FFX: Fast, Scalable, Deterministic Symbolic Regression Technology

Trent McConaghy
Solido Design Automation Inc.
Canada

Outline

- Introduction
- Background
- FFX: Fast Function Extraction
- Results
- Scaling Higher?
- Discussion

Technology

Technology


The Exciting New F2 ("Fork Fan")
Designed by World Renown Entrepeneur: Rod Ryan
Cools down all those "too hot" to eat foods before they get to your mouth!
Never burn your tounge again!
Go ahead, be in a hurry. Never wait for your food to cool down ever again.
Featuring:
* High Tech Ergonomic Design
* Two Speed "Whisper Quiet" Fan
* Right and Left Handed Compatible
* Stainless Steel Anti-Corrosion Materials
* Dishwasher Safe!
"This is the BEST new kitchen innovation I have ever seen! Ideal for prison food!" Martha Stewart
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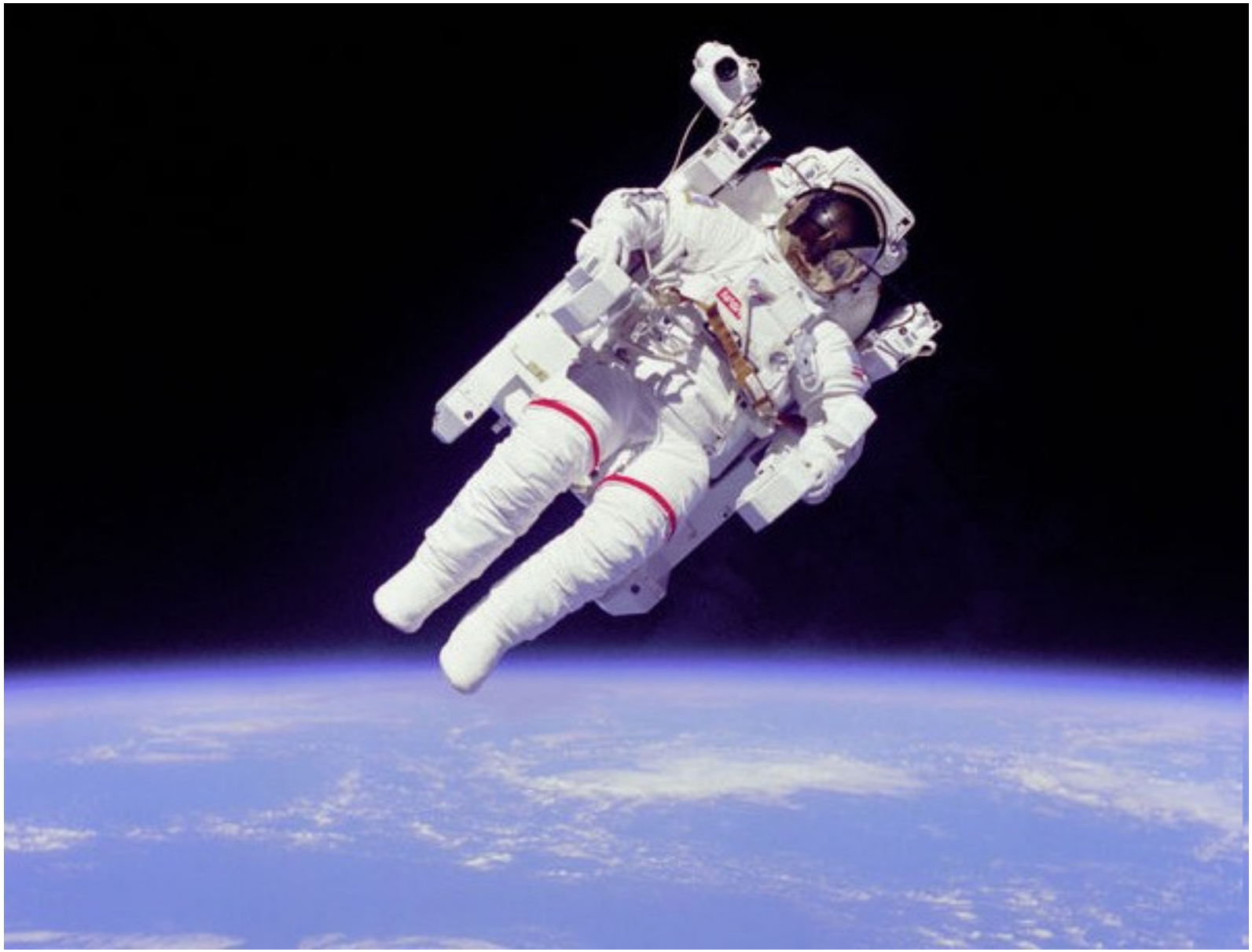
Technology

Technology

Technology



Technology

Technology – Alternate Definition

"We can say that solving least-squares problems … is a (mature) *technology*, that can be reliably used by many people who do not know, and do not need to know, the details."

- Boyd and Vandenberghe, Convex Optimization, 2004

Technology – Alternate Definition

I would say that least squares is a mature technology. ...This is the highest praise. …What it means is that other people know enough about the theory, the algorithms, and the implementations are so good and so reliable that the rest of us can just type “A / B”.

– Transcript of Steve Boyd Stanford lecture on convex optimization.
http://see.stanford.edu/materials/lsocoee364a/transcripts/ConvexOptimizationI-Lecture01.pdf

Technology – Alternate Definition

Here's the really cool part about linear programming .. [these problems] are solved. Unless your problem is huge or you have some super real time thing like in communications, then [once you formulate the problem and run LP] there's a sense in which you're kind of done.

– Transcript of Steve Boyd Stanford lecture on convex optimization. http://see.stanford.edu/materials/lsocoee364a/transcripts/ConvexOptimizationI-Lecture01.pdf

SVM Envy?

- SVMs were introduced in the late 90s
  - And have become a standard tool in the practitioners' toolbox
- Convex optimization was popularized in the late 90s
  - And is becoming a standard tool in practitioners' toolbox
- GP was popularized in the early 90s
  - And is not a standard tool in the practitioners' toolbox

GP and Technology

Last year, a gauntlet was thrown:

> "How can GP be scoped so that it becomes another standard, off-the-shelf method in the "toolboxes" of scientists and engineers around the world? Can GP follow in the same vein of linear programming?
>
> "Scalability is always relative. GP has attacked fairly large problems, but how can GP be improved to solve problems that are 10x, 100x, 1,000,000x harder?"

– McConaghy, Riolo, and Vladislavleva, "Genetic programming theory and practice: an introduction", GPTP VIII, Springer, 2010

On Symbolic Regression (SR)

GP is a popular approach to do SR

Many successful GP-based applications

- Finance, medicine, industrial processing, …

SR is a popular app among GP researchers

So, a meaningful advance in SR can influence overall GP theory and practice

~~GP~~ SR and Technology

For this GPTP, my gauntlet to myself:

"How can ~~GP~~ SR be scoped so that it becomes another standard, off-the-shelf method in the "toolboxes" of scientists and engineers around the world? Can ~~GP~~ SR follow in the same vein of linear programming?

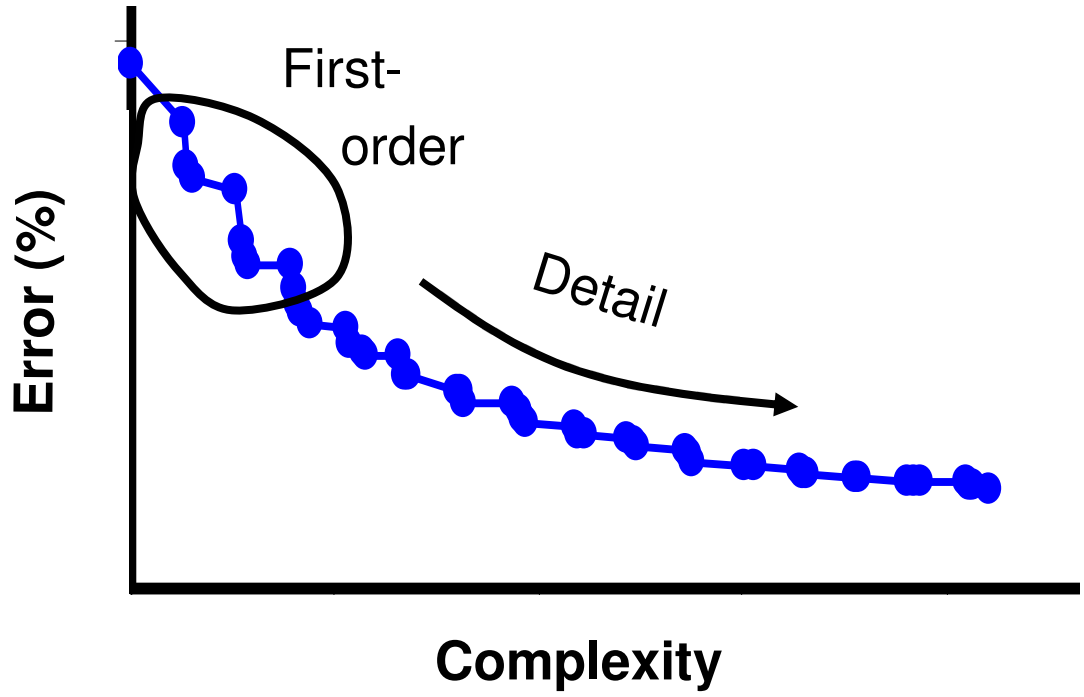
"Scalability is always relative. ~~GP~~ SR has attacked fairly large problems, but how can ~~GP~~ SR be improved to solve problems that are 10x, 100x, 1,000,000x harder?"

Summary:
Aiming for SR* as a Technology

*** SR ≠ Shopping Robot**

SR Problem Definition

- Given (X,y)
- Find a whitebox model (or models)
- That minimizes error
- And minimizes complexity



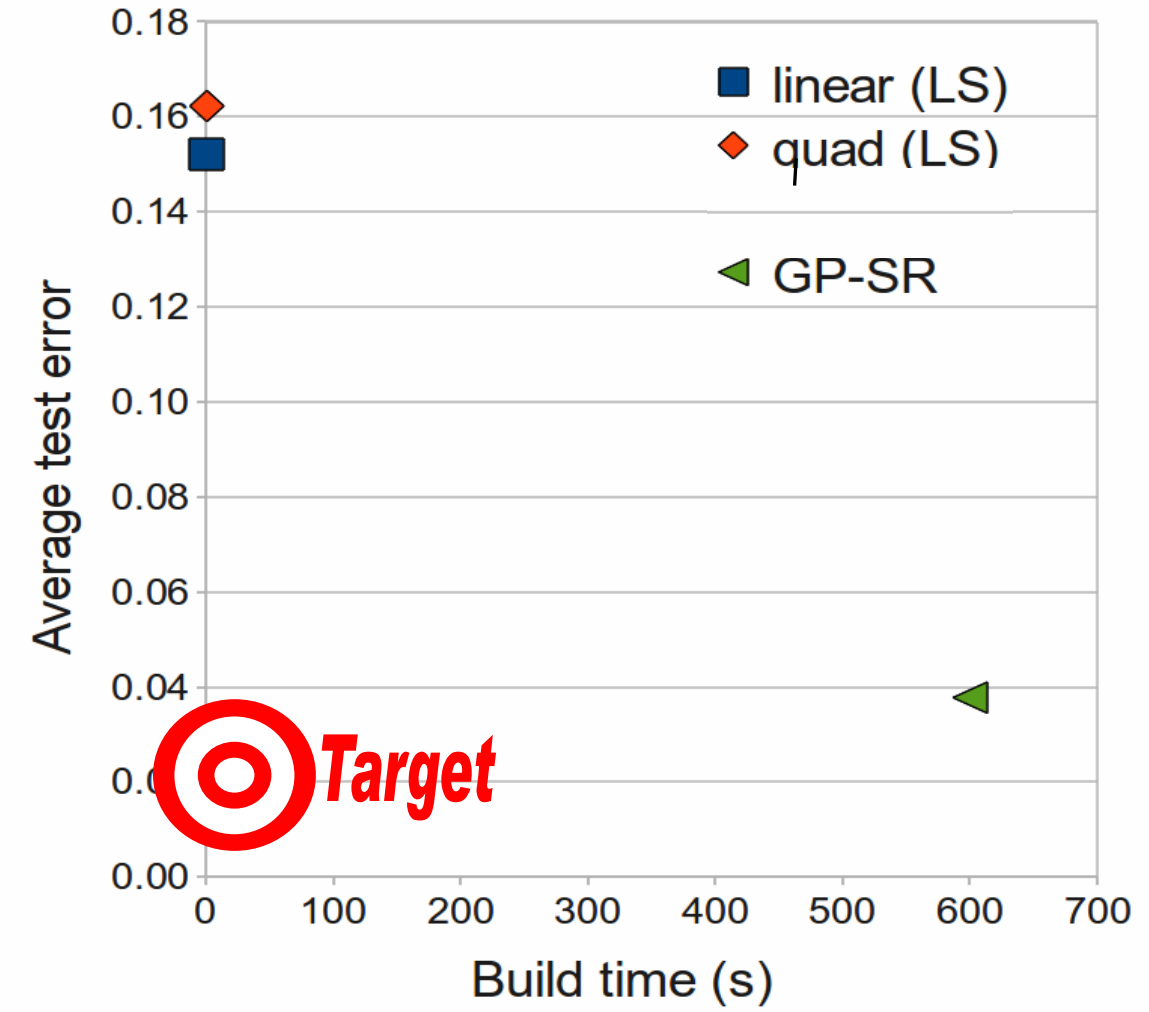
SR Problem Definition

- Given (X,y)
- Find a whitebox model (or model*s*)
- That minimizes error
- And minimizes complexity

Desirable Features:

- Scalable (# variables, # samples)
- Fast
- Reliable, consistent results
  - Derandomized → deterministic? (CMAES → X/y)
- Ideal: simple algorithm
  - Arch. Altering Ops → Push → …
  - FFNNs → SVMs
- Ideal: hits global optimum (on problem formulation)

Summary of Goal
Speed of LS, Accuracy of GP-SR



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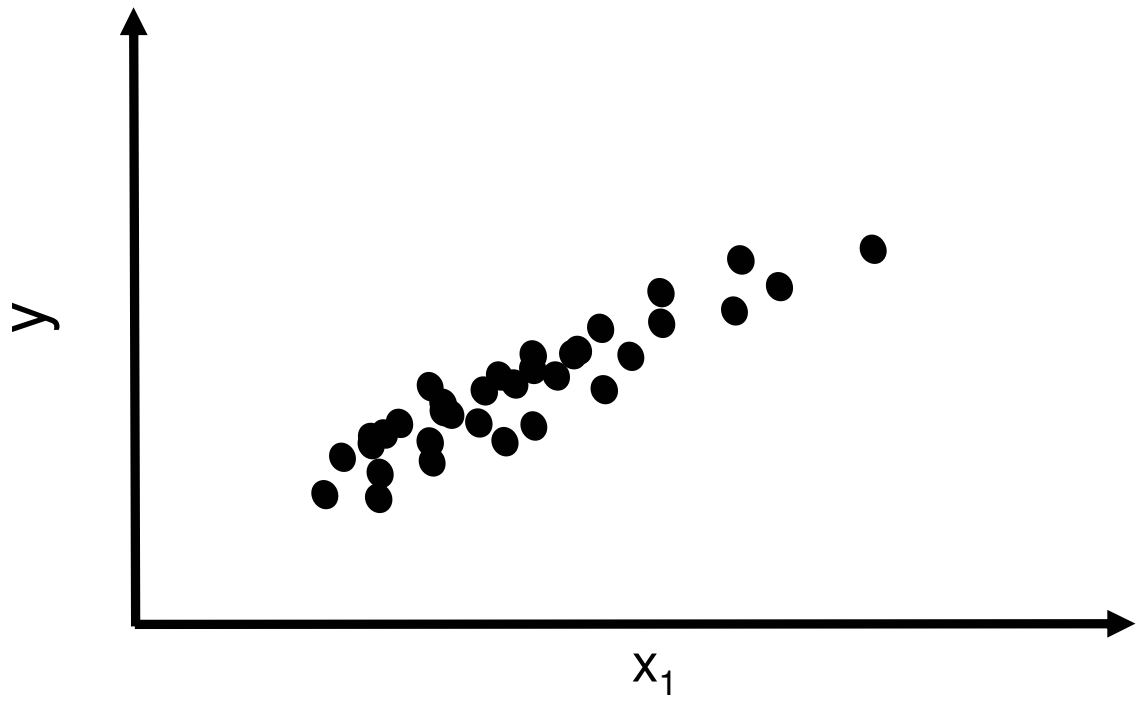
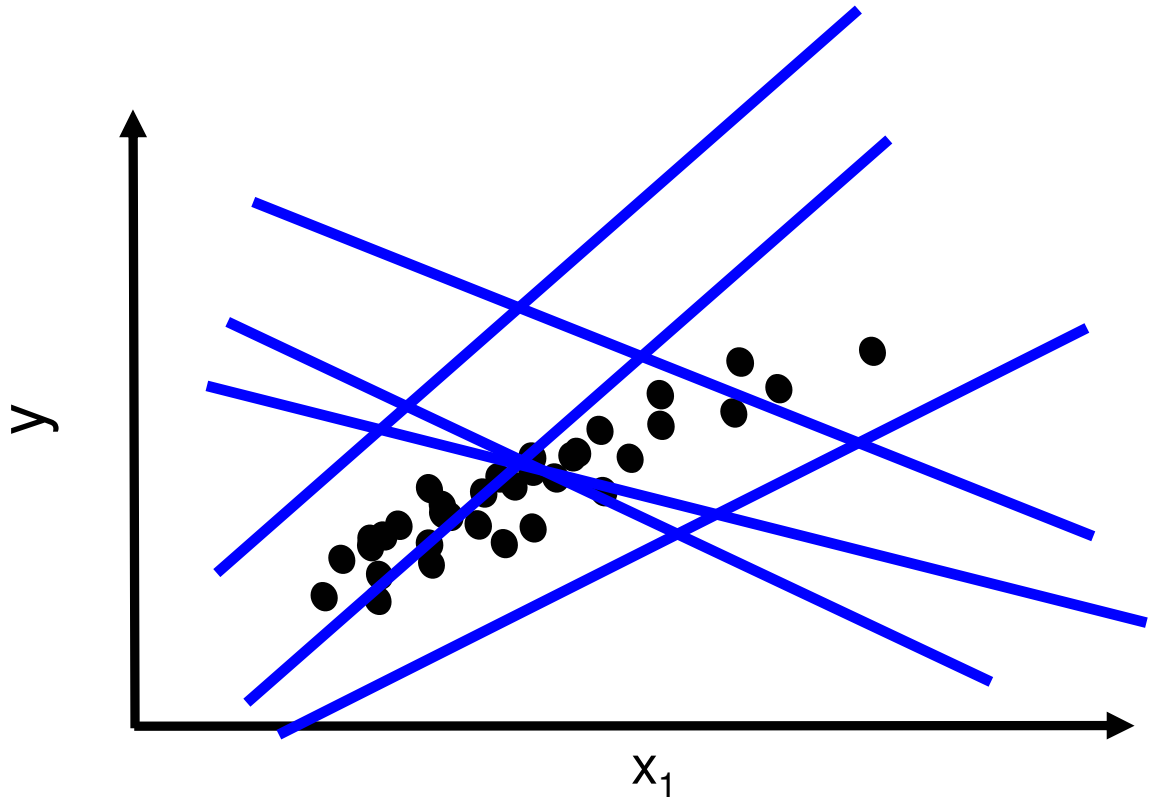
Background

1D Linear Least-Squares Regression



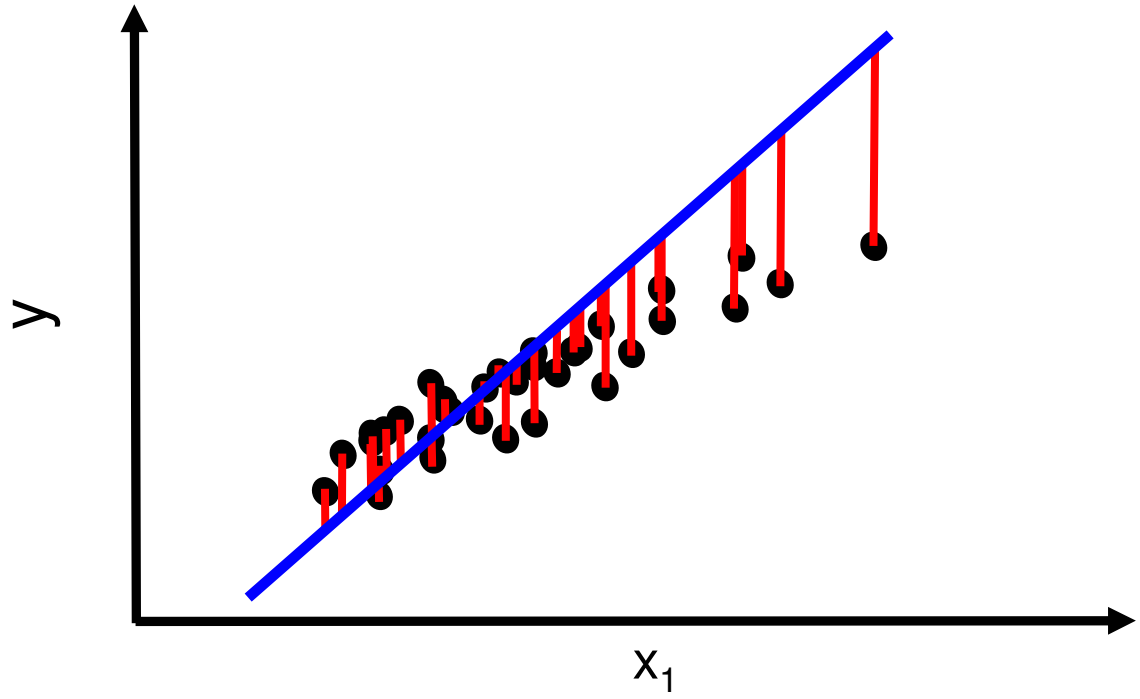
1D Linear LS Regression

Many possible linear models!



