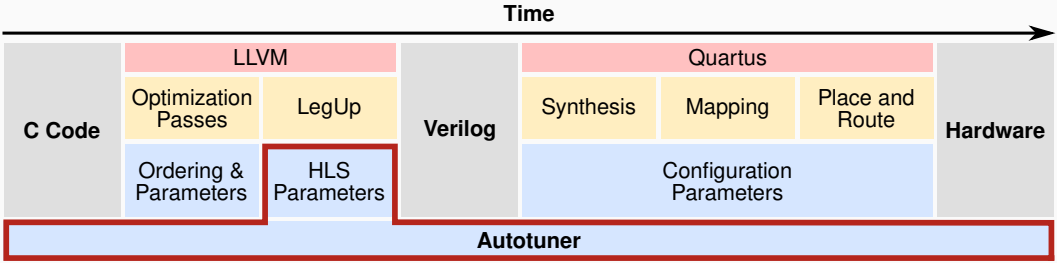
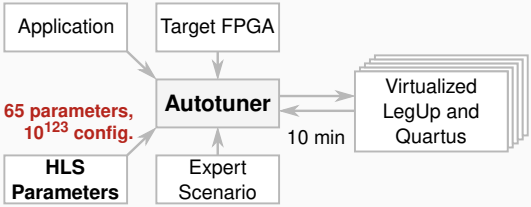
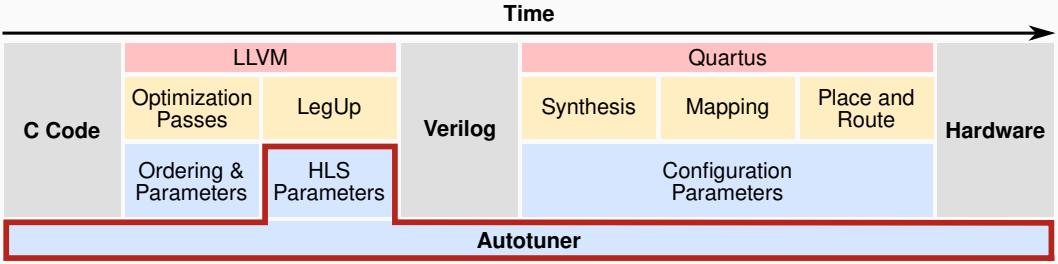


Search Space



Application: High-Level Synthesis for FPGAs



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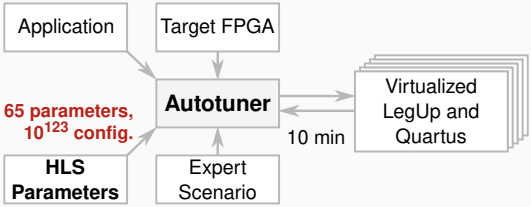


Performance Metrics

- Weighted average of 8 hardware metrics
- Metrics for the usage of registers, memory, DSP units, frequency and clock speed
- An expert devised weights for optimizing for area, latency, performance, or for multiple criteria

Results

Experimental Settings

- 11 problems
- Up to 300 measurements per problem
- Compared to optimized LegUp configurations for the target FPGA

Improvements

- 10% improvement on weighted average
- 2 and 5 times improvements for some metrics and scenarios

Implementation in OpenTuner

- Ensemble with Simulated Annealing, Genetic Algorithms, and Nelder-Mead

Performance: darker blues are better

	WNS	LUTs	Pins	BRAM	Regs	Blocks	Cycles	DSP	FMax
aes	0.82	0.75	1.00	1.00	0.92	1.00	1.05	1.00	0.63
adpcm	0.84	0.94	1.17	1.00	0.96	1.00	0.94	0.69	0.74
sha	0.92	1.00	1.06	1.00	0.92	1.00	0.88	1.00	0.96
motion	0.99	1.00	1.00	1.00	1.01	1.00	1.00	1.00	0.98
mips	0.90	1.00	1.06	1.00	0.93	1.00	1.03	0.83	0.80
gsm	0.95	0.92	1.00	1.00	0.95	1.00	0.90	1.00	1.02
dfsin	0.87	1.11	1.06	1.00	1.27	1.00	1.25	0.53	0.56
dfmul	0.77	1.00	1.17	0.83	0.85	0.83	1.04	0.21	0.70
dfdiv	0.81	1.00	1.06	1.00	1.03	1.00	1.25	0.50	0.59
dfadd	0.97	1.00	1.00	1.00	0.97	1.00	1.00	1.00	0.94
blowfish	0.94	1.00	1.00	1.00	0.98	1.00	0.91	1.00	0.95