1D Linear LS Regression

Find linear model that
minimizes $\sum(yhat_i - y_i)^2$
for all *i* in training data



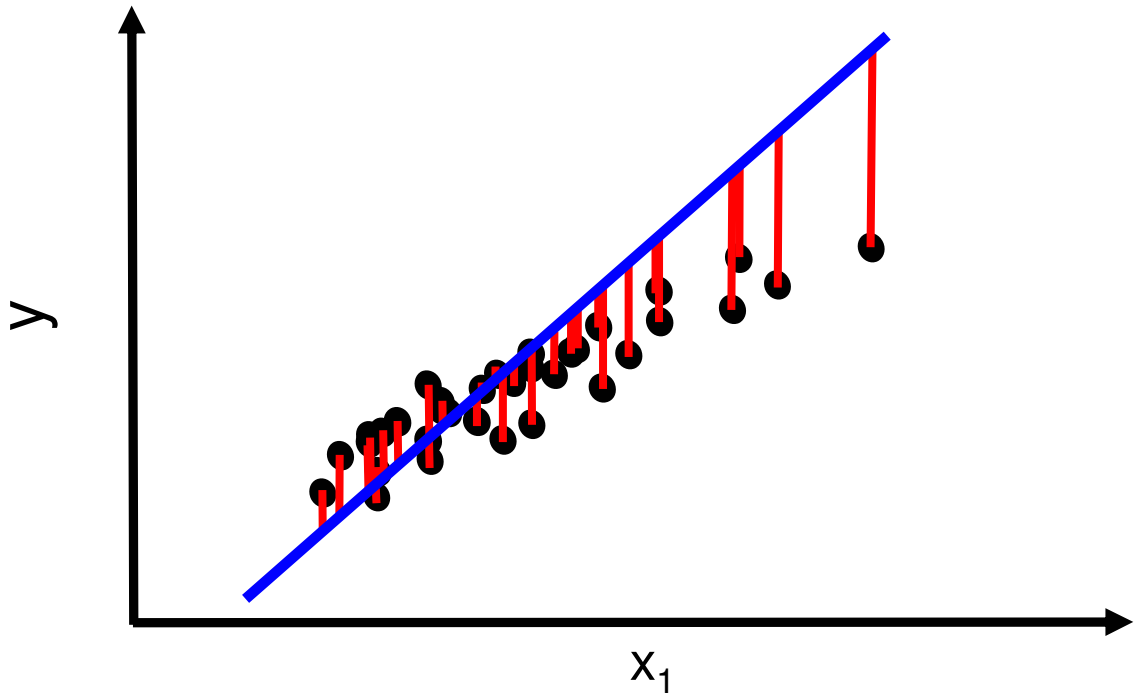
1D Linear LS Regression

Find linear model that minimizes $\sum(yhat_i - y_i)^2$

That is:

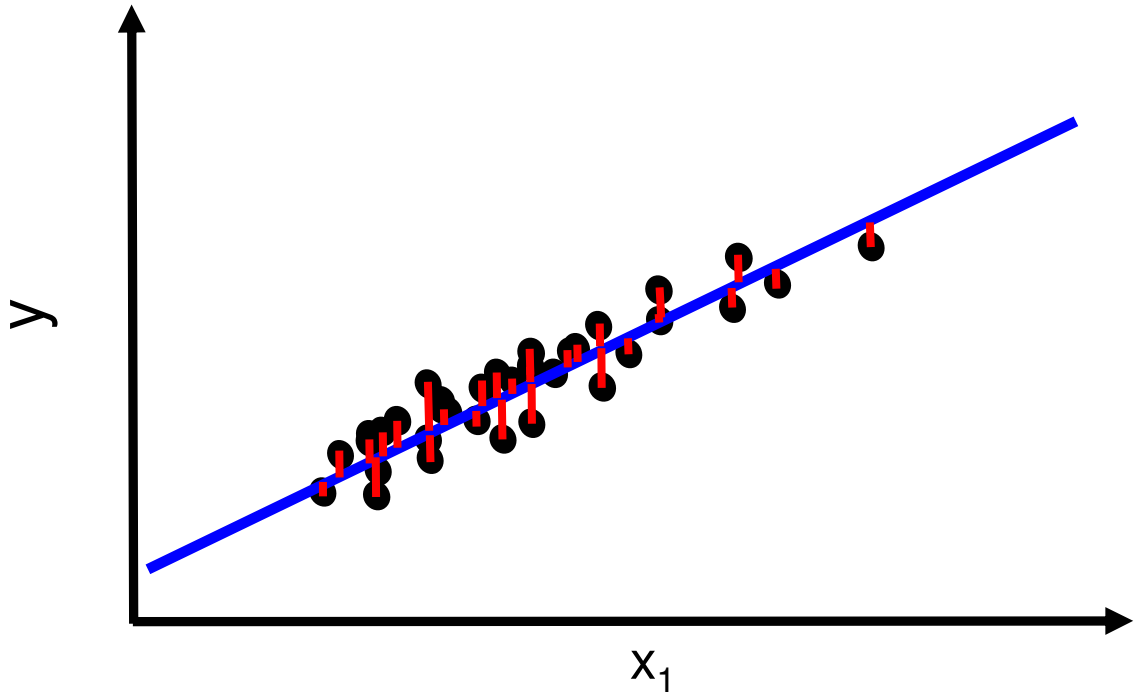
$[w_0, w_1]^* = \text{argmin} \sum(yhat_i - y_i)^2$

where $yhat(x_1) = w_0 + w_1 * x_1$



1D Linear LS Regression

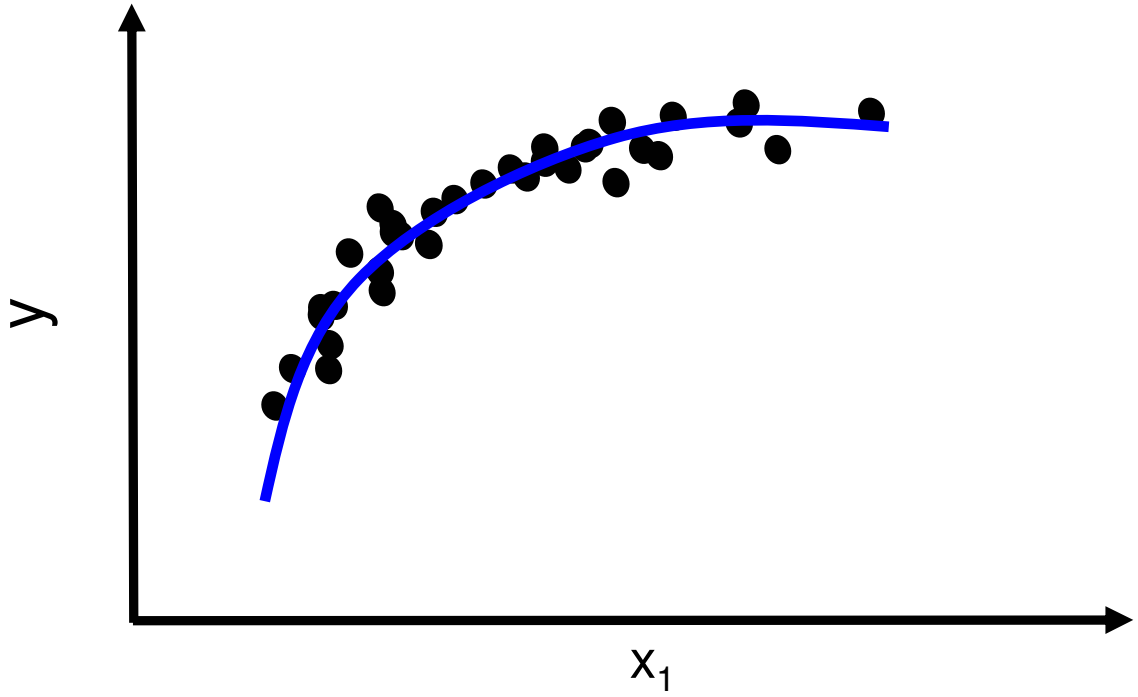
$y = 1.1 + 2.3 * x_1$
i.e. $w_0=1.1$, $w_1=2.3$
Found with "least-squares learning"
(amounts to ≈matrix inversion)



1D *Quadratic* LS Regression

$[w_0, w_1, w_{11}]^* = \text{argmin} \sum(yhat_i - y_i)^2$
where $yhat(x_1) = w_0 + w_1 * x_1 + w_{11} * x_1^2$

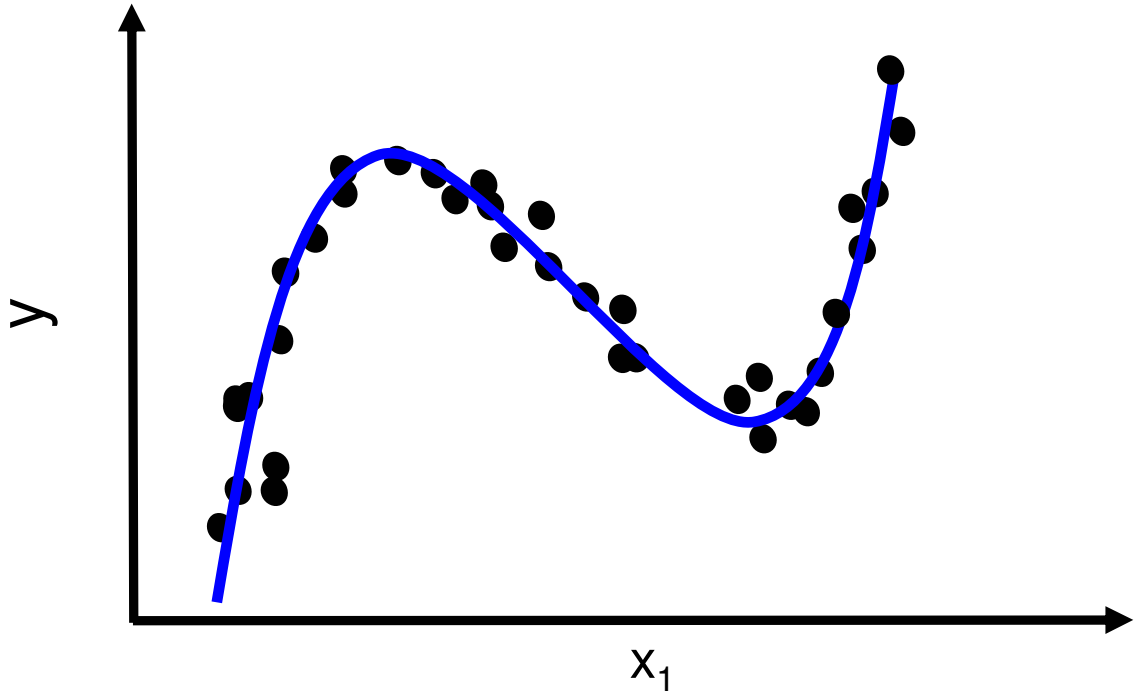
We are applying linear (LS) learning on linear & nonlinear basis functions. OK!



1D *Nonlinear* LS Regression

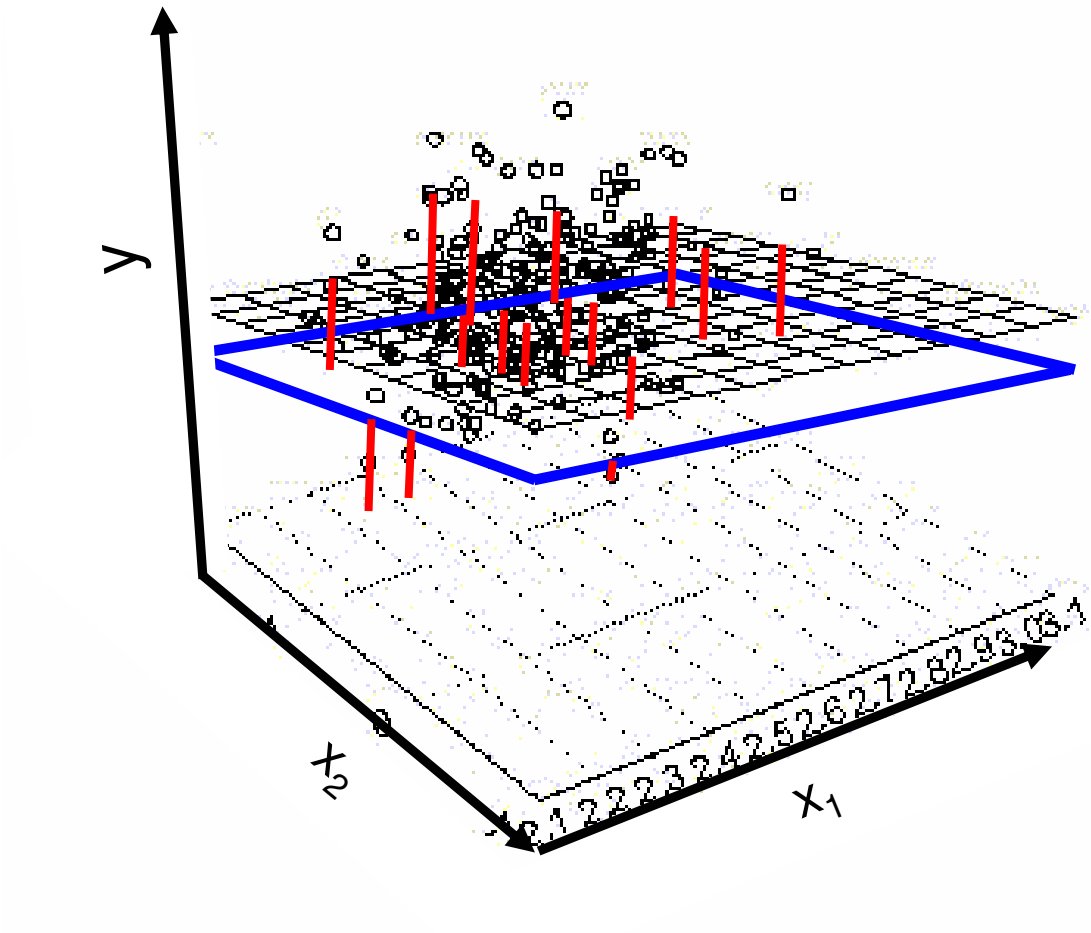
$[w_0, w_1, w_{sin}]^* = \text{argmin} \sum(yhat_i - y_i)^2$
where $yhat(x_1) = w_0 + w_1 * x_1 + w_{sin} * \sin(x_1)$

We are applying linear (LS) learning on linear & nonlinear basis functions. OK!



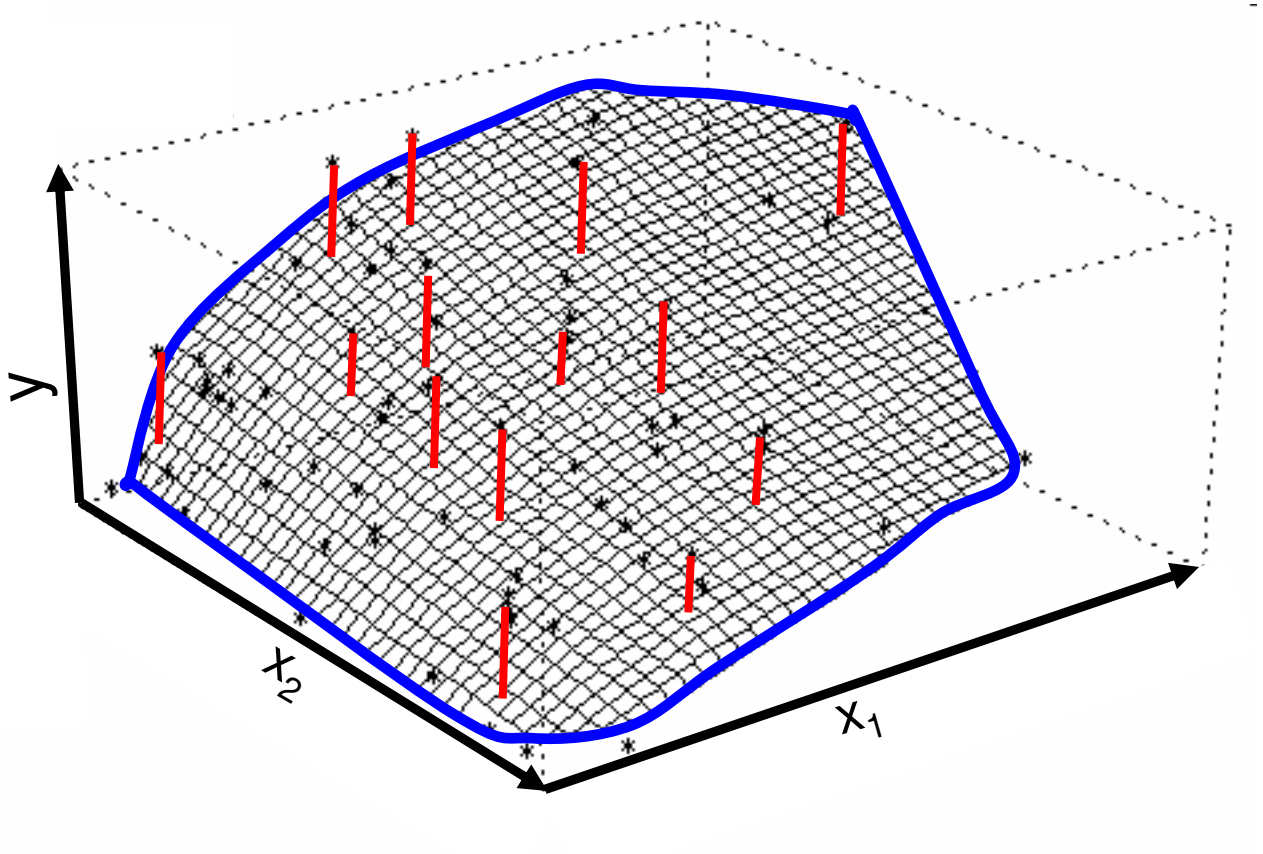
2D Linear LS Regression

$[w_0, w_1, w_2]^* = \text{argmin} \sum(\text{yhat}_i - y_i)^2$
where $\text{yhat}(\mathbf{x}) = w_0 + w_1 * x_1 + w_2 * x_2$



2D Quadratic LS Regression

$[w_0, w_1, w_2, w_{11}, w_{22}, w_{12}]^* = \text{argmin} \sum(\text{yhat}_i - y_i)^2$
where $\text{yhat}(\mathbf{x}) = w_0 + w_1 * x_1 + w_{11} * x_1^2 + w_{22} * x_2^2 + w_{12} * x_1 * x_2$



Generalized Linear Model (GLM)

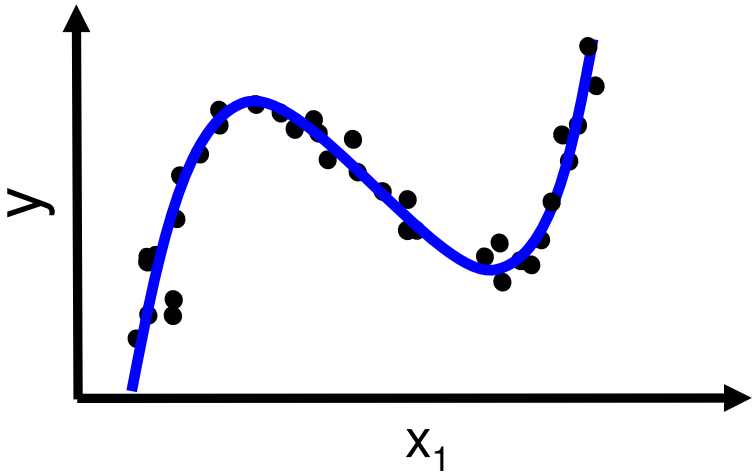
G*eneralized linear model (GLM) of B basis functions.*

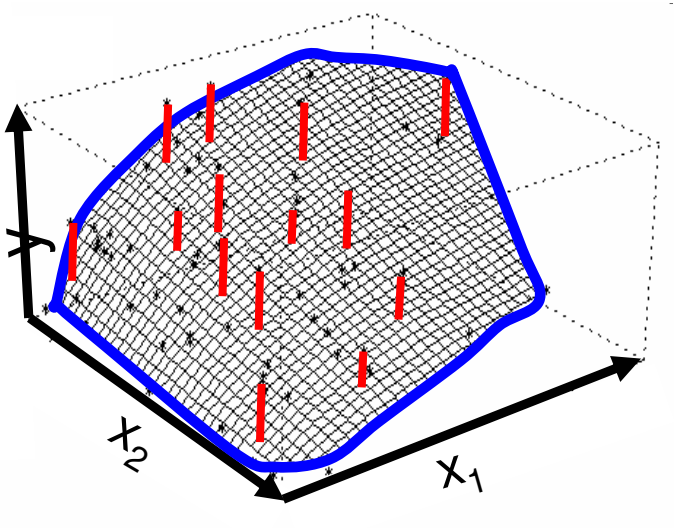
$$yhat(\mathbf{x}) = w_0 + w_1 * f_1(\mathbf{x}) + w_2 * f_2(\mathbf{x}) + \ldots + w_B * f_B(\mathbf{x})$$

Just treat each basis function as an input variable, and LS-learn!

Examples:

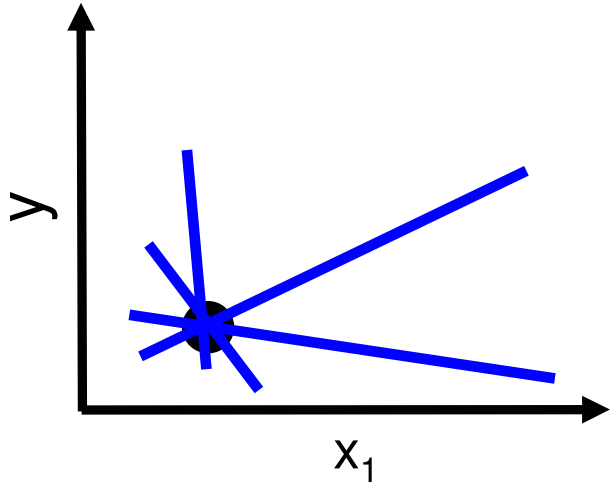
- $yhat(x_1) = w_0 + w_1 * x_1 + w_{11} * x_1^2$
- $yhat(x_1) = w_0 + w_1 * x_1 + w_{sin} * \sin(x_1)$
- $yhat(\mathbf{x}) = w_0 + w_1 * x_1 + w_{11} * x_{12} + w_{22} * x_{22} + w_{12} * x_1 * x_2$
- polynomials, SVMs, FFNNs, many GP SR. Universal approximator!