Weighted Average for all Scenarios

	Balanced	Area	Performance	Perf. & Lat.
aes	0.94	0.96	0.82	0.83
adpcm	0.84	0.83	0.84	0.76
sha	0.98	0.96	0.92	0.88
motion	0.98	0.97	0.99	0.98
mips	0.95	0.91	0.90	0.95
gsm	0.95	0.89	0.95	0.92
dfsin	0.93	0.94	0.87	0.97
dfmul	0.85	0.82	0.77	0.86
dfdiv	0.84	0.77	0.81	0.82
dfadd	1.00	0.99	0.97	0.98
blowfish	0.99	0.99	0.94	0.96
Average	0.93	0.91	0.89	0.90

Discussion

Autotuning with Heuristics

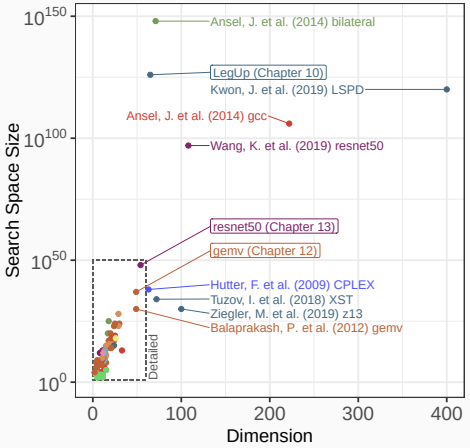
- Lack of structured exploration prevented statistical analyses and interpretation

Needle in a Haystack

- Global optimum in 10^{123} configurations?
- Are there better configurations to find?
- For how long should we continue exploring?

Proprietary Software Stack for FPGAs

- LegUp is now proprietary software



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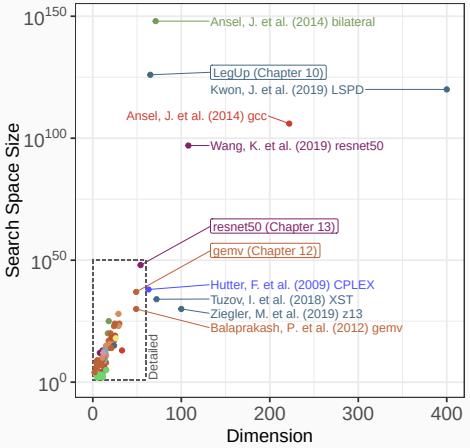


Sequential Design of Experiments

Structure explorations using modeling hypotheses to guide sampling and optimization

Applying Sequential Design of Experiments

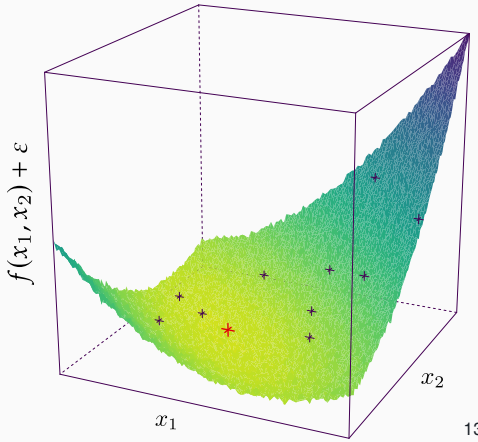
Search Space Hypotheses with Linear Models

Learning: Building Surrogates

- $f : \mathcal{X} \to \mathbb{R}$
- Model: $f(\mathbf{x}) = \mathbf{x}^\mathsf{T}\boldsymbol{\theta} + \varepsilon$, with $\varepsilon \sim \mathcal{N}(0, \sigma^2)$
- Data: $(\mathbf{x}_k, y_k = f(\mathbf{x}_k))$
- $\mathbf{x}_{1,\dots,n}$ in a given design $\mathbf{X}$

10 Measurements of Booth's Function

$$f(\mathbf{x}) = (x_1 + 2x_2 - 7)^2 + (2x_1 + x_2 - 5)^2 + \varepsilon$$



Search Space Hypotheses with Linear Models

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Minimize a Surrogate instead of f

- Surrogate: $\hat{f}_\theta(\mathbf{x}') = \mathbf{x}'^\intercal \hat{\boldsymbol{\theta}}$
- Estimator: $\hat{\boldsymbol{\theta}} = (\mathbf{X}^\intercal \mathbf{X})^{-1} \mathbf{X}^\intercal \mathbf{y}$

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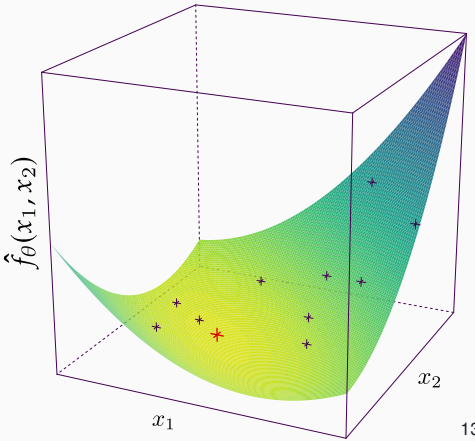

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- Estimator: $\hat{\boldsymbol{\theta}} = (\mathbf{X}^\intercal \mathbf{X})^{-1} \mathbf{X}^\intercal \mathbf{y}$

Variance of $\hat{\theta}$ is independent of $\mathbf{y}$

$$\mathrm{Var}(\hat{\boldsymbol{\theta}}) = (\mathbf{X}^\intercal \mathbf{X})^{-1} \sigma^2$$

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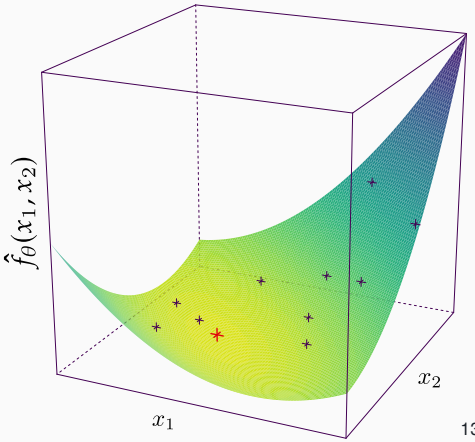


Design of Experiments

Choosing the Design $\mathbf{X}$

- Minimize Var$(\hat{\theta})$
- Decrease number of experiments in $\mathbf{X}$
- Enable testing hypotheses

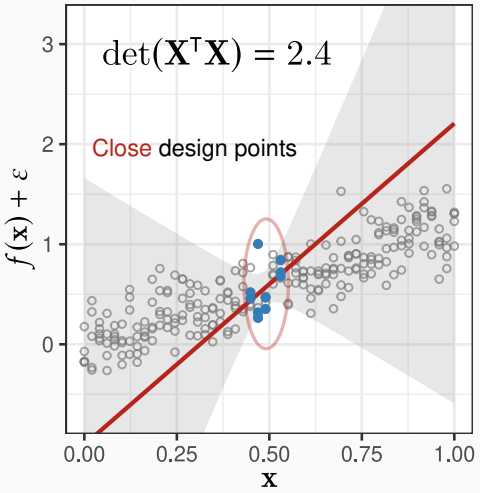
Components

- $\mathbf{X}_{n \times p}$: design matrix
- $\mathbf{x}_{1 \times n} \in \mathbf{X}$: factor columns
- $x_1, \ldots, x_p \in \mathbf{x}$: chosen factor levels

Examples

- Factorial designs, screening, Latin Hypercube and low-discrepancy sampling, optimal design