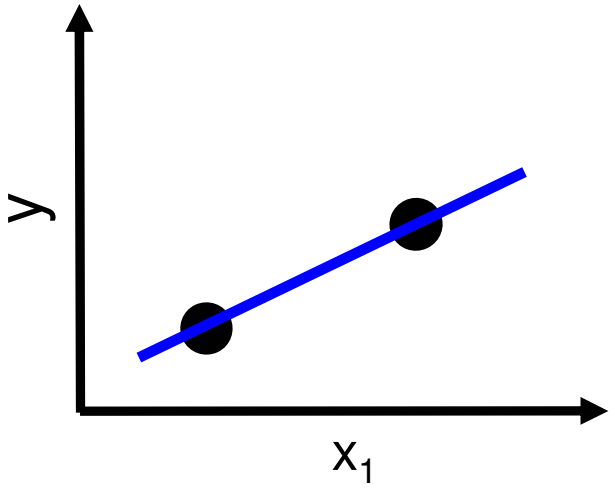


Constraint on LS Regression?

(1D Example)



1 Sample – too few



2 Samples – enough

General rule?

Constraint on LS Regression

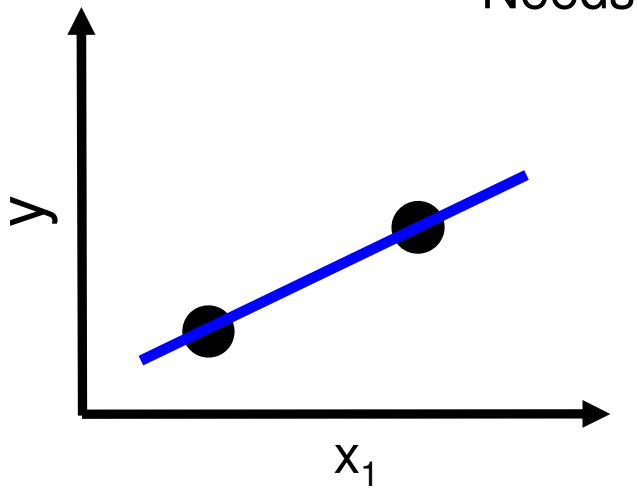
General Rule:

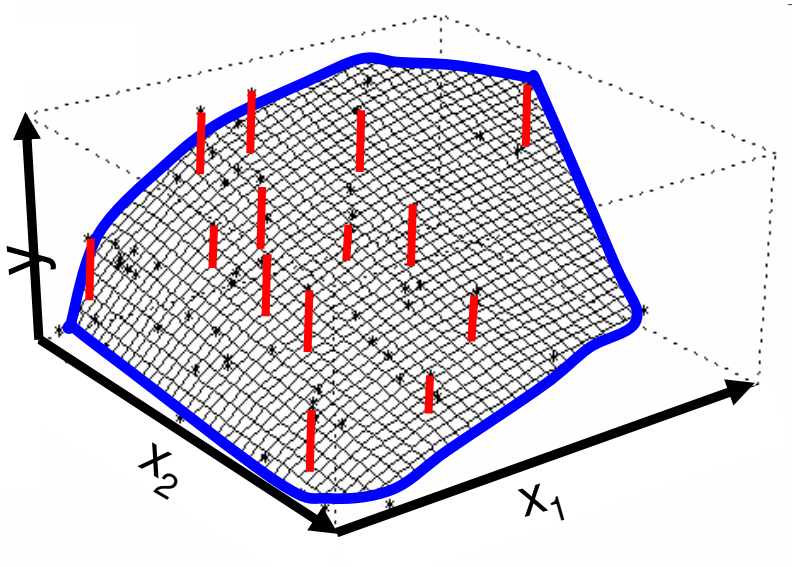
- **If *n* variables, need N ≥ N+1 training samples**

Examples:

1D Lin: $[w_0, w_1]^* = \text{argmin} \sum(\text{yhat}_i - y_i)^2$
Needs ≥ 1+1 = 2 training samples.

2D Quad $[w_0, w_1, w_2, w_{11}, w_{22}, w_{12}]^* = \text{argmin} \sum(\text{yhat}_i - y_i)^2$
Needs ≥ 6+1 = 7 training samples.





LS Regression On High Dimensionality

Consider 10,000 basis functions in a GLM
Q: Can we fit this with LS-learning?
A: Yes! (As long as ≥10,001 samples)*

Consider 1M basis functions in a GLM
Q: Can we fit this with LS-learning?
A: Yes! (As long as ≥1M+1 samples)*

*and no memory issues etc

90˚ turn…

genetic programming

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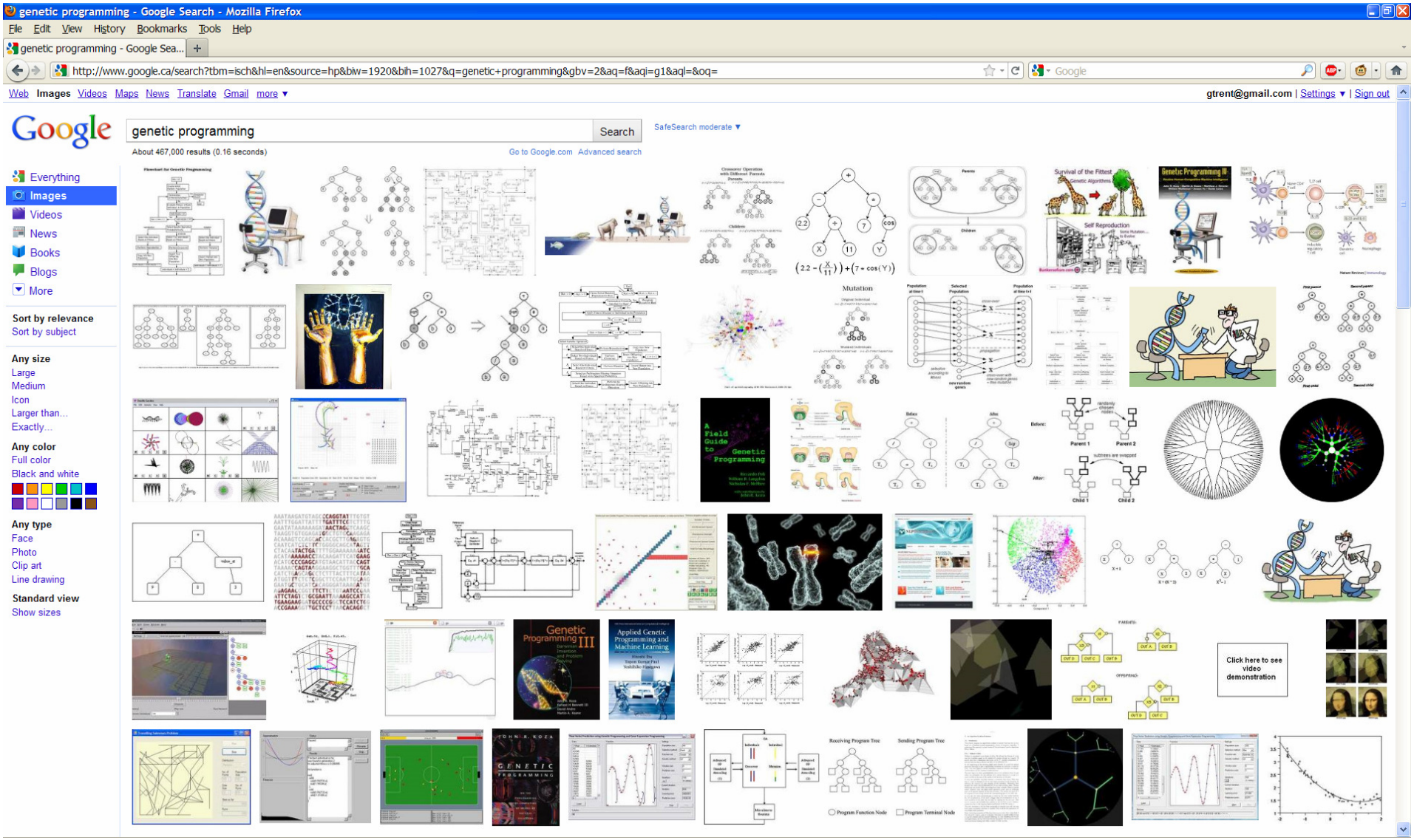
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Standard view
Show sizes
A Field Guide to Genetic Programming
Genetic Programming III
Applied Genetic Programming and Machine Learning
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Trivia Q: State of the art in image search? (NIPS ’09)

A: BHALR!*

Q: State of the art in image search? (NIPS ’09)
A: BHALR!*

*__B__ig, __H__airy, __A__udacious __L__inear __R__egression

1000 pixels x 1000 pixels = 1M input variables
100-1000 samples.
Then apply linear regression or classification

Q: State of the art in image search? (NIPS ’09)
A: BHALR!*

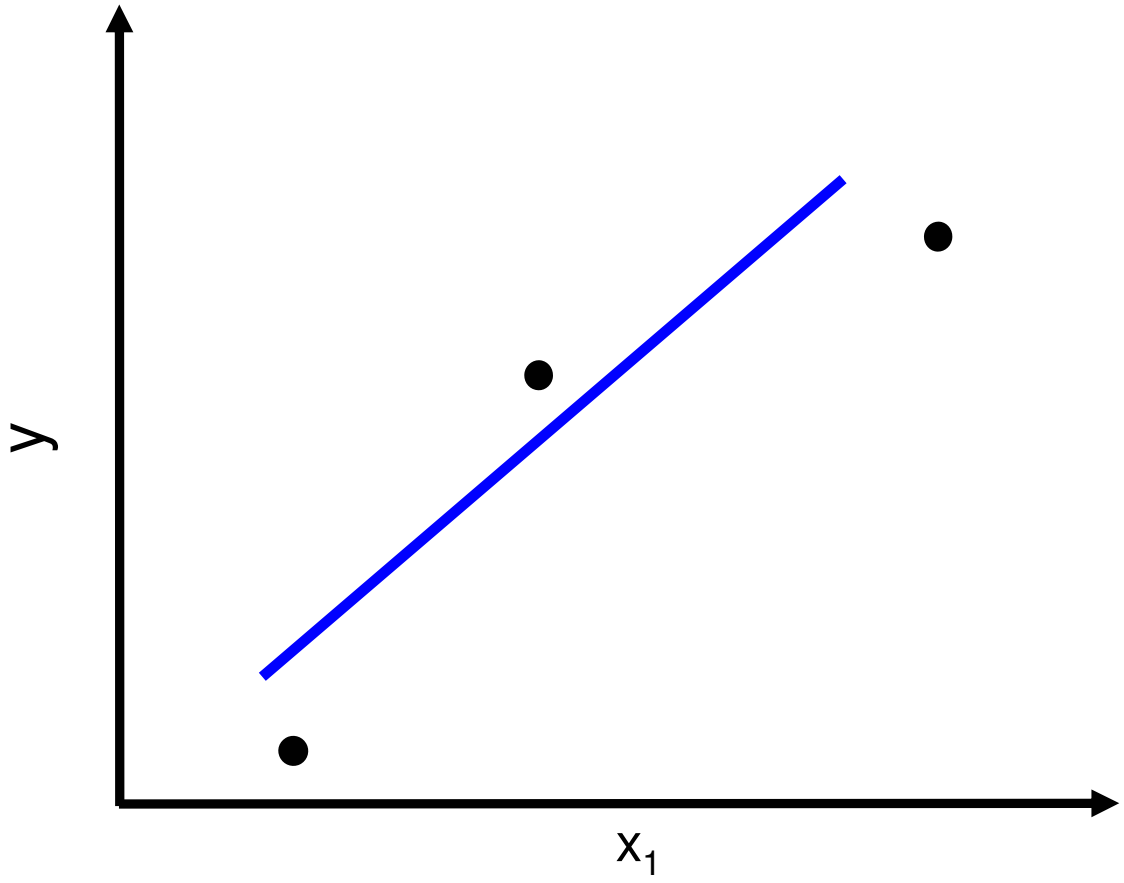
*__B__ig, __H__airy, __A__udacious __L__inear __R__egression

1000 pixels x 1000 pixels = 1M input variables
100-1000 samples.
Then apply linear regression or classification

But 100 << 1M. *HOW DO THEY DO IT??*

Linear Regression

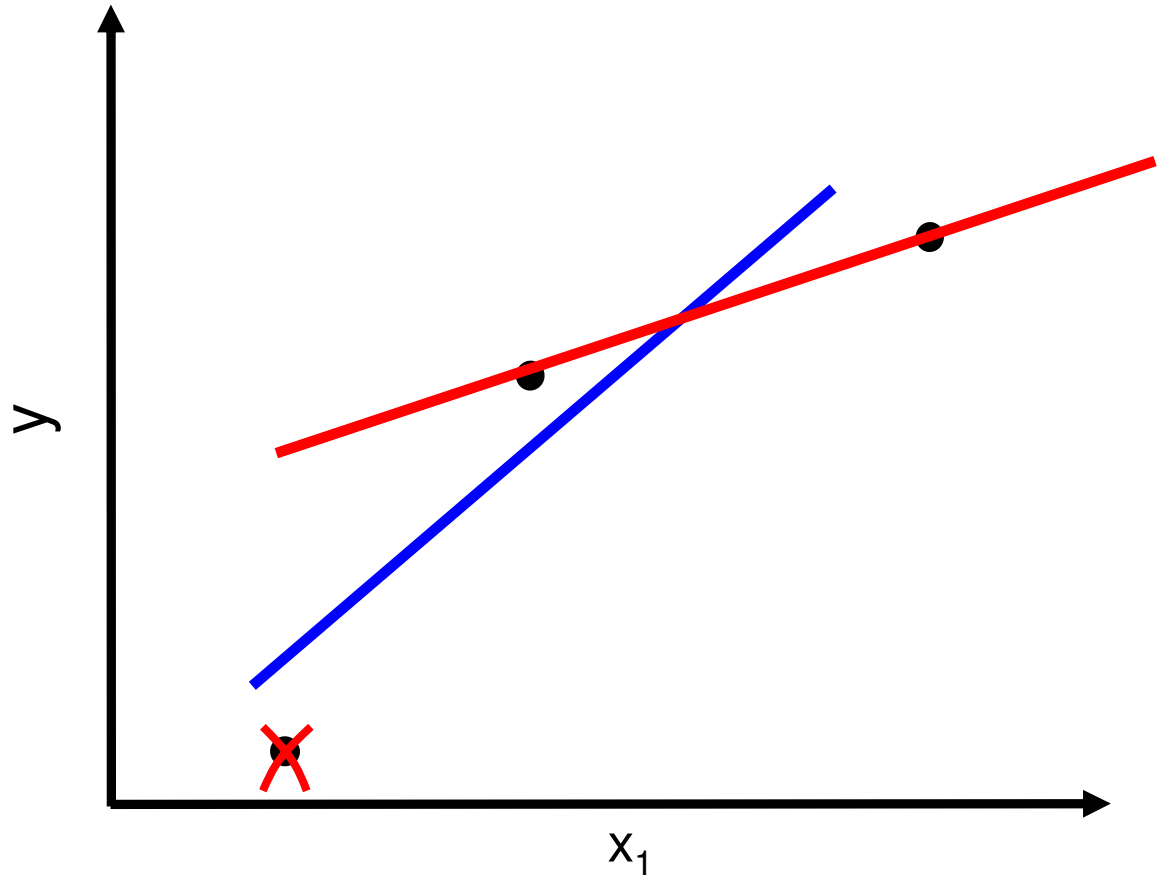
Q: What happens when samples $N \rightarrow$ # variables n ?



Linear Regression

Q: What happens when # samples $N \rightarrow$ # variables n ?

A: Model gets more sensitive!



Linear Regression

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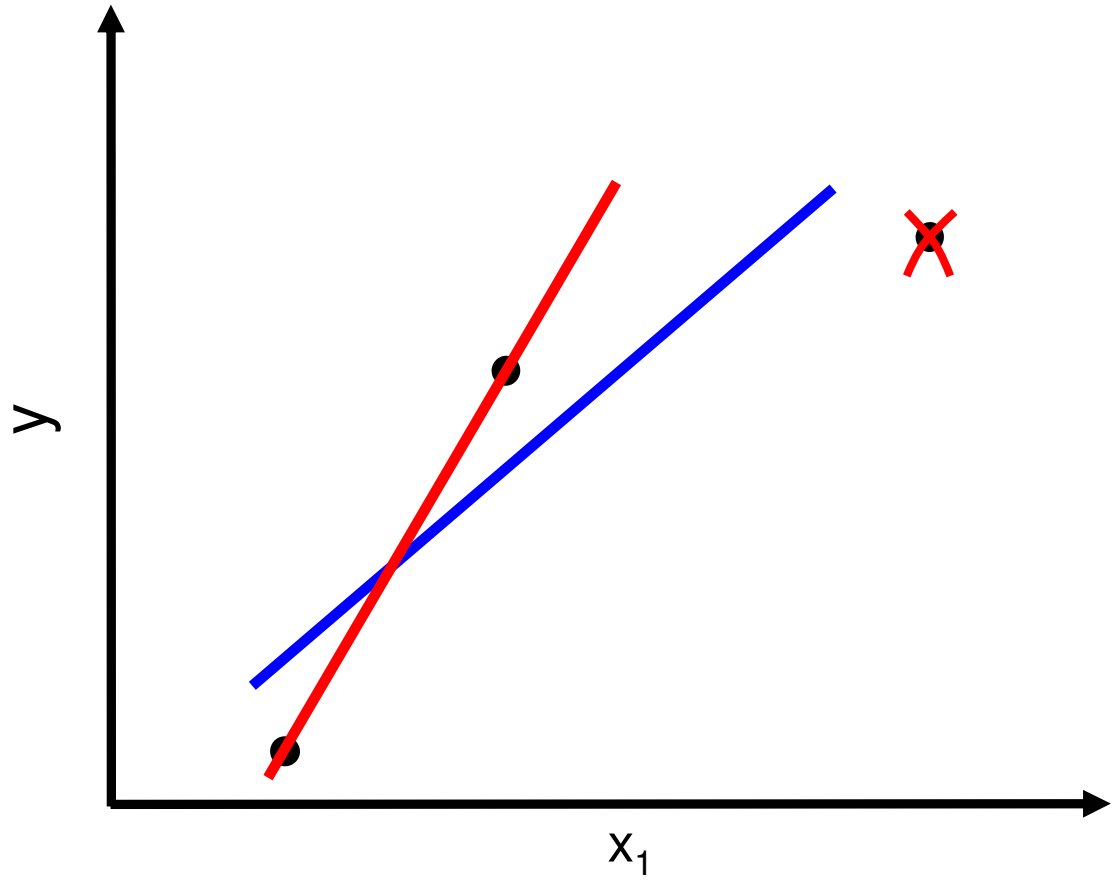
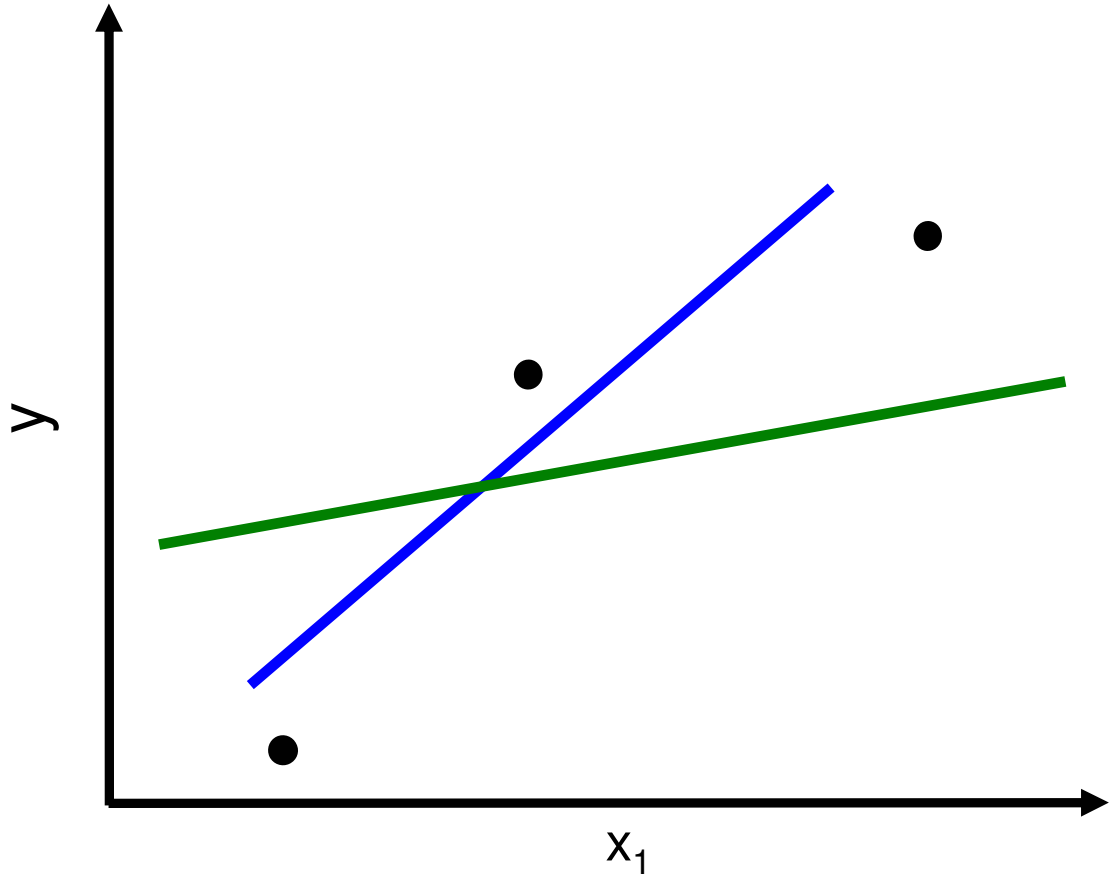


Linear Regression

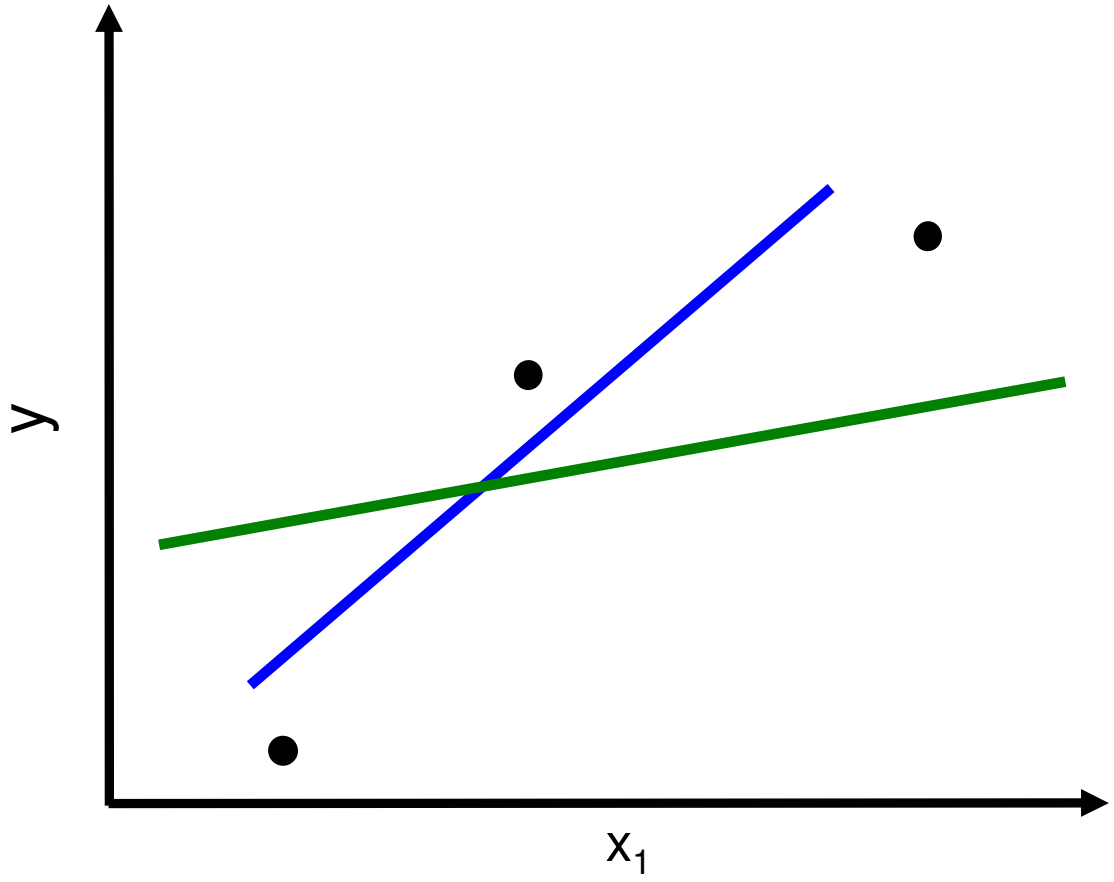
A model that's "less sensitive"



Linear Regression

A model that's "less sensitive"

Smaller |dy/dx| means less sensitive

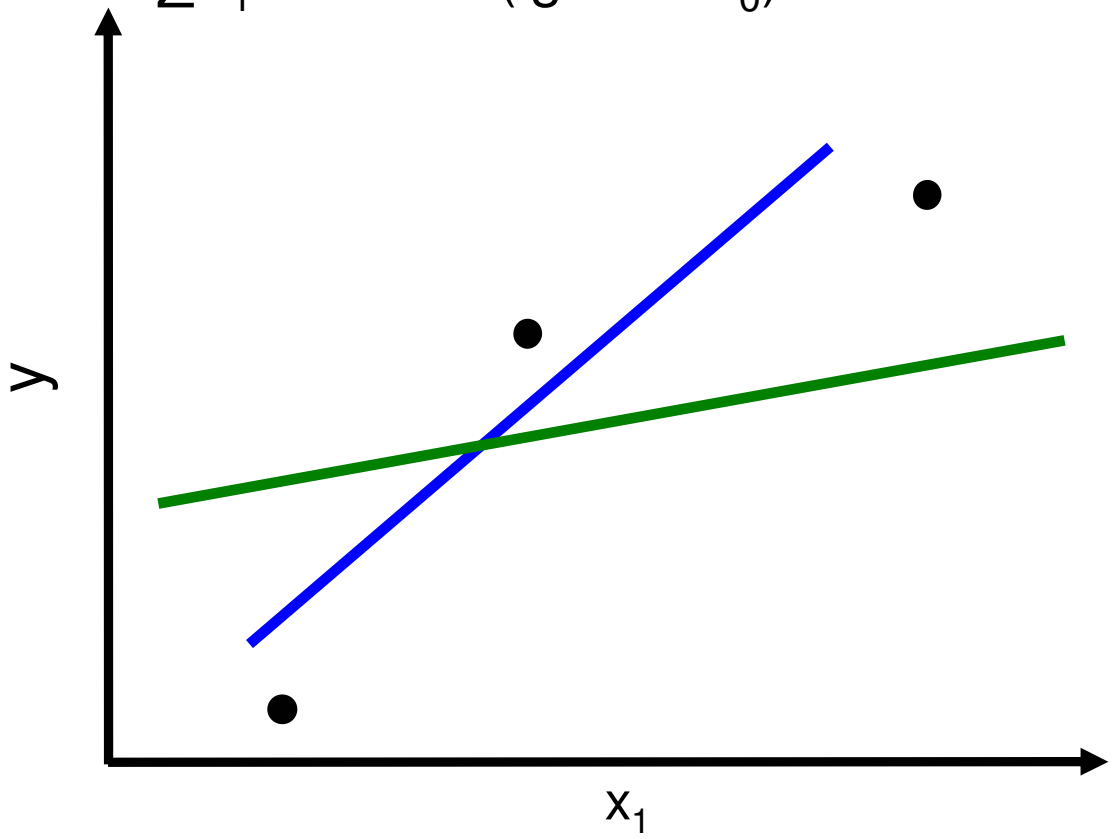


Linear Regression

A model that's "less sensitive"

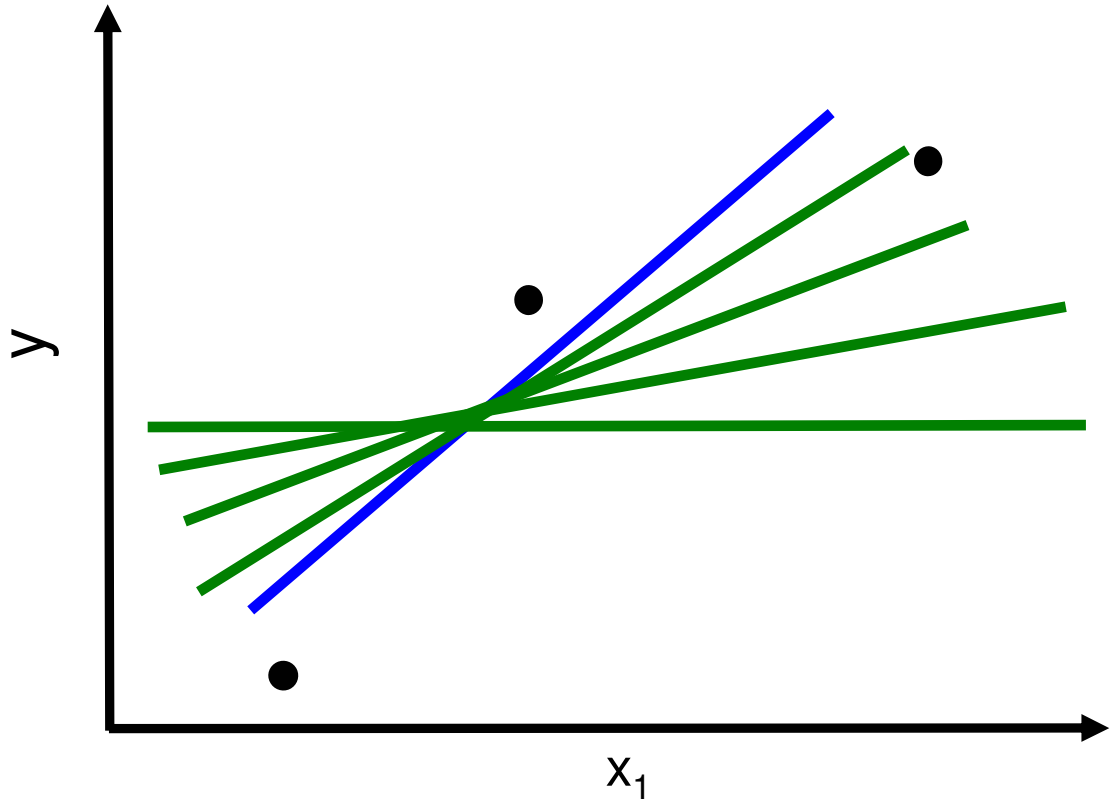
Smaller |dy/dx| means less sensitive

i.e. given $\hat{y}(x_1) = w_0 + w_1 * x_1$
A smaller $|w_1|$ means less sensitive
or smaller $\sum w_i$ for n > 1 (ignore w_0)



Linear Regression

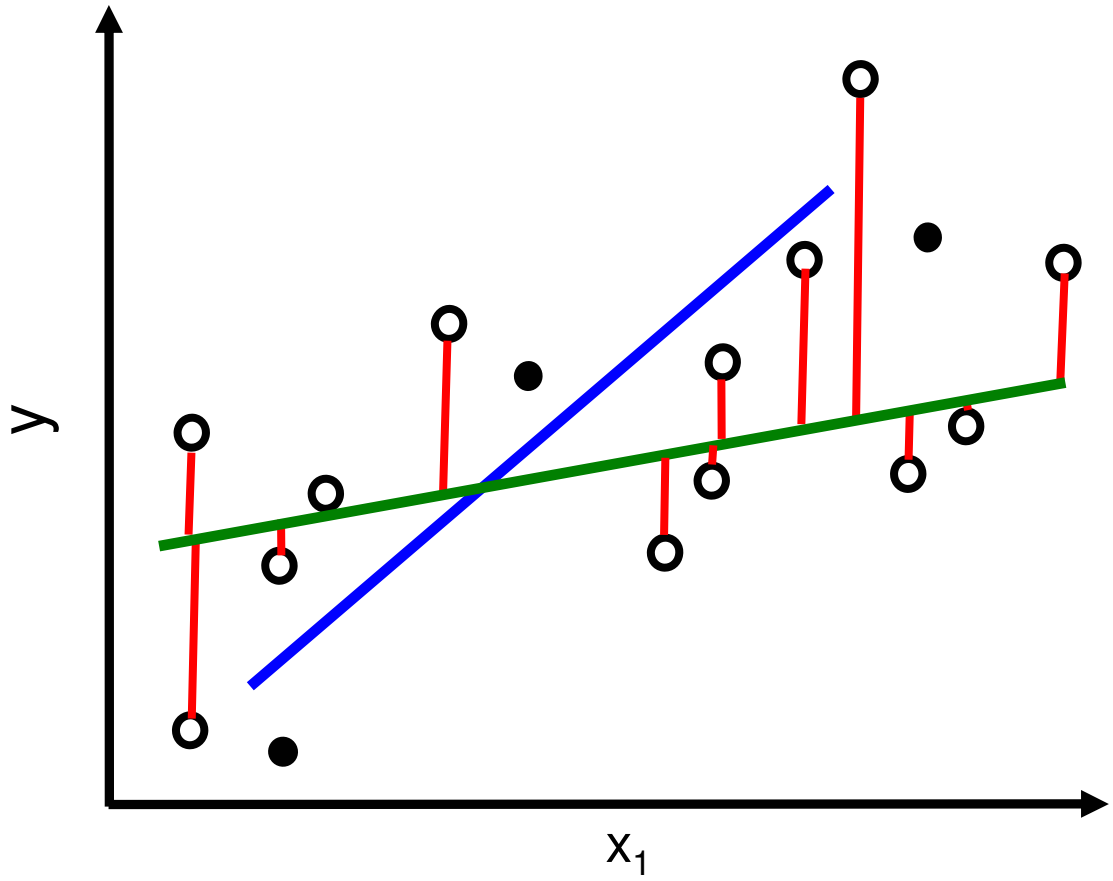
Least-sensitive model has slope of 0
(By definition)
(And also when viewed pragmatically as a model)



Linear Regression

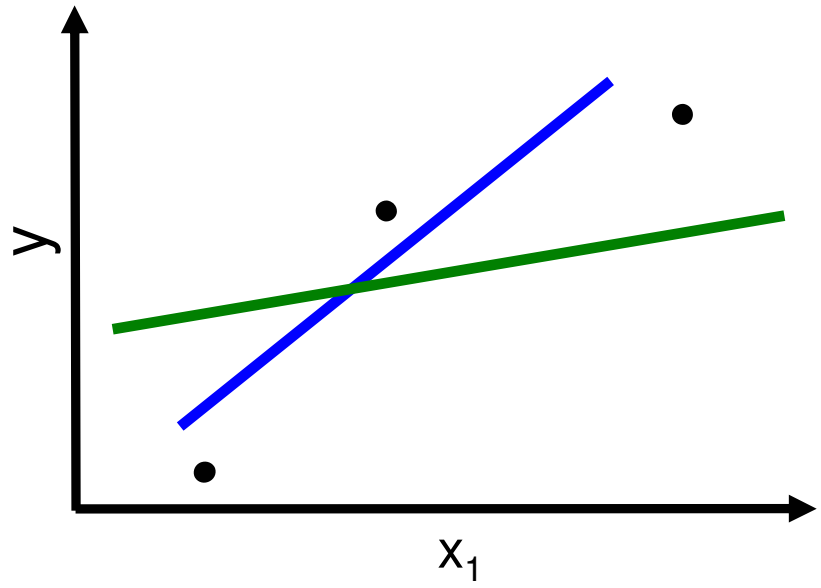
A model that's "less sensitive"

"less sensitive" ≈ lower future prediction error
(in light of less training data)



Linear Regression

- Aim: minimize *future* prediction error
- Pragmatic Issue: we only have access to training data!
- Trick: minimize sensitivity ≈ minimize future prediction error
- But *do* consider training data to bias the model (otherwise we end up with a constant – useless!)
- So: **minimize a combination of training error vs. sensitivity** (bias vs. variance tradeoff) (explanation-of-data vs. overfitting)

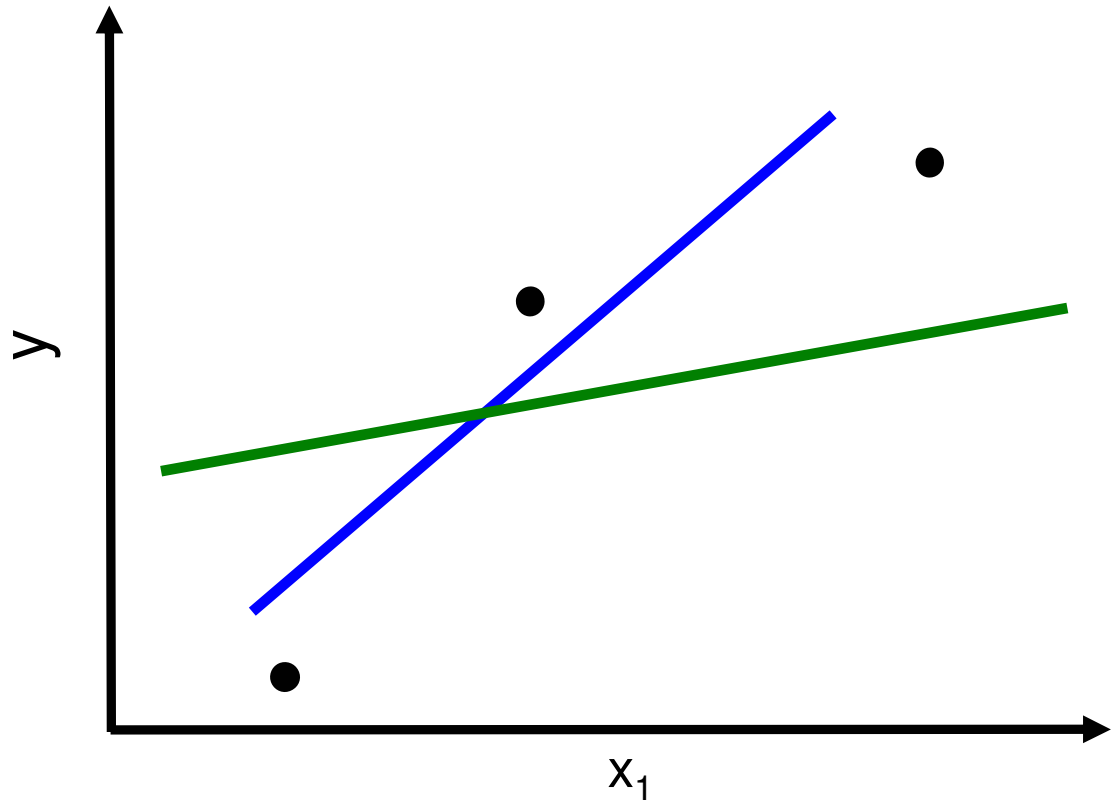


Linear Regression

- Minimize a combination of training error and model sensitivity
- Formulation:

$$\mathbf{w}^* = \text{argmin} \left(\sum(\hat{y}_i(\mathbf{w}) - y_i)^2 + \lambda * \sum|w_i| \right)$$

training error **model sensitivity**



Linear Regression

- Minimize a combination of training error and sensitivity

- Formulation:

$$\mathbf{w}^* = \text{argmin} \left(\sum(\text{yhat}_i(\mathbf{w}) - y_i)^2 + \lambda * \sum|w_i| \right)$$

[Lasso]

OR

$$\mathbf{w}^* = \text{argmin} \left(\sum(\text{yhat}_i(\mathbf{w}) - y_i)^2 + \lambda * \sum w_i^2 \right)$$

[Ridge Regression]

… [Elastic Net, Gradient Directed Regularization, …]

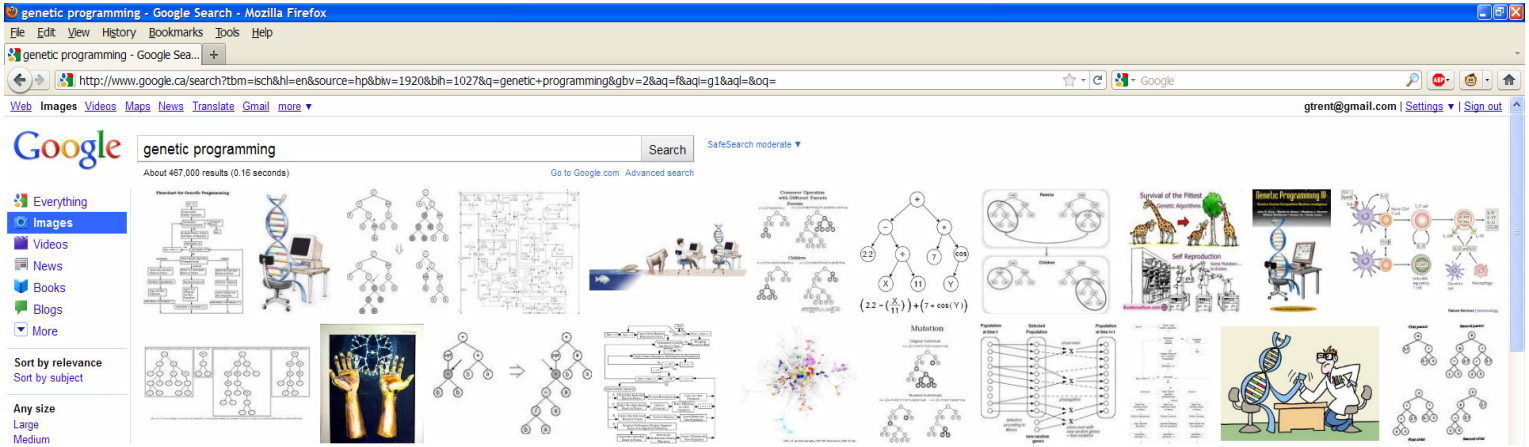
This is regularized linear learning

Regularized Linear Regression

- **Cool property #1:** solving a regularized learning problem is just as fast (or faster) than solving a least-squares learning problem!
    - Why: convex optimization problem – one big hill

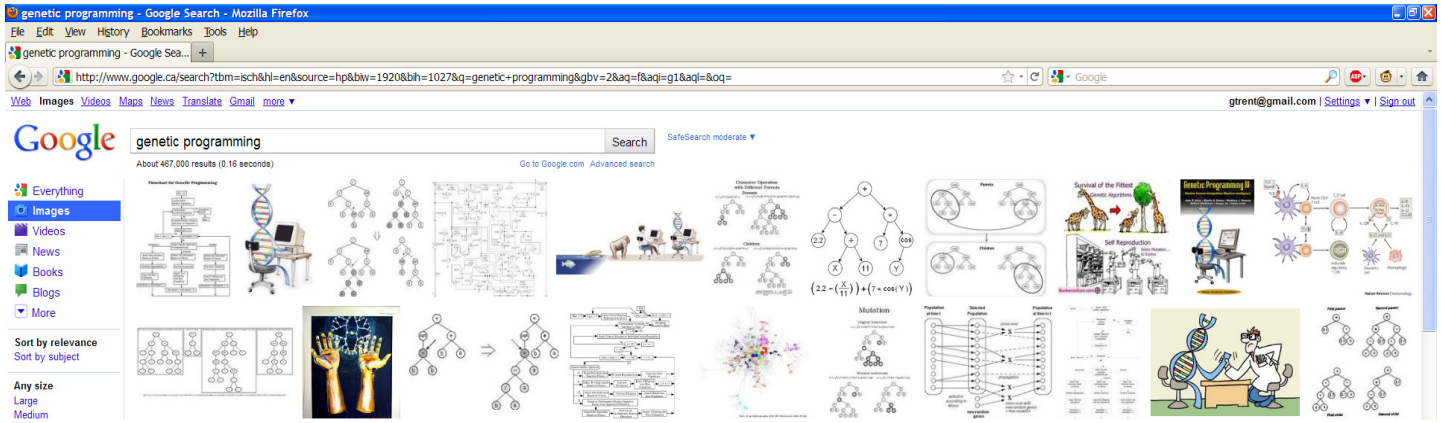
Regularized Linear Regression

- Remember BHALR image search problem?
  - n = 1M variables, N=1000 samples



Regularized Linear Regression

- Remember BHALR image search problem?
  - *n* = 1M variables, *N*=1000 samples



- **Cool property #2:** can have more coefficients than samples! That is, can handle *n* >> *N*!
  - Because the regularization term minimizes the sensitivity, i.e. the "degree of screwup"

$$\mathbf{w}^* = \text{argmin} \left(\sum(\text{yhat}_i(\mathbf{w}) - y_i)^2 + \lambda * \sum|w_i| \right)$$

Regularized Linear Regression

When solving $\mathbf{w}^* = \text{argmin}\ (\ \sum(\hat{y}_i(\mathbf{w}) - y_i)^2 + \lambda * \sum|w_i|)$,
What is a good value for λ?