Distance of Experiments Impacts Var$(\hat{\theta})$



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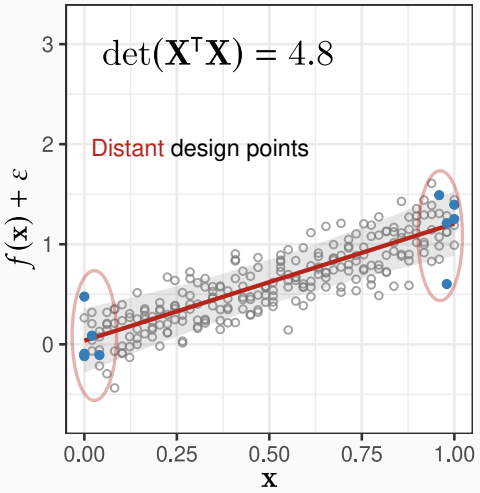

Optimal Design: Parsimony

Designs

- Building surrogates within a constrained budget
- Exploiting known search space structure
- Testing modeling hypotheses

Maximizing $\det(\mathbf{X}^T\mathbf{X})$ by Swapping Rows

- Requires an initial **model**
- Choose best rows for $\mathbf{X}$ from a large set
- $D(\mathbf{X}) \propto \det(\mathbf{X}^T\mathbf{X})$

Sampling with Different Models

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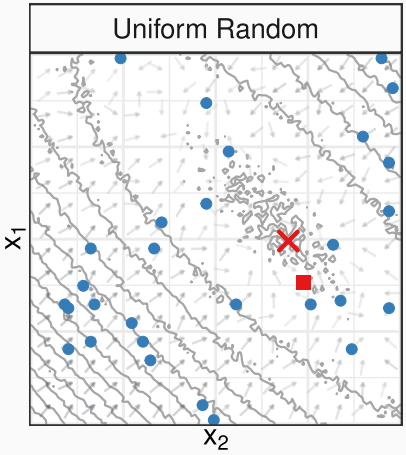

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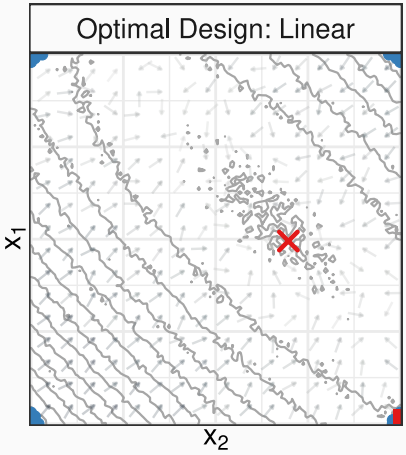

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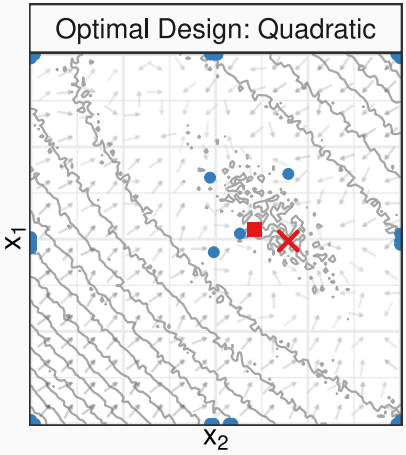

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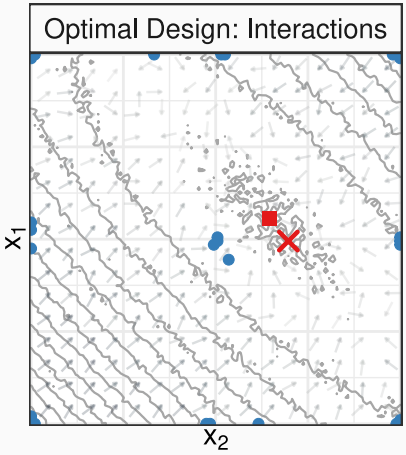

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Best design is independent of measurements

Sampling with Different Models

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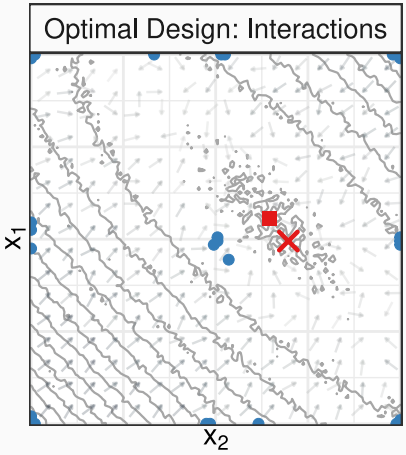

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Interpreting Significance with Analysis of Variance

Analysis of Variance (ANOVA)

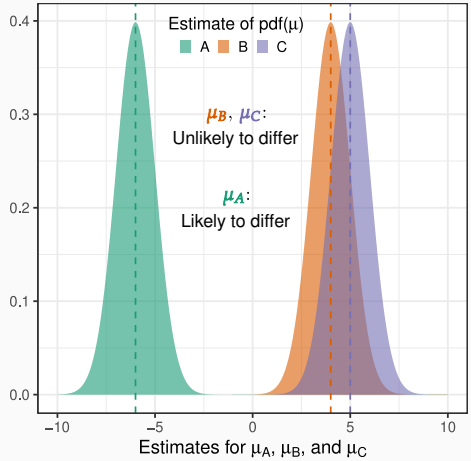
- Identify which factors and levels are significant

Steps

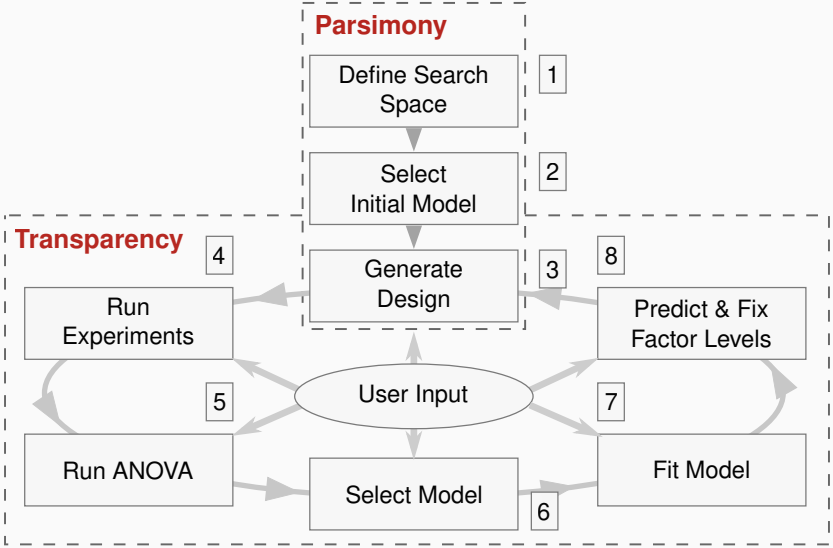
- Group observations by factor and factor levels
- Estimate distributions for each group mean μ
- Run F-tests for significance of differences between means

Enables refining initial hypotheses

One-Way ANOVA for Levels A, B, C



A Transparent and Parsimonious Approach to Autotuning



Application: OpenCL GPU Laplacian Kernel

Edge Detection with the Laplacian

The OpenCL Kernel

- Highly optimized
- Efficiently parametrized
- Generated by BOAST
- Completely evaluated previously

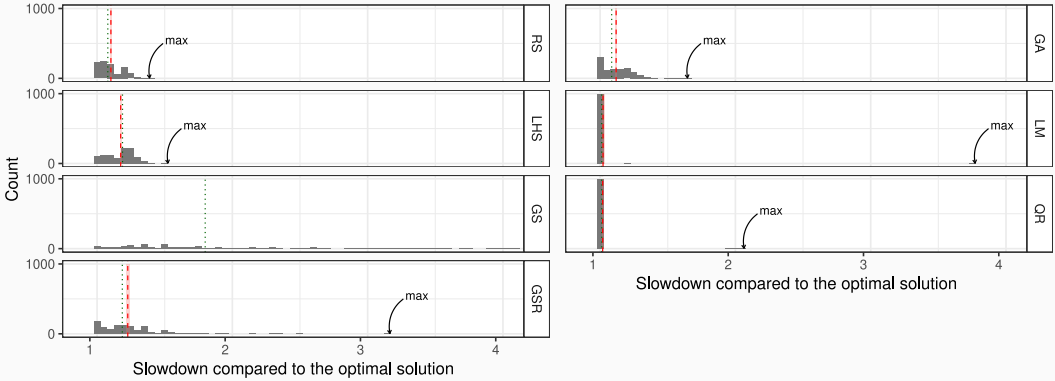
Search Space with 10^4 Valid Configurations