- **Case: λ=0** $\sum(\hat{y}_i(\mathbf{w}) - y_i)^2 + \lambda * \sum|w_i|$ → **0**

…reduces to least-squares

Regularized Linear Regression

When solving $\mathbf{w}^* = \text{argmin}\ (\ \sum(\hat{y}_i(\mathbf{w}) - y_i)^2 + \lambda * \sum|w_i|)$,
What is a good value for λ?

- **Case: λ=0** $\sum(\hat{y}_i(\mathbf{w}) - y_i)^2 + \lambda * \sum|w_i|$ → 0

…reduces to least-squares

- **Case: λ=∞** $\sum(\hat{y}_i(\mathbf{w}) - y_i)^2 + \lambda * \sum|w_i|$ → 0

…gives a constant (w_0=const; w_1=w_2=… = 0)

Regularized Linear Regression

When solving $\mathbf{w}^* = \text{argmin}\ (\ \sum(\hat{y}_i(\mathbf{w}) - y_i)^2 + \lambda * \sum|w_i|)$,
What is a good value for λ?

- **Case: λ=0** $\sum(\hat{y}_i(\mathbf{w}) - y_i)^2 + \lambda * \sum|w_i|$ → 0

…reduces to least-squares

- **Case: λ=∞** $\sum(\hat{y}_i(\mathbf{w}) - y_i)^2 + \lambda * \sum|w_i|$ → 0

…gives a constant (w_0=const; w_1=w_2=… = 0)

- **Case: λ in-between**

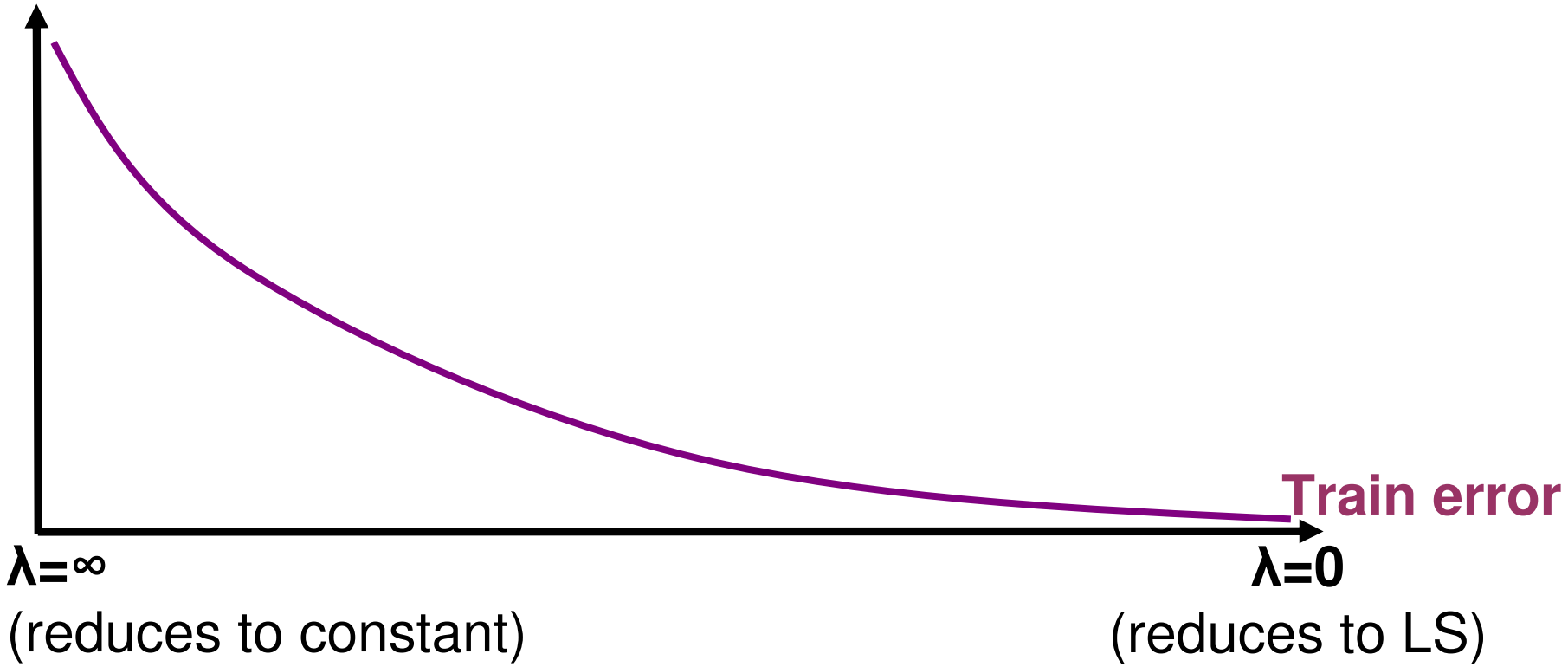
…is a balance between constant & LS.

Regularized Linear Regression

When solving $\mathbf{w}^* = \text{argmin}\ (\ \sum(\text{yhat}_i(\mathbf{w}) - y_i)^2 + \lambda * \sum|w_i|)$,

~~**What is a good value for λ?**~~

Learn w* at *many* values of λ



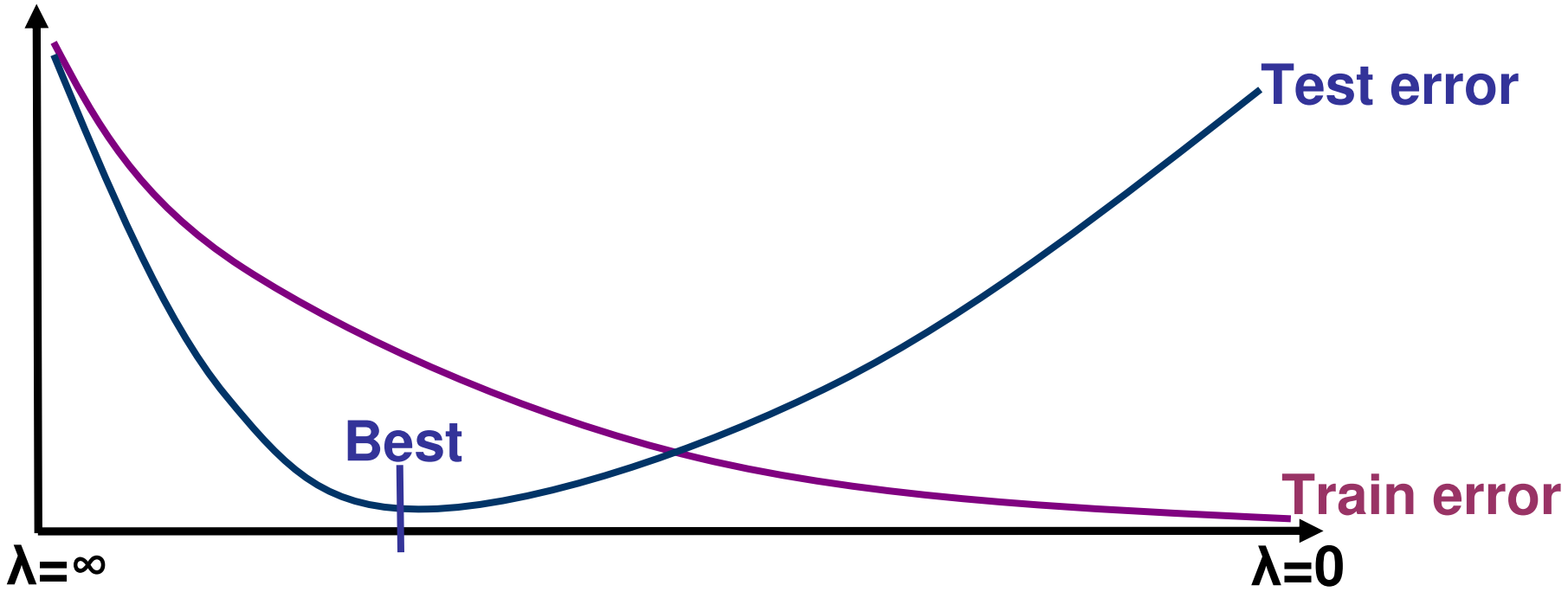
Regularized Linear Regression

When solving $\mathbf{w}^* = \text{argmin}\ (\ \sum(\text{yhat}_i(\mathbf{w}) - y_i)^2 + \lambda * \sum|w_i|)$,

~~**What is a good value for λ?**~~

Learn w* at *many* values of λ, and keep "best"

("Best" = best error on a left-out test set.)



(reduces to constant)

(reduces to LS)

Regularized Linear Regression

Algorithm

λ= huge (e.g. 1e40)

w = **0**

while λ > 1e-10

    λ = λ / 10

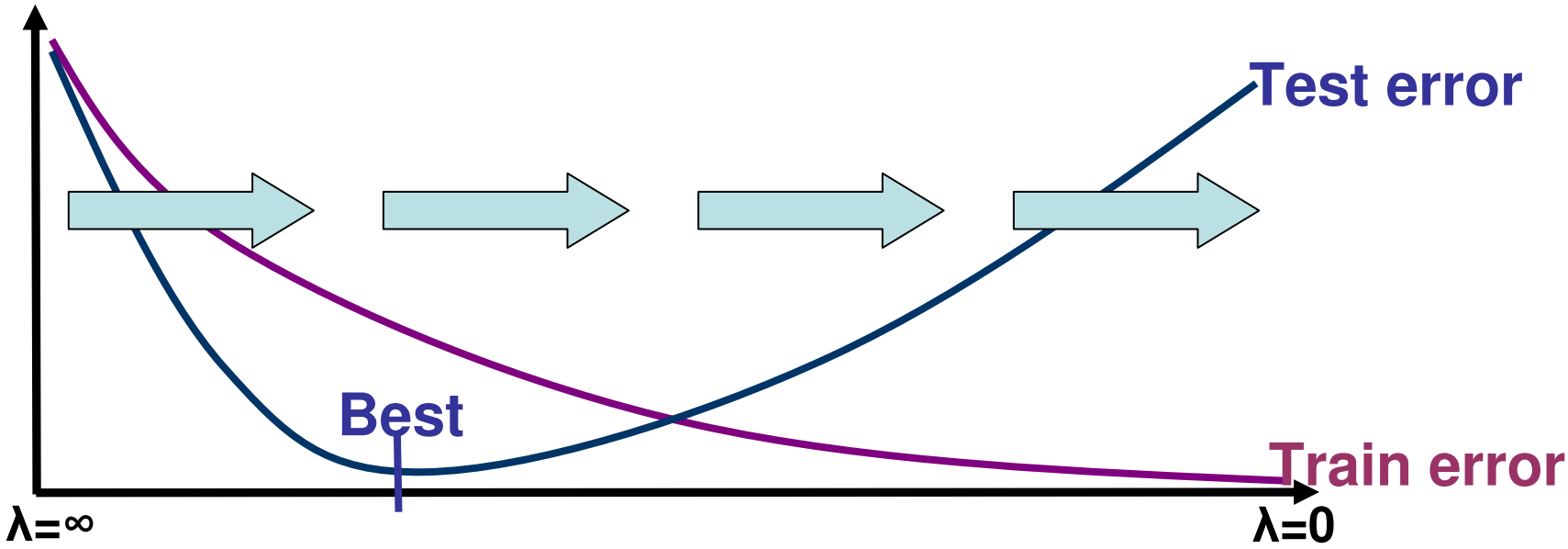
    w = solveAt($\mathbf{X}_{\mathbf{train}}$, $\mathbf{y}_{\mathbf{train}}$, λ, $\mathbf{w}_{\mathbf{init}}$=**w**)

    Compute error on test set

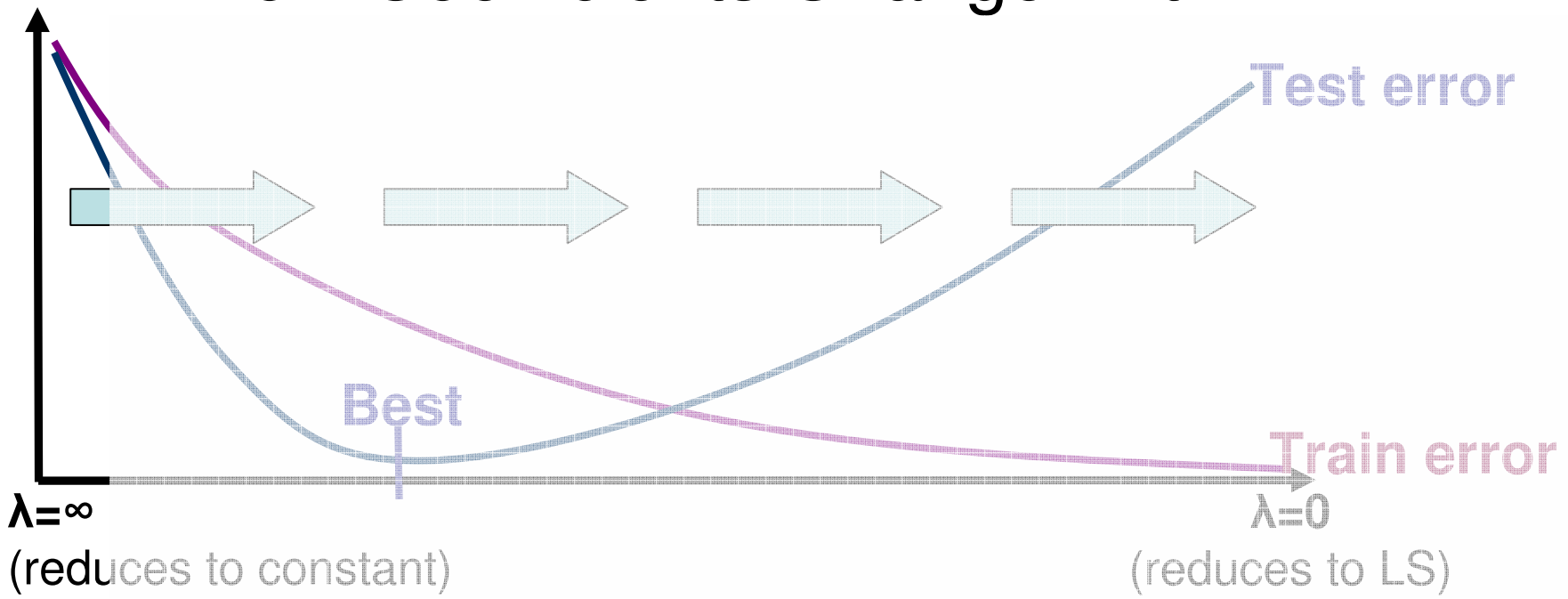
Return **w** with best test error

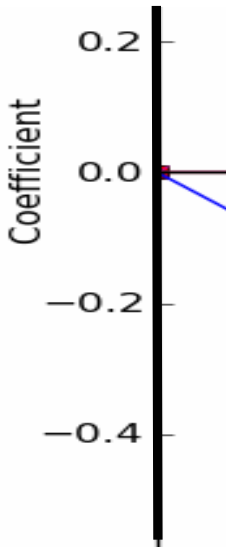
Solves

$\mathbf{w}^* = \text{argmin} \left(\sum(\text{yhat}_i(\mathbf{w}) - y_i)^2 + \lambda * \sum|w_i| \right)$



Regularized Linear Regression: How Coefficients Change With λ

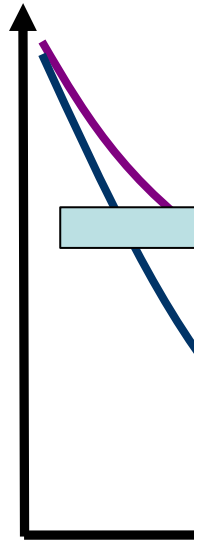




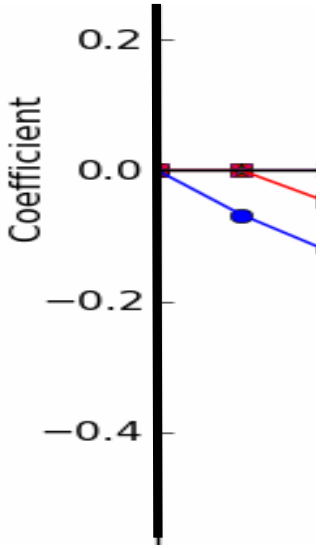
w_3 "pops in"

(All other w_i=0)

Regularized Linear Regression: How Coefficients Change With λ

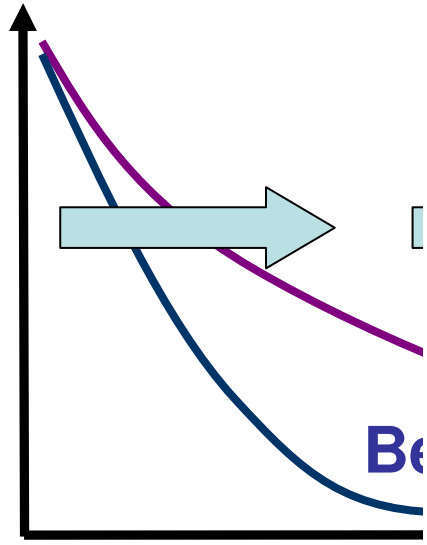


λ=∞
(reduces



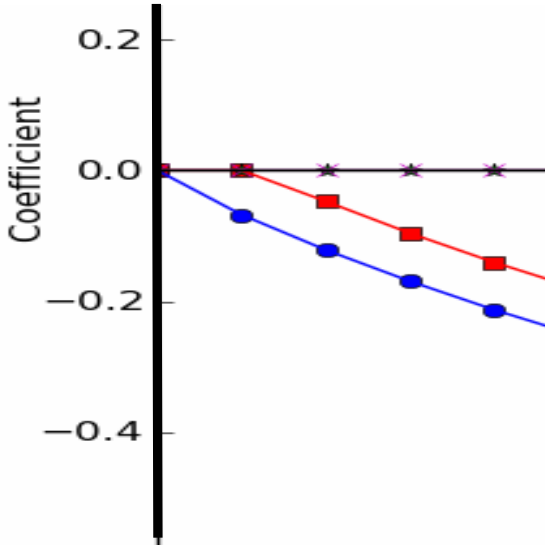
w_6 “pops in”

Regularized Linear Regression: How Coefficients Change With λ

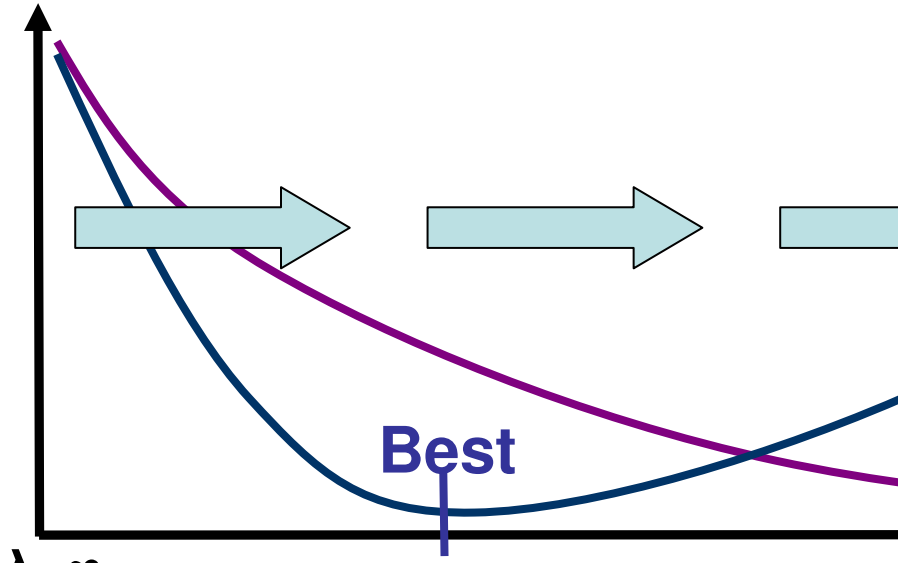


λ=∞

(reduces to consta

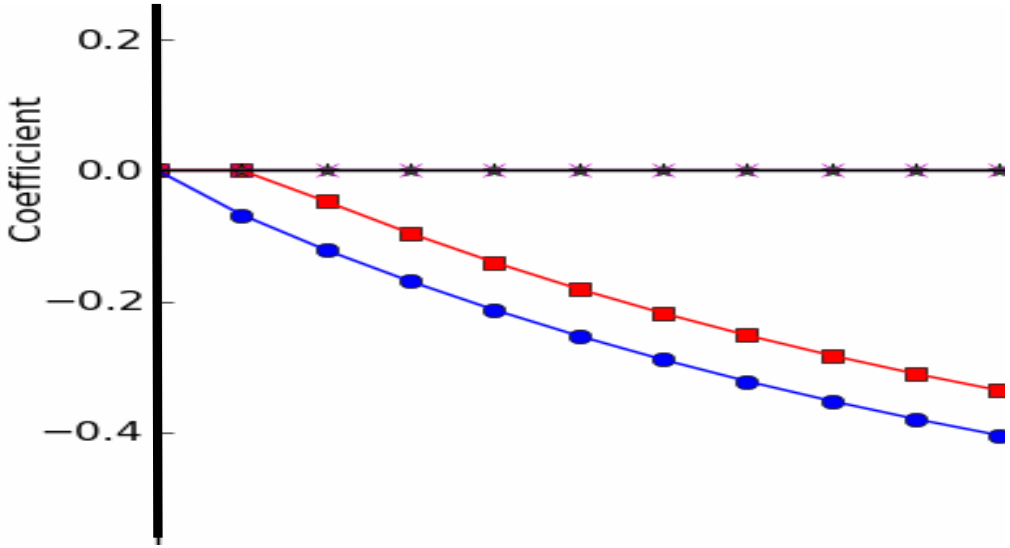


Regularized Linear Regression: How Coefficients Change With λ

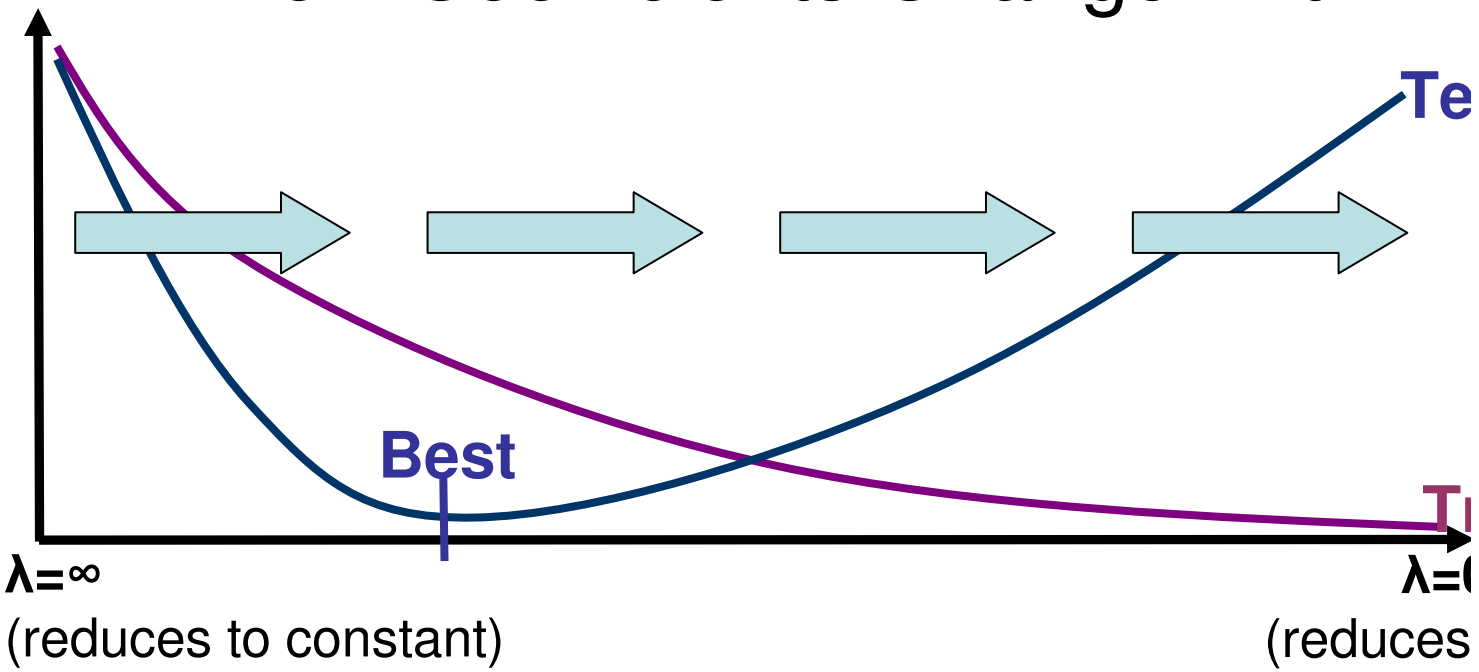


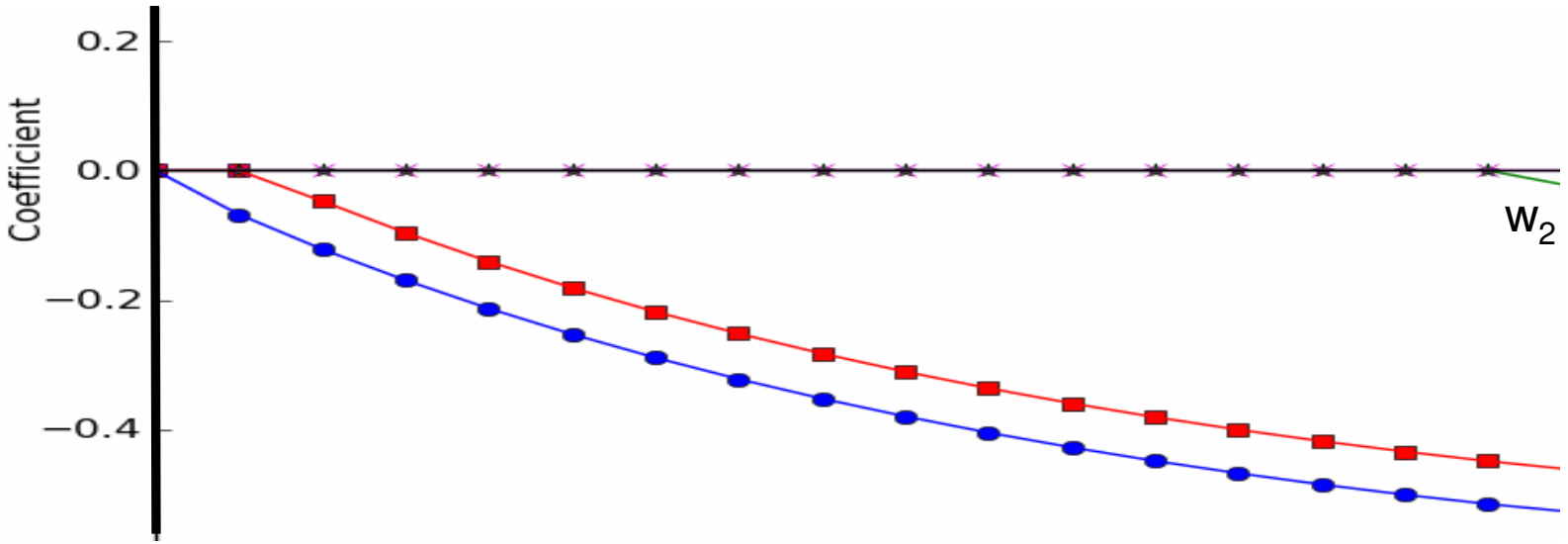
λ=∞

(reduces to constant)



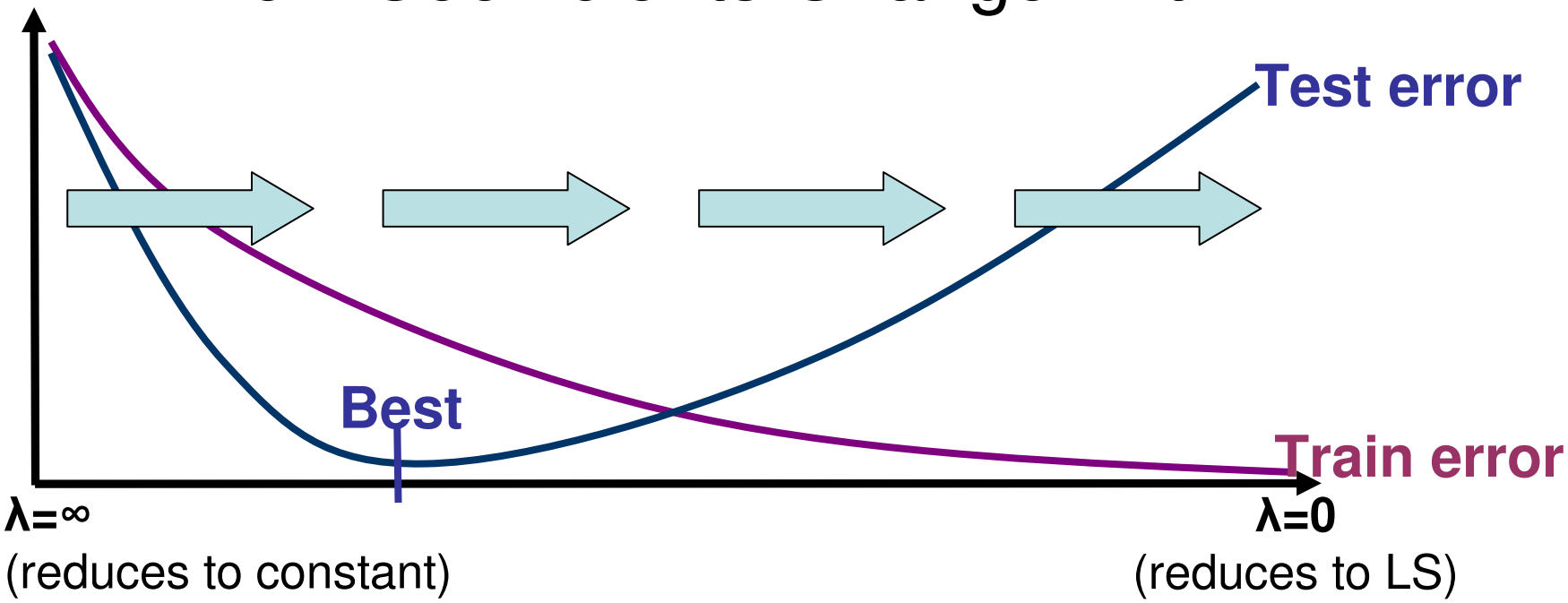
Regularized Linear Regression: How Coefficients Change With λ

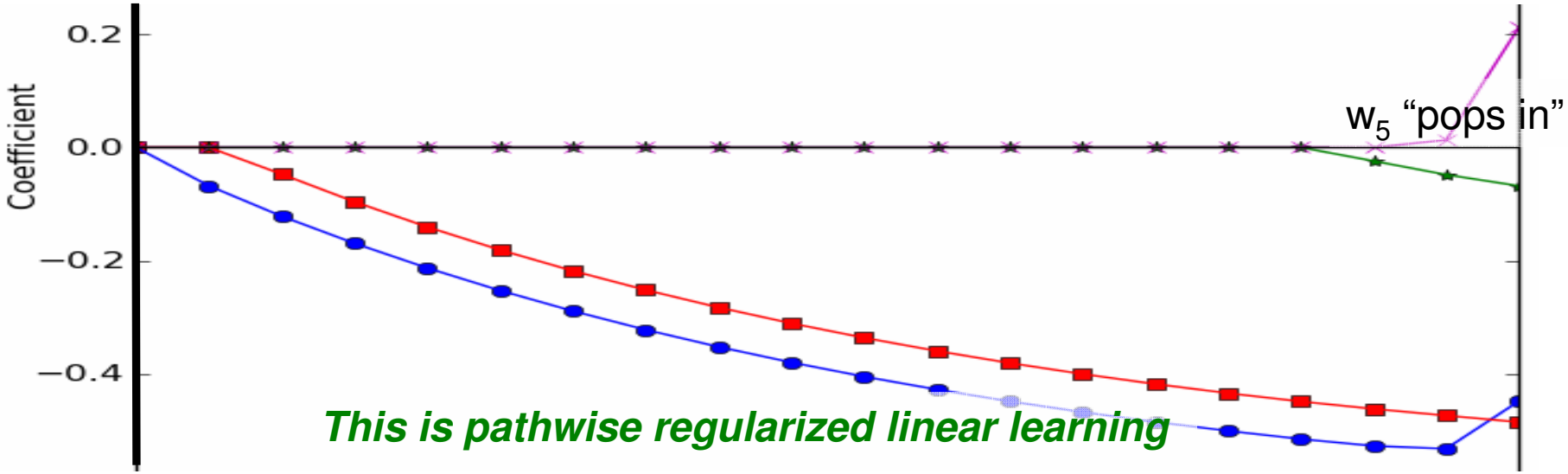




w_2 “pops in”

Regularized Linear Regression: How Coefficients Change With λ





Regularized Linear Regression

• **Cool property #3:** solving a full regularized path is ≈ as fast as solving single regularized problem
(or a least-squares learning problem)

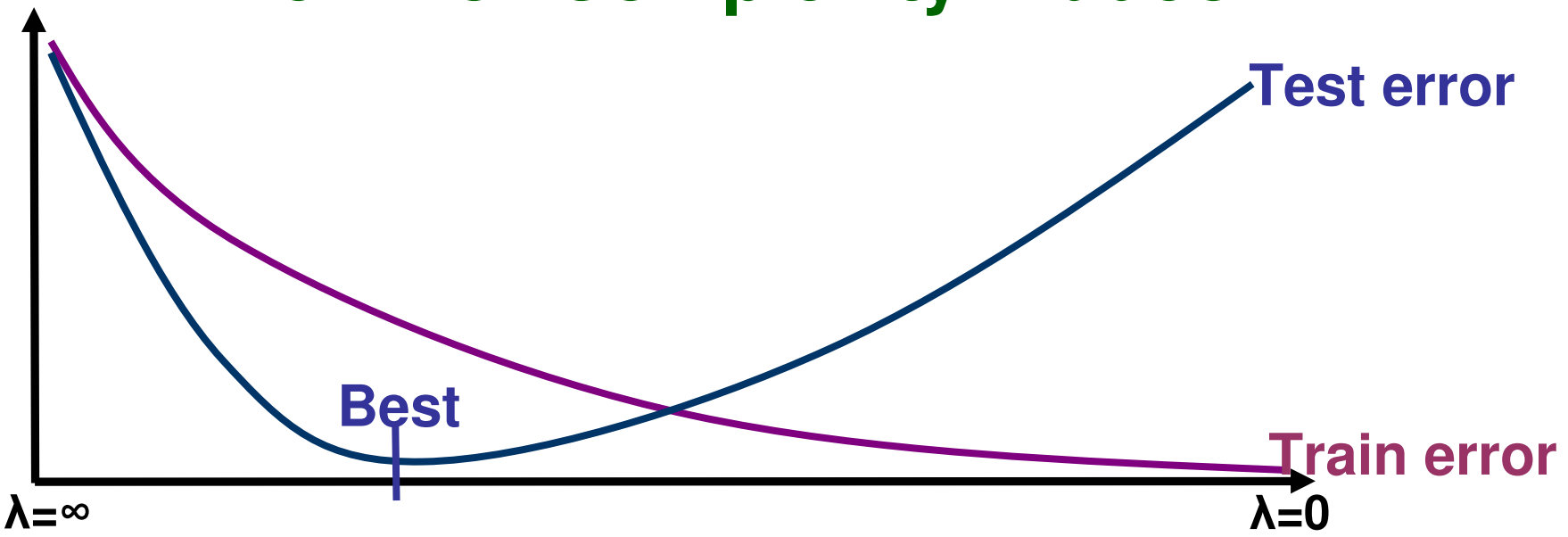
Why fast:

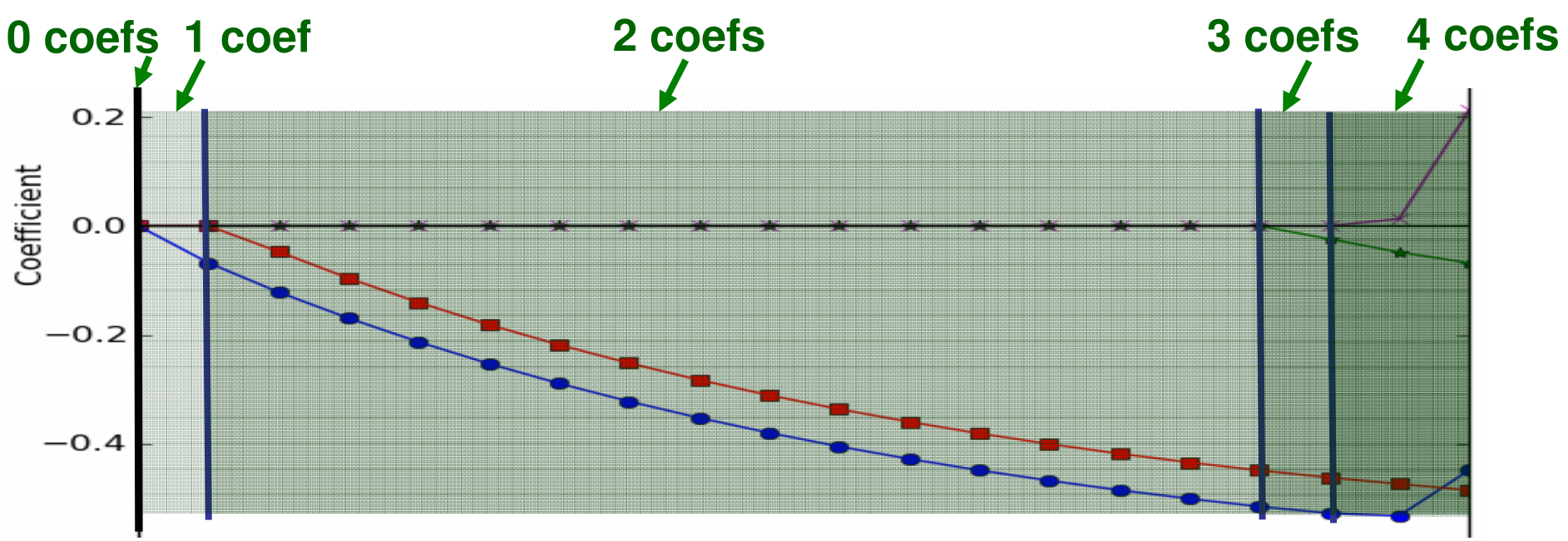
Hot starts on local optimize

Algorithm

λ= huge (e.g. 1e40)
w = **0**
while λ > 1e-10
    λ = λ / 10
    w = solveAt($\mathbf{X}_{\text{train}}$, $\mathbf{y}_{\text{train}}$, λ, $\mathbf{w}_{\text{init}}$=**w**)
    Compute error on test set
Return **w** with best test error

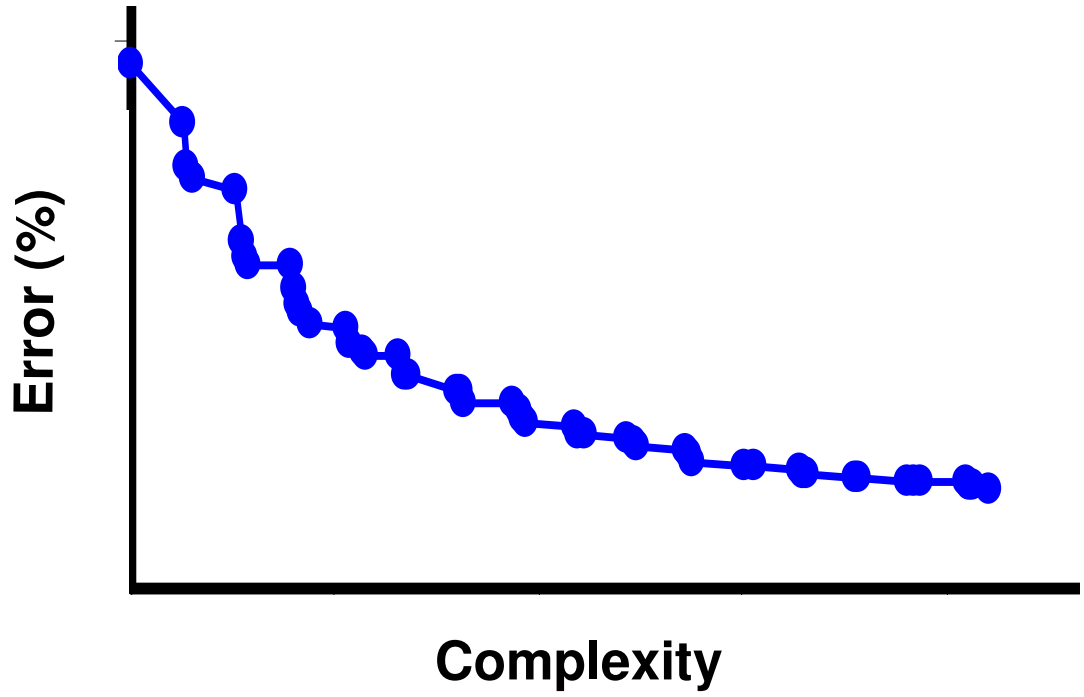
Regularized Linear Regression:
The Error-Complexity Tradeoff





Regularized Linear Regression

- **Cool property #4:** solving a full regularized path gives us error-complexity tradeoffs!
  - train error versus # coefs (bases)
  - test error versus # coefs (bases)



Recap on Linear Regression

• Generalized linear models: **nonlinear basis functions** with linearly-learned coefficients!

Path-based Regularized Linear Regression:
• Can have more coefficients than samples! That is, can handle ***n >> N***!
    • **BHALR**: 1M basis functions for 1K samples
• Solving path is ≈ as **fast** as solving a least-squares learning problem! (Convex problem!)
• Solving path gives **error vs. complexity tradeoffs**!

One final trick:
• Can cast a **rational-learning** problem f(x)/(1+g(x)) as a linear-learning problem. See paper for details.