Factor	Levels	Short Description
vector_length	$2^0, \ldots, 2^4$	Size of vectors
load_overlap	*true*, *false*	Load overlaps in vectorization
temporary_size	$2, 4$	Byte size of temporary data
elements_number	$1, \ldots, 24$	Size of equal data splits
y_component_number	$1, \ldots, 6$	Loop tile size
threads_number	$2^5, \ldots, 2^{10}$	Size of thread groups
lws_y	$2^0, \ldots, 2^{10}$	Block size in y dimension

Performance Metric and Starting Model

$$\begin{aligned} \mathit{time\_per\_pixel} \sim & \mathit{y\_component\_number} + \frac{1}{\mathit{y\_component\_number}} + \\ & \mathit{temporary\_size} + \mathit{vector\_length} + \mathit{load\_overlap} + \\ & \mathit{lws\_y} + \frac{1}{\mathit{lws\_y}} + \mathit{elements\_number} + \frac{1}{\mathit{elements\_number}} + \\ & \mathit{threads\_number} + \frac{1}{\mathit{threads\_number}} \end{aligned}$$

Results: 1000 Repetitions with a Budget of 120 Measurements



RS: Random Sampling, LHS: Latin Hypercube Sampling, GS: Greedy Search,
GSR: Greedy Search w. Restart, GA: Genetic Algorithm, LM: Linear Model, QR: Quantile Regression

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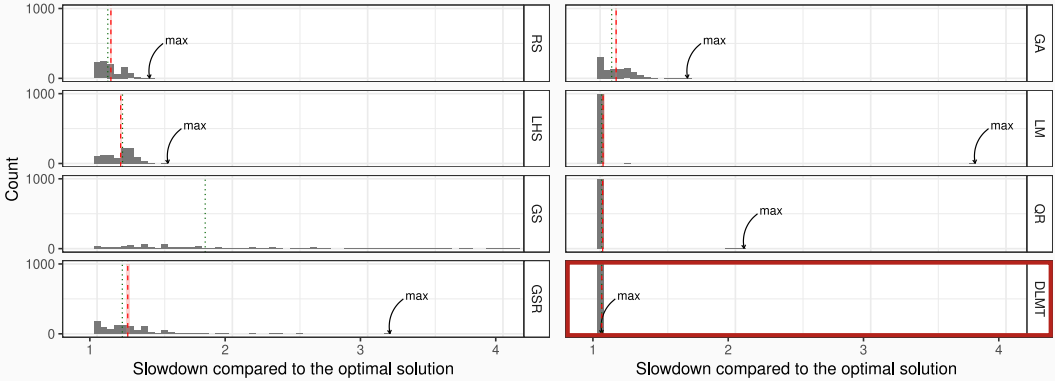

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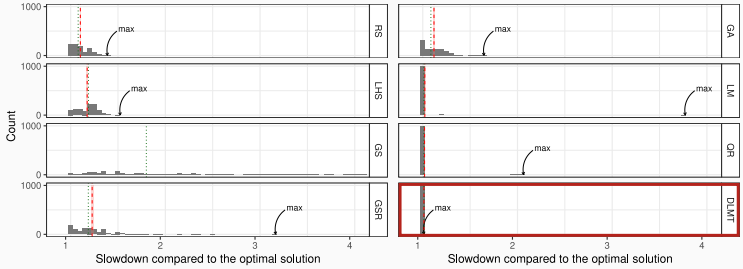
DLMT: D-Optimal Designs, Linear Model w. Transform