Outline

- Introduction
- Background
- FFX: Fast Function Extraction
- Results
- Scaling Higher?
- Discussion

FFX Step 1/3: GenerateBases()

Inputs: X #input training data
Outputs: B #list of bases

```
# Generate univariate bases
1.  B1 = {}
2.  for each input variable v = {x1, x2, ...}
3.      for each exponent exp = {0.5, 1.0, 2.0}
4.          let expression b_exp = v^exp
5.          if ok(eval(b_exp, X))
6.              add b_exp to B1
7.              for each operator op = {abs(), log10, ...}
8.                  let expression b_op = op(b_exp)
9.                  if ok(eval(b_op, X))
10.                     add b_op to B1

# Generate interacting-variable bases
11. B2 = {}
12. for i = 1 to length(B1)
13.     let expression b_i = B1[i]
14.     for j = 1 to i - 1
15.         let expression b_j = B1[j]
16.         if b_j is not an operator # disallow op() * op()
17.             let expression b_inter = b_i * b_j
18.             if ok(eval(b_inter, X))
19.                 add b_inter to B2
20. return B = B1 ∪ B2
```

"Replace linear bases with a crazy amount of nonlinear ones"

FFX Step 2/3: PathFollow() [using BHALR]

Inputs: X, y, B #input data, output data, bases
Outputs: A #list of coefficent-vectors

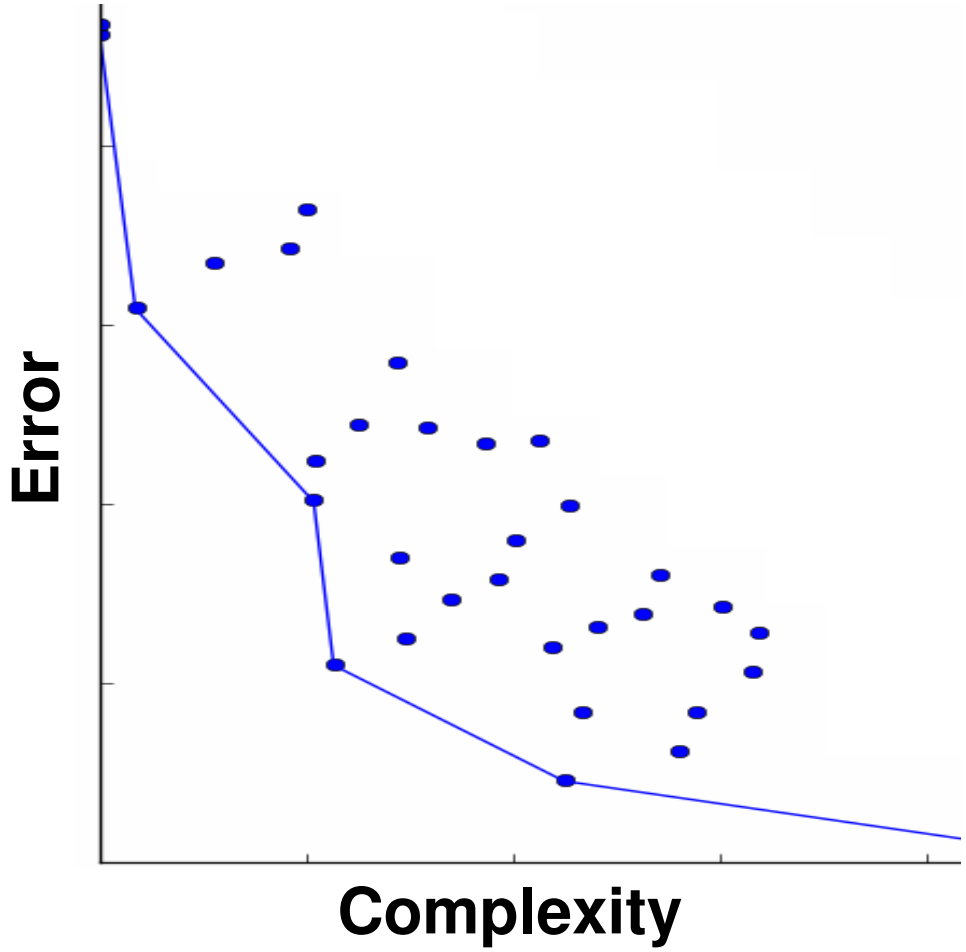
Compute X_B
1. for i = 1 to length(B)
2. $X_B[i]$ = eval($B[i]$, X)

Generate λ_{vec} = range of λ values
3. $\lambda_{max} = max(|X^T y|)/(N * \rho)$
4. $\lambda_{vec} = logspace(log_{10}(\lambda_{max} * eps), log_{10}(\lambda_{max}), N_\lambda)$

Main path-following
5. $A = \{\}$
6. $N_{bases} = 0$
7. $i = 0$
8. $a = \{0, 0, \ldots\}$
9. while $N_{bases} < N_{max-bases}$ and $i <$ length(λ_{vec})
10. $\lambda = \lambda_{vec}[i]$
11. a = elasticNetLinearFit(X_B, y, λ, ρ, a)
12. N_{bases} = number of nonzero values in a (not counting offset)
13. if $N_{bases} < N_{max-bases}$
14. add a to A
15. $i = i + 1$
16. return A

"Generate set of models, at increasing complexity"

FFX Step 3/3: NondominatedFilter()



Outline

- Introduction
- Background
- FFX: Fast Function Extraction
- Results
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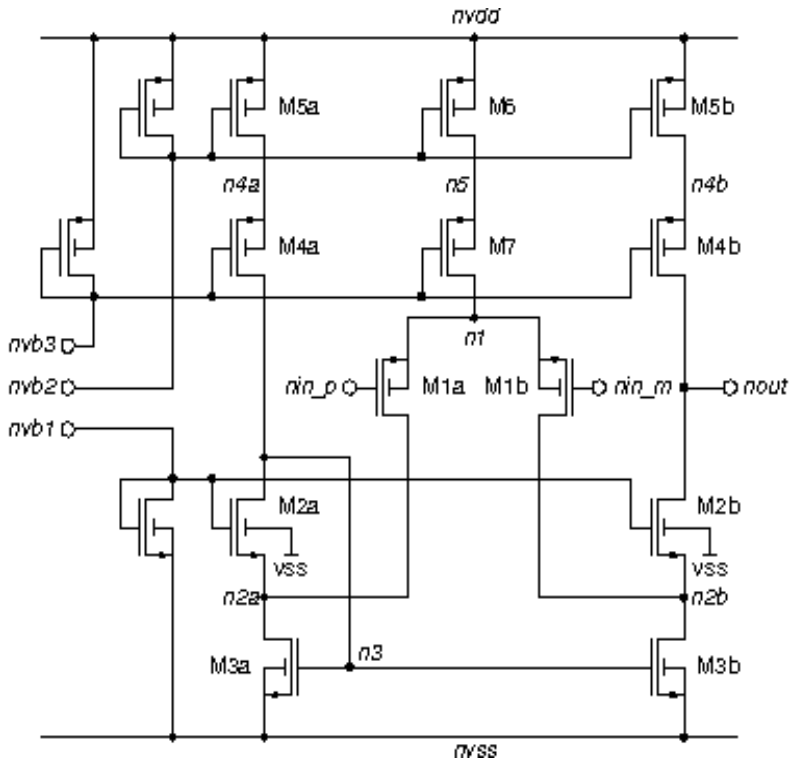
FFX Experiments

- **High Speed CMOS OTA**
- **13 design variables**
  - **Vds, Vgs, Ids (operating-point driven formulation)**
- **orthogonal hypercube sampling**
- **243 training samples**
- **243 testing samples**



FFX Setup

Up to $N_{max-bases}$=5 bases are allowed. Operators allowed are: $abs(x)$, $log_{10}(x)$, $min(0, x)$, $max(0, x)$; and exponents on variables are $x^{1/2}$ (=$\sqrt{(x)}$), x^1 (=x), and x^2. By default, denominators are allowed; but if turned off, then negative exponents are also allowed: $x^{-1/2}$ (=$1/\sqrt{(x)}$), x^{-1} (=$1/x$), and x^{-2} (=$1/x^2$). The elastic net settings followed good defaults: ρ = 0.5, eps = 1e-40, and N_{lambda} = 1000.

Because the algorithm is not GP, there are no settings for population size, number of generations, mutation/crossover rate, selection, etc. We emphasize that the settings in the previous paragraph are very simple, with no tuning needed by users.

FFX Step 1: The 176 Candidate 1-Variable Bases

$v_{sg1}^{0.5},\ abs(v_{sg1}^{0.5}),\ max(0, v_{sg1}^{0.5}),\ min(0, v_{sg1}^{0.5}),\ log_{10}(v_{sg1}^{0.5}),\ v_{sg1},\ abs(v_{sg1}),\ max(0, v_{sg1}),\ min(0, v_{sg1}),$
$log_{10}(v_{sg1}),\ v_{sg1}^{2},\ max(0, v_{sg1}^{2}),\ min(0, v_{sg1}^{2}),\ log_{10}(v_{sg1}^{2}),\ v_{gs2}^{0.5},\ abs(v_{gs2}^{0.5}),\ max(0, v_{gs2}^{0.5}),\ min(0, v_{gs2}^{0.5}),$
$log_{10}(v_{gs2}^{0.5}),\ v_{gs2},\ abs(v_{gs2}),\ max(0, v_{gs2}),\ min(0, v_{gs2}),\ log_{10}(v_{gs2}),\ v_{gs2}^{2},\ max(0, v_{gs2}^{2}),\ min(0, v_{gs2}^{2}),$
$log_{10}(v_{gs2}^{2}),\ v_{ds2}^{0.5},\ abs(v_{ds2}^{0.5}),\ max(0, v_{ds2}^{0.5}),\ min(0, v_{ds2}^{0.5}),\ log_{10}(v_{ds2}^{0.5}),\ v_{ds2},\ abs(v_{ds2}),\ max(0, v_{ds2}),$
$min(0, v_{ds2}),\ log_{10}(v_{ds2}),\ v_{ds2}^{2},\ max(0, v_{ds2}^{2}),\ min(0, v_{ds2}^{2}),\ log_{10}(v_{ds2}^{2}),\ v_{sg3}^{0.5},\ abs(v_{sg3}^{0.5}),\ max(0, v_{sg3}^{0.5}),$
$min(0, v_{sg3}^{0.5}),\ log_{10}(v_{sg3}^{0.5}),\ v_{sg3},\ abs(v_{sg3}),\ max(0, v_{sg3}),\ min(0, v_{sg3}),\ log_{10}(v_{sg3}),\ v_{sg3}^{2},\ max(0, v_{sg3}^{2}),$
$min(0, v_{sg3}^{2}),\ log_{10}(v_{sg3}^{2}),\ v_{sg4}^{0.5},\ abs(v_{sg4}^{0.5}),\ max(0, v_{sg4}^{0.5}),\ min(0, v_{sg4}^{0.5}),\ log_{10}(v_{sg4}^{0.5}),\ v_{sg4},\ abs(v_{sg4}),$
$max(0, v_{sg4}),\ min(0, v_{sg4}),\ log_{10}(v_{sg4}),\ v_{sg4}^{2},\ max(0, v_{sg4}^{2}),\ min(0, v_{sg4}^{2}),\ log_{10}(v_{sg4}^{2}),\ v_{sg5}^{0.5},\ abs(v_{sg5}^{0.5}),$
$max(0, v_{sg5}^{0.5}),\ min(0, v_{sg5}^{0.5}),\ log_{10}(v_{sg5}^{0.5}),\ v_{sg5},\ abs(v_{sg5}),\ max(0, v_{sg5}),\ min(0, v_{sg5}),\ log_{10}(v_{sg5}),\ v_{sg5}^{2},$
$max(0, v_{sg5}^{2}),\ min(0, v_{sg5}^{2}),\ log_{10}(v_{sg5}^{2}),\ v_{sd5}^{0.5},\ abs(v_{sd5}^{0.5}),\ max(0, v_{sd5}^{0.5}),\ min(0, v_{sd5}^{0.5}),\ log_{10}(v_{sd5}^{0.5}),\ v_{sd5},$
$abs(v_{sd5}),\ max(0, v_{sd5}),\ min(0, v_{sd5}),\ log_{10}(v_{sd5}),\ v_{sd5}^{2},\ max(0, v_{sd5}^{2}),\ min(0, v_{sd5}^{2}),\ log_{10}(v_{sd5}^{2}),$
$v_{sd6}^{0.5},\ abs(v_{sd6}^{0.5}),\ max(0, v_{sd6}^{0.5}),\ min(0, v_{sd6}^{0.5}),\ log_{10}(v_{sd6}^{0.5}),\ v_{sd6},\ abs(v_{sd6}),\ max(0, v_{sd6}),\ min(0, v_{sd6}),$
$log_{10}(v_{sd6}),\ v_{sd6}^{2},\ max(0, v_{sd6}^{2}),\ min(0, v_{sd6}^{2}),\ log_{10}(v_{sd6}^{2}),\ i_{d1},\ abs(i_{d1}),\ max(0, i_{d1}),\ min(0, i_{d1}),\ i_{d1}^{2},$
$max(0, i_{d1}^{2}),\ min(0, i_{d1}^{2}),\ log_{10}(i_{d1}^{2}),\ i_{d2}^{0.5},\ abs(i_{d2}^{0.5}),\ max(0, i_{d2}^{0.5}),\ min(0, i_{d2}^{0.5}),\ log_{10}(i_{d2}^{0.5}),\ i_{d2},\ abs(i_{d2}),$
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$min(0, i_{b1}^{0.5}),\ log_{10}(i_{b1}^{0.5}),\ i_{b1},\ abs(i_{b1}),\ max(0, i_{b1}),\ min(0, i_{b1}),\ log_{10}(i_{b1}),\ i_{b1}^{2},\ max(0, i_{b1}^{2}),\ min(0, i_{b1}^{2}),$
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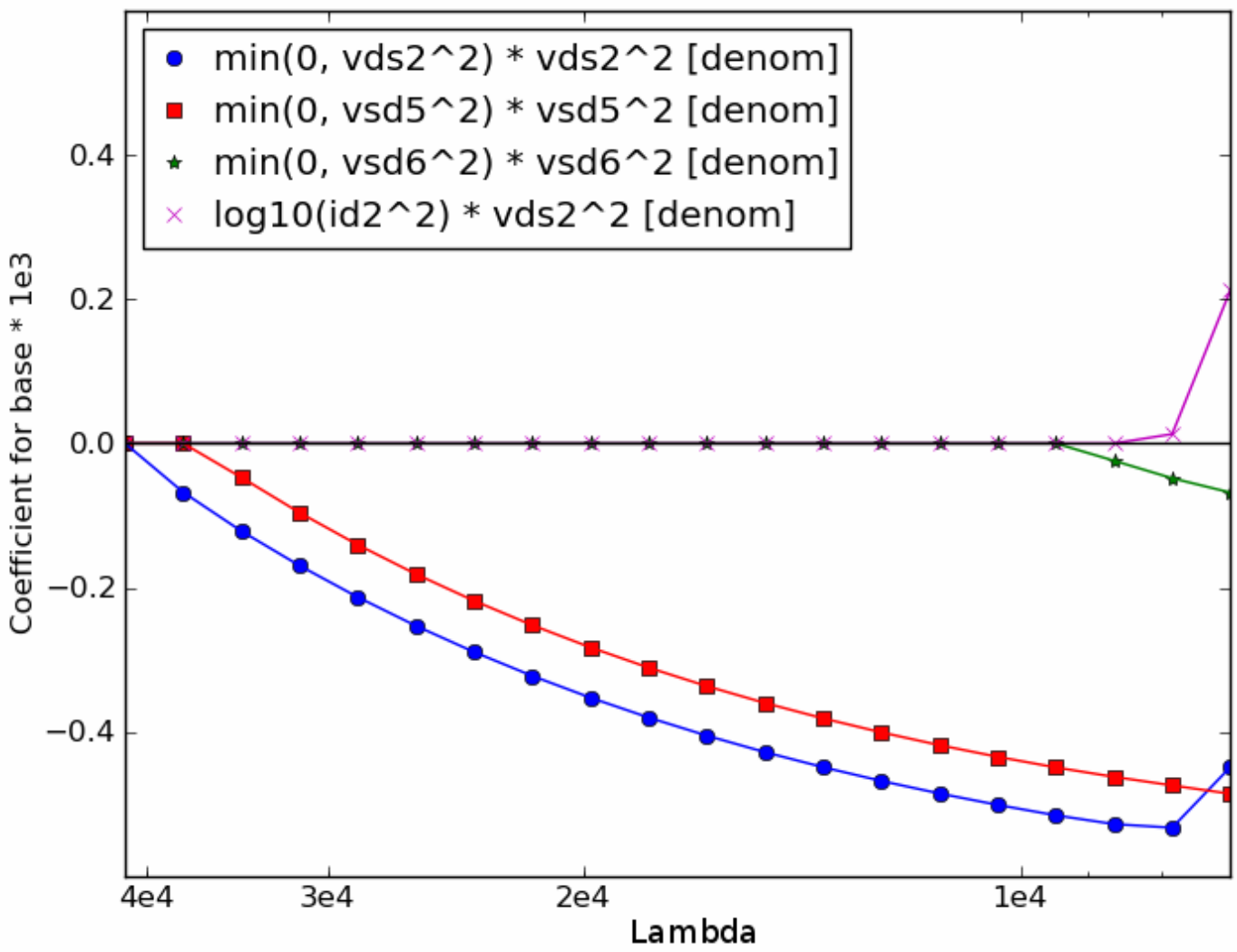
$log_{10}(i_{b2}),\ i_{b2}^{2},\ max(0, i_{b2}^{2}),\ min(0, i_{b2}^{2}),\ log_{10}(i_{b2}^{2}),\ i_{b3}^{0.5},\ abs(i_{b3}^{0.5}),\ max(0, i_{b3}^{0.5}),\ min(0, i_{b3}^{0.5}),\ log_{10}(i_{b3}^{0.5}),$
$i_{b3},\ abs(i_{b3}),\ max(0, i_{b3}),\ min(0, i_{b3}),\ log_{10}(i_{b3}),\ i_{b3}^{2},\ max(0, i_{b3}^{2}),\ min(0, i_{b3}^{2}),\ log_{10}(i_{b3}^{2})$

FFX Step 1: Some Candidate 2-Variable Bases (3374 total)

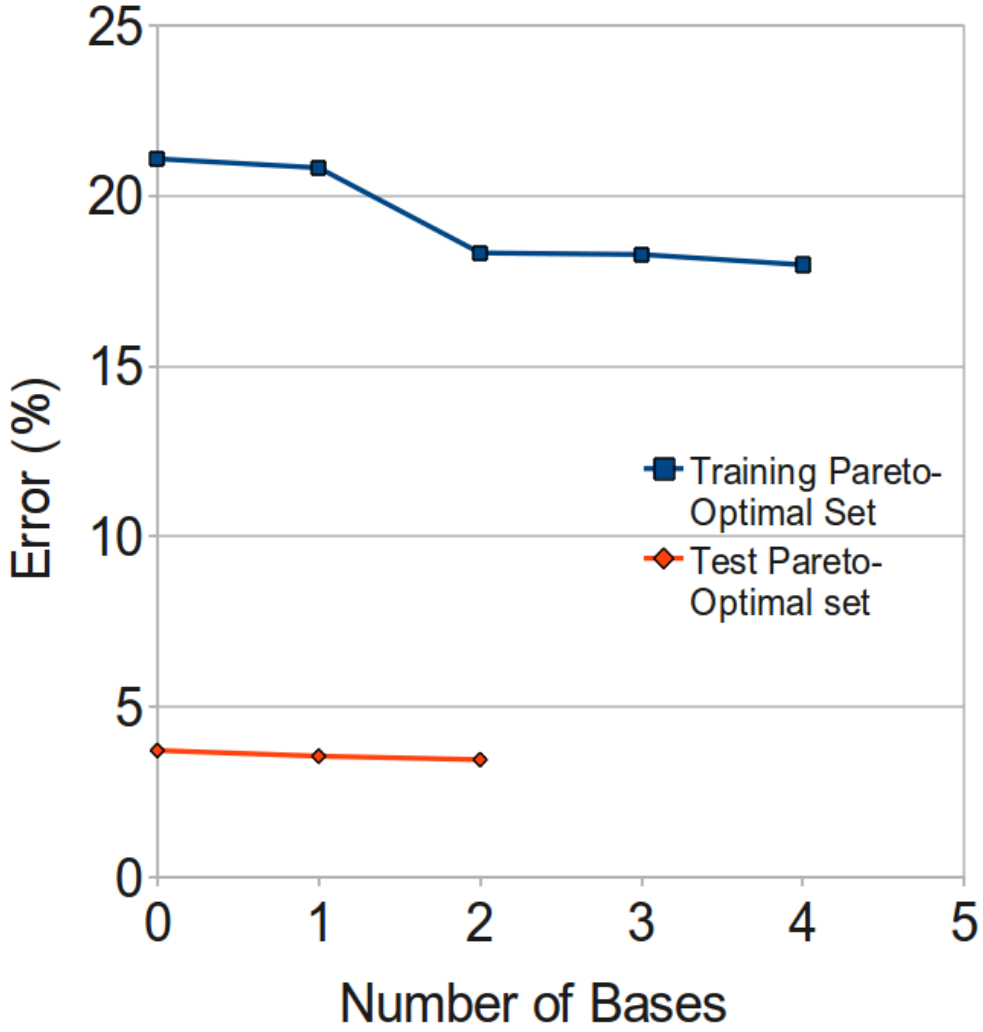
$log_{10}(i_{b3}^2) * i_{d2}^2, log_{10}(i_{b3}^2) * i_{b1}^{0.5}, log_{10}(i_{b3}^2) * i_{b1}, log_{10}(i_{b3}^2) * i_{b1}^2, log_{10}(i_{b3}^2) * i_{b2}^{0.5}, log_{10}(i_{b3}^2) * i_{b2}, log_{10}(i_{b3}^2) * i_{b2}^2, log_{10}(i_{b3}^2) * i_{b3}^{0.5}, log_{10}(i_{b3}^2) * i_{b3}, log_{10}(i_{b3}^2) * i_{b3}^2$

(and 3364 more)

FFX Step 2: PathFollow: First Four Bases (A_{LF} problem)



FFX Step 3: Nondominated Filter Error vs. # Bases (A_{LF} problem)



FFX Step 3: Final Pareto-Optimal Set

Total Runtime <5 s (1 GHz CPU)

This is Fast Function Extraction

Test error (ϵ_{test}) (%)	**Extracted Function**
3.72	37.619
3.55	$\frac{37.379}{1.0-6.78e\text{-}5*min(0,v_{ds2}^2)*v_{ds2}^2}$
3.45	$\frac{37.020}{1.0-1.22e\text{-}4*min(0,v_{ds2}^2)*v_{ds2}^2-4.72e\text{-}5*min(0,v_{sd5}^2)*v_{sd5}^2}$

FFX Functions with Lowest Test Error on 6 Different Problems.