Results: Parsimony Regarding the Budget



Method	Slowdown Mean	Slowdown Min.	Slowdown Max.	Budget Mean	Budget Max.
Random Sampling (RS)	1.10	1.00	1.39	120.00	120
Latin Hypercube Sampling (LHS)	1.17	1.00	1.52	98.92	125
Greedy Search (GS)	6.46	1.00	124.76	22.17	106
Greedy Search w. Restart (GSR)	1.23	1.00	3.16	120.00	120
Genetic Algorithm (GA)	1.12	1.00	1.65	120.00	120
Linear Model (LM)	1.02	1.01	3.77	119.00	119
Quantile Regression (QR)	1.02	1.01	2.06	119.00	119
D-Opt., Linear Model w. Transform (DLMT)	1.01	1.01	1.01	54.84	56

Interpreting the Optimization

Application: SPAPT kernels

Search Spaces and Performance Metric

Results

- Pick one?
- Is there anything to find?
- Leave GPR for later

Interpreting the Optimization

- Maybe remove?

Discussion

- Sequential and incremental
  - Definitive restrictions
  - Improvements by batch
  - Low model flexibility (rigid models)
- Motivating results in the Laplacian kernel
- It is possible to interpret results, guide optimization
  - sometimes simpler models give better results
- For SPAPT kernels, it is still unclear:
  - if there is something to find, and when to stop exploring
  - is there a global optimum, is it "hidden"?
    - how to find it, if so? (can learning do it?)
- Random Sampling has good performance
  - Abundance of local optima?
- What is the most effective level of abstraction for optimizing a program?
  - Compiler, kernel, machine, model, dependencies?

Active Learning with Gaussian Processes

More Flexibility with Gaussian Process Regression

- Introduce notation:
  - Model of f: $f(\mathbf{x}) \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$
  - Surrogate $\hat{f}_\theta(\mathbf{x}) \sim f(\mathbf{x}) \mid \mathbf{X}, \mathbf{y}$

Space-filling Designs

- Curse of dimensionality for sampling:
  - Most sampled points will be on the "shell"
- LHS: Partition and then sample, need to optimize later
- Low-discrepancy: deterministic space-filling sequences

Expected Improvement: Balancing Exploitation and Exploration

- How to decide where to measure next?

Application: GPU Laplacian and SPAPT

- GPR was applied to these problems too
- Quickly Present Results Here Too
- GPR is good too, but the simpler model is more consistent

Application: Quantization for Convolutional Neural Networks

Search Space, Constraints, and Performance Metrics

- Comparing with a Reinforcement Learning approach in the original paper
- ImageNet

Results

Interpreting the Optimization

- Sobol indices, inconclusive

Discussion

- Low-discrepancy sampling in high dimension
- Constraints complicate exploration
- Multi-objective optimization
- A more complex method usually produces less interpretable results, but not always achieves better optimizations

Conclusion

Toward Transparent and Parsimonious Autotuning

Contributions of this Thesis

- Developing transparent and parsimonious autotuning methods based on the Design of Experiments
- Evaluating different autotuning methods in different HPC domains

Transparent

- Use statistics to justify code optimization choices
- Learn about the search space

Parsimonious

- Carefully choose which experiments to run
- Minimize f using as few measurements as possible

Domain	Method
CUDA compiler parameters	F, D
FPGA compiler parameters	F
OpenCL Laplacian Kernel	F, L, D
SPAPT Kernels	L, D
CNN Quantization	L, D

F: Function Minimization, L: Learning,
D: Design of Experiments
: In this presentation

Reproducibility of Performance Tuning Experiments

- Redoing all the work for different problems
- Complementary approaches:
  - Completely evaluate small sets of a search space
  - Collaborative optimizing for different architectures, problems

Key Discussions

Curse of Dimensionality for Autotuning Problems

- Implications for Sampling and Learning
- Space-filling helps, but does not solve
- Constraints

Which method to use?

- Design of Experiments for transparency and parsimony when building and interpreting statistical models
- Linear models for simpler spaces and problems
- Gaussian Process Surrogates for more complex situations

It is often unclear if there is something to find

- Abundance of local optima
- Is there a global optimum, is it "hidden"?
  - How to find it, if so? (can learning do it?)
- What is the most effective level of abstraction for optimizing a program?
  - Compiler, kernel, machine, model, dependencies?
- When to stop?

Conclusion

Toward Transparent and Parsimonious Methods for Automatic Performance Tuning

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July 9 2021