Problem	**Test error** (ϵ_{test}) (%)	**Extracted Function**
A_{LF}	3.45	$\frac{37.020}{1.0-1.22e\text{-}4*min(0,v_{ds2}^2)*v_{ds2}^2-4.72e\text{-}5*min(0,v_{sd5}^2)*v_{sd5}^2}$
PM	1.51	$\frac{90.148}{1.0-8.79e\text{-}6*min(0,v_{sg1}^2)*v_{sg1}^2+2.28e\text{-}6*min(0,v_{ds2}^2)*v_{ds2}^2}$
SR_n	2.10	$\frac{-5.21e7}{1.0-8.22e\text{-}5*min(0,v_{gs2}^2)*v_{gs2}^2}$
SR_p	4.74	$2.35e7$
V_{offset}	2.16	$-0.0020 - 1.22e\text{-}23 * min(0, v_{gs2}^2) * v_{gs2}^2$
$log_{10}(f_u)$	2.17	$0.74 - 1.10e\text{-}5 * min(0, v_{sg1}^2) * v_{sg1}^2$ $+1.88e\text{-}5 * min(0, v_{ds2}^2) * v_{ds2}^2$

Reference GP-SR Setup (CAFFEINE)

up to 15 bases functions, population size 200, and 5000 generations. All operators had equal probability, except parameter mutation was 5x more likely (to encourage tuning of a compact function). It has many speedups including subtree caching (Keijzer, 2004) and linear regression to compute linear coefficients. Unary operators allowed are: $\sqrt{(x)}$, $log_{10}(x)$, $1/x$, x^2, $sin(x)$, $cos(x)$, $tan(x)$, $max(0, x)$, $min(0, x)$, 2^x, and 10^x, where x is an expression. Binary operators allowed are $x_1 + x_2$, $x_1 * x_2$, $max(x_1, x_2)$, $min(x_1, x_2)$, $power(x_1, x_2)$, and x_1/x_2. Conditional operators included $\leq (testExpr, condExpr, exprIfLessThanCond, elseExpr)$ and $\leq (testExpr, 0, exprIfLessThanCond, elseExpr)$. Any input variable could have an exponent in the range $\{\ldots, -1, 1, 2, \ldots\}$. Details are in (McConaghy and Gielen, 2009).

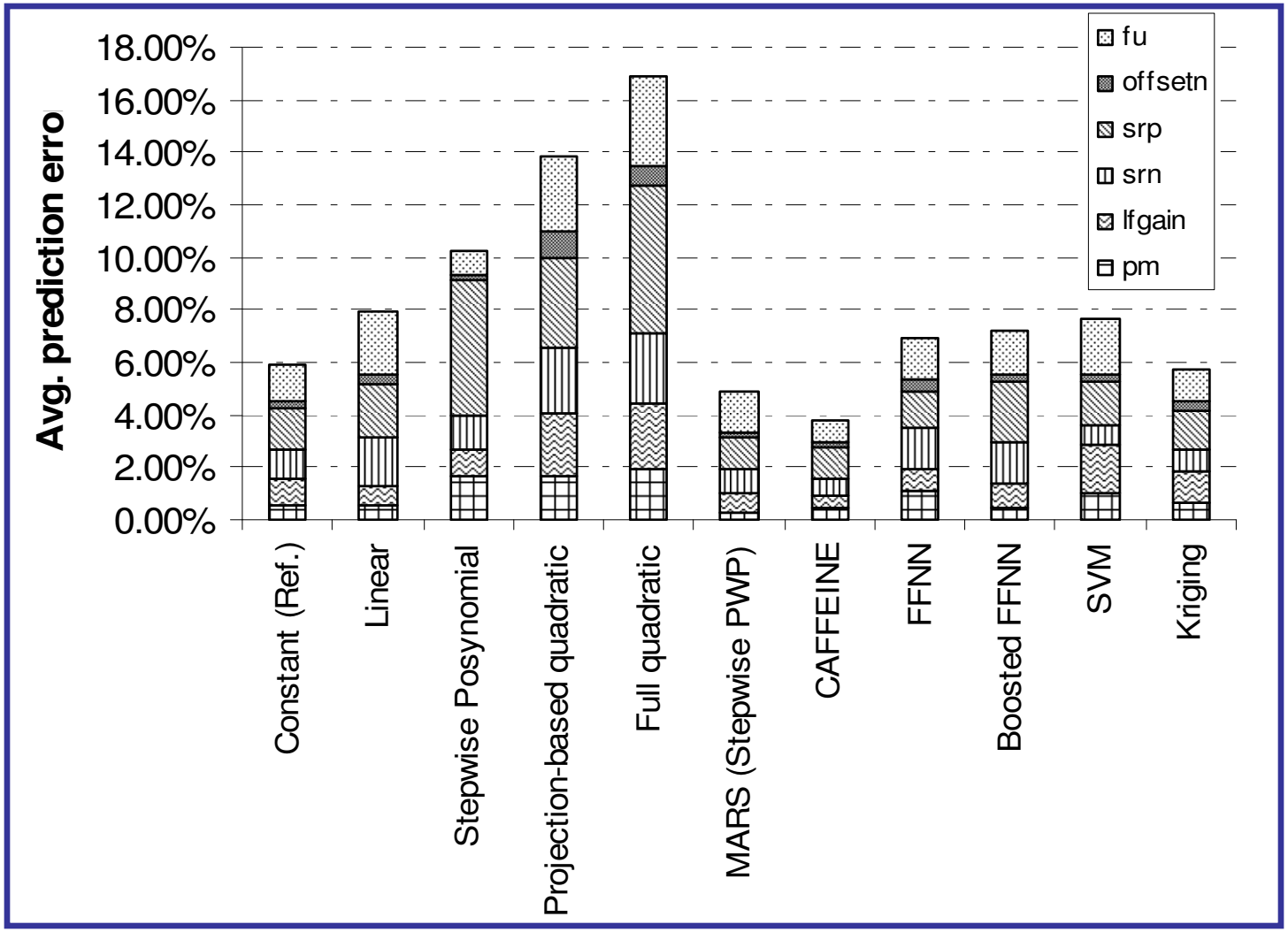
Each CAFFEINE run took $\approx$ 10 minutes on a 1-GHz CPU.

CAFFEINE models with <10% error

Perf.	Expression
A_{LF}	-10.3 + 7.08e-5 / id1 + 1.87 * ln(-1.95e+9 + 1.00e+10 / (vsg1*vsg3) + 1.42e+9 *(vds2*vsd5) / (vsg1*vgs2*vsg5*id2))
f_u	10^(5.68 - 0.03 * vsg1 / vds2 - 55.43 * id1+ 5.63e-6 / id1)
PM	90.5 + 190.6 * id1 / vsg1 + 22.2 * id2 / vds2
v_{offset}	- 2.00e-3
SR_p	2.36e+7 + 1.95e+4 * id2 / id1 - 104.69 / id2 + 2.15e+9 * id2 + 4.63e+8 * id1
SR_n	- 5.72e+7 - 2.50e+11 * (id1*id2) / vgs2 + 5.53e+6 * vds2 / vgs2 + 109.72 / id1

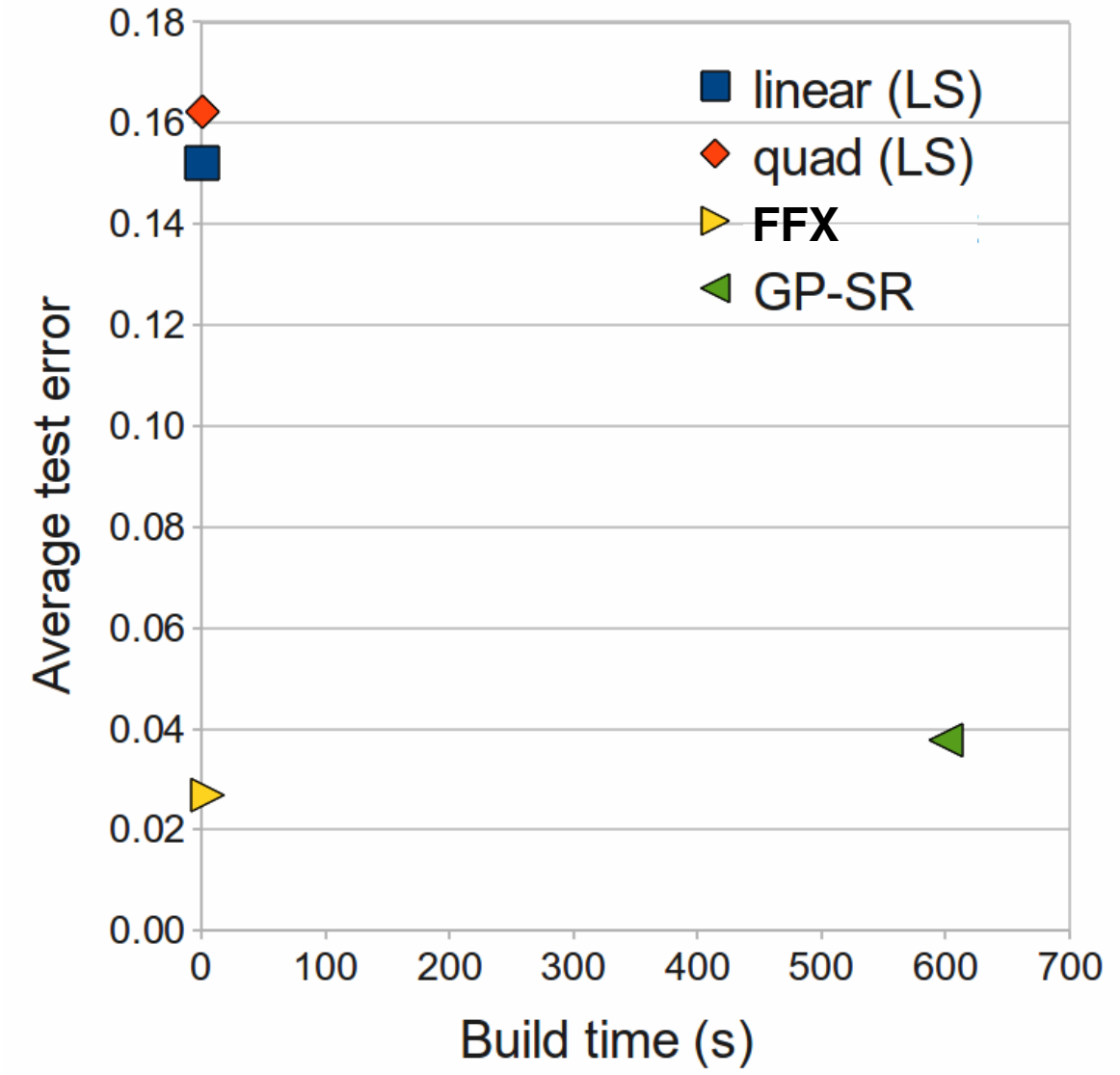
CAFFEINE Prediction Performance

- CAFFEINE models actually predict better than several state-of-the-art blackbox regression techniques (shown: benchmark suite of 6 circuit problems)



Compare FFX vs. GP-SR

Average test time & build errors over 6 problems



Outline

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FFX So Far

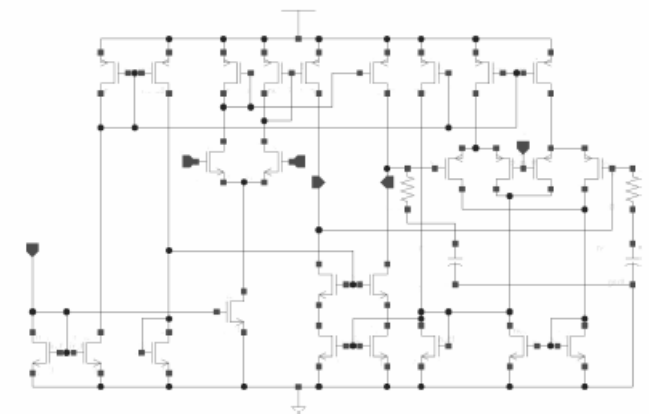
- Problems: 13 input variables, 256 samples
- Results: <5 s, best error
- Pretty good!

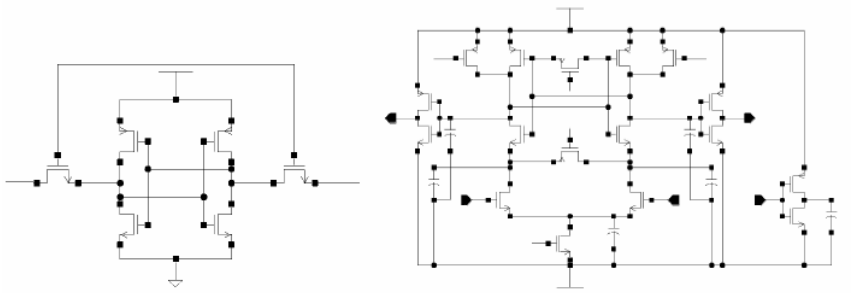
- What about 100-1000 input variables…?

12 Larger Problems
Up to 1468 input variables

Circuit	# Devices	# Process variables	Outputs Modeled
opamp	30	215	AV (gain), BW (bandwidth), PM (phase margin), SR (slew rate)
bitcell	6	30	$cell_i$ (read current)
sense amp	12	125	$delay$, pwr (power)
voltage reference	11	105	$DVREF$ (difference in voltage), PWR (power)
GMC filter	140	1468	$ATTEN$ (attenuation), IL
comparator	62	639	BW (bandwidth)

The opamp and voltage reference had 800 Monte Carlo sample points, the comparator and GMC filter 2000, and bitcell and sense amp 5000.





Other Approaches on 30T Opamp Problems

(215 input vars.) [McConaghy GPTP 2009]

Problem	GP (CAFF-EINE)	Boost tree (SGB)	Bootstr. tree (RF)	LVSR-GDR	LVSR-GDR-tune
30T AV	$\gg$10.0	0.6418	0.8183	0.0765	0.1073
30T BW	$\gg$10.0	0.5686	0.7730	0.0378	0.0442
30T PM	$\gg$10.0	0.5894	0.7656	0.0732	0.0693
30T SR	$\gg$10.0	0.5208	0.7436	0.1642	0.1403

- A “direct” GP-SR approach did terrible
- Resorted to a latent-variable SR approach for good results

Scaling Up FFX

- What about 100-1000 input variables…?
- Summary of results:
  - *Out of memory*
  - *Time for some theory…*

Computational Complexity of FFX?

- **Step one.** Let e be the number of exponents and o be the number of nonlinear operators. Therefore the number of univariate bases per variable is $(o + 1) * e$. (The $+1$ is when no nonlinear operator is applied; or, equivalently, unity). With n as the number of input variables, then the total number of univariate bases is $(o+1)*e*n$. With N samples, the univariate part of step one has a complexity of $O((o + 1) * e * n * N)$. Since e and o are constants, this reduces to $O(n * N)$. The number of bivariate bases is $p = O(n^2)$, so the bivarate part of step one has complexity $O(n^2 * N)$.

Computational Complexity of FFX?

- **Step two.** Elastic net path-following is the dominant part. The cost of an older elastic-net learning technique, LARS, was approximately that of one least-squares (LS) fitting according to p.93 of (Hastie et al., 2008). Since then, the coordinate descent algorithm (Friedman et al., 2010) has been shown to be 10x faster. Nonetheless, we will use LS as a baseline. With p input variables, LS fitting with QR decomposition has complexity $O(N * p^2)$. Because $p = O(n^2)$, FFX has approximate complexity $O(N * n^4)$.

Computational Complexity of FFX?

- **Step three.** Reference (Deb et al., 2002) shows that nondominated filtering has complexity $O(N_o * N_{nondom})$ where N_o is the number of objectives, and N_{nondom} is the number of nondominated individuals. In the SR cases, N_o is a constant (at 2) and $N_{nondom} \leq N_{max-bases}$ where $N_{max-bases}$ is a constant (≈ 5). Therefore, FFX step three complexity is $O(1)$.

The complexity of FFX is the maximum of steps one, two, and three, which is ***O(N * n^4)***.

 # samples ***# input variables***

Improving FFX

A batch-style riff on MARS.

Revised FFX Algorithm:

1. Learn univariate coefficients
2. Only combine the $k \leq O(\sqrt{n})$ most important basis functions
3. Pathwise-learn univariate & combination
4. Nondominated filter

Complexity down to **$O(N*n^2)$** !

Improving FFX

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Complexity down to **$O(N*n^2)$** !

Two more tricks:

- Add MARS-style "hinge" bases: $\max(0, x_i\text{-thr})$, $\max(0, \text{thr-}x_i)$
  - Buys us ≈universal approximation ☺
- Repeat steps 1-3 six times: maybe interactions, maybe rational, maybe hinge functions, maybe log/abs.

Improving Complexity to *O(N*n^2):*

A batch-style riff on MARS.

Revised algorithm:

1. First learn univariate coefficients
2. Only combine the k ≤ O(√n) most important basis functions
3. Pathwise-learn univariate & combination
4. Nondominated filter

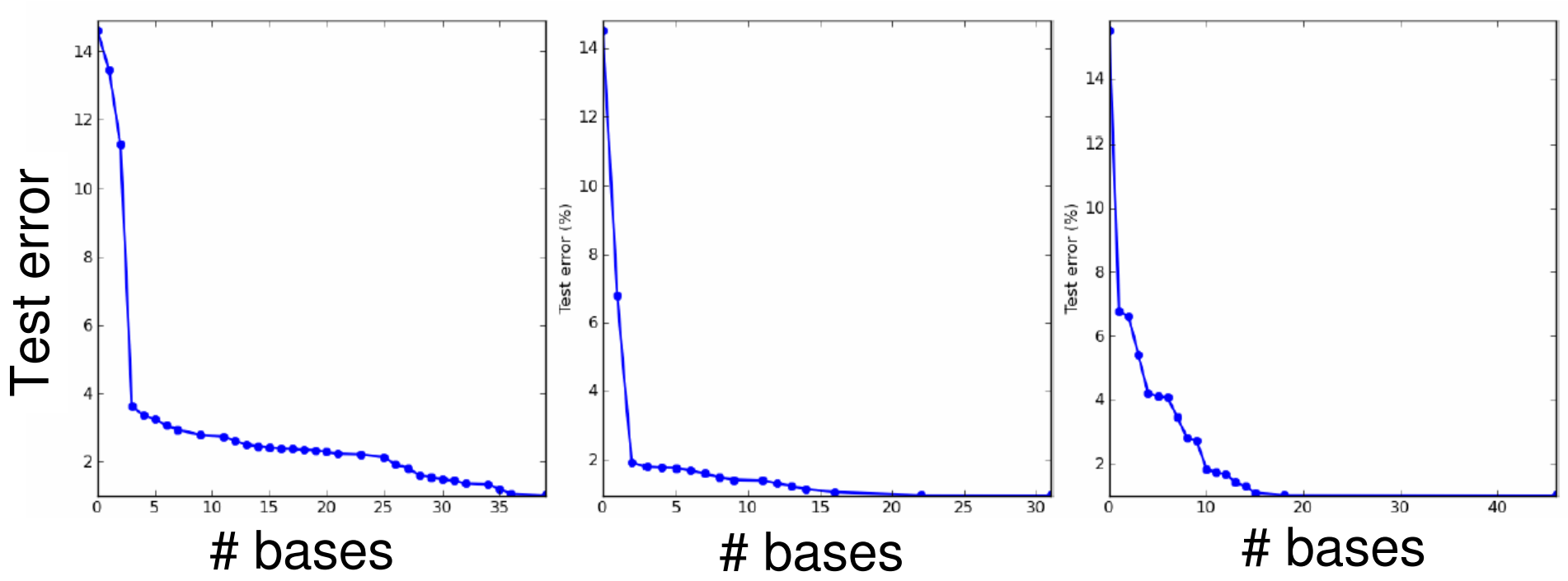
Complexity down to O(N*n^2) !

Two more tricks:

- Add MARS-style “hinge” bases: max(0, x_i-thr), max(0, thr-x_i)
- Repeat steps1-3 six times: maybe interactions, maybe rational, maybe hinge functions, maybe log/abs.

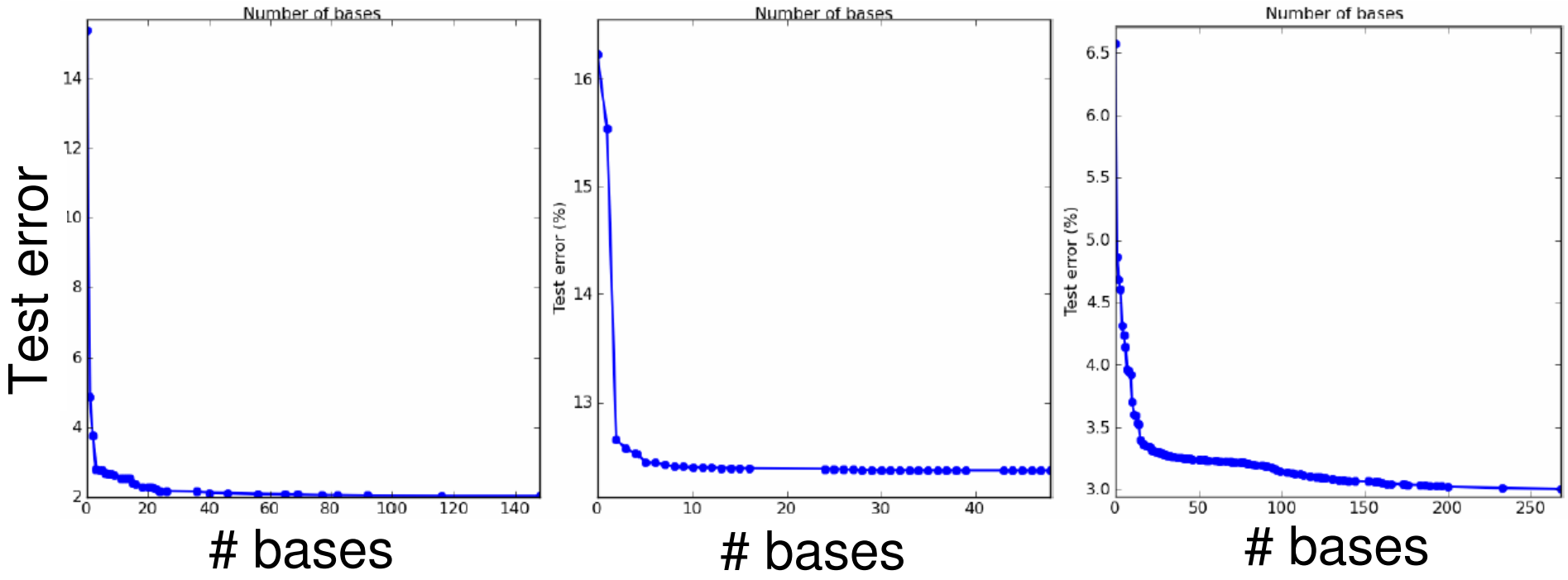
Overall runtime 5-30 s

Test Error vs. Complexity
Large Problems 1-3 (of 12). <30 s!



Opamp AV **Opamp BW** **Opamp PM**

Test Error vs. Complexity
Large Problems 4-6 (of 12). <30 s!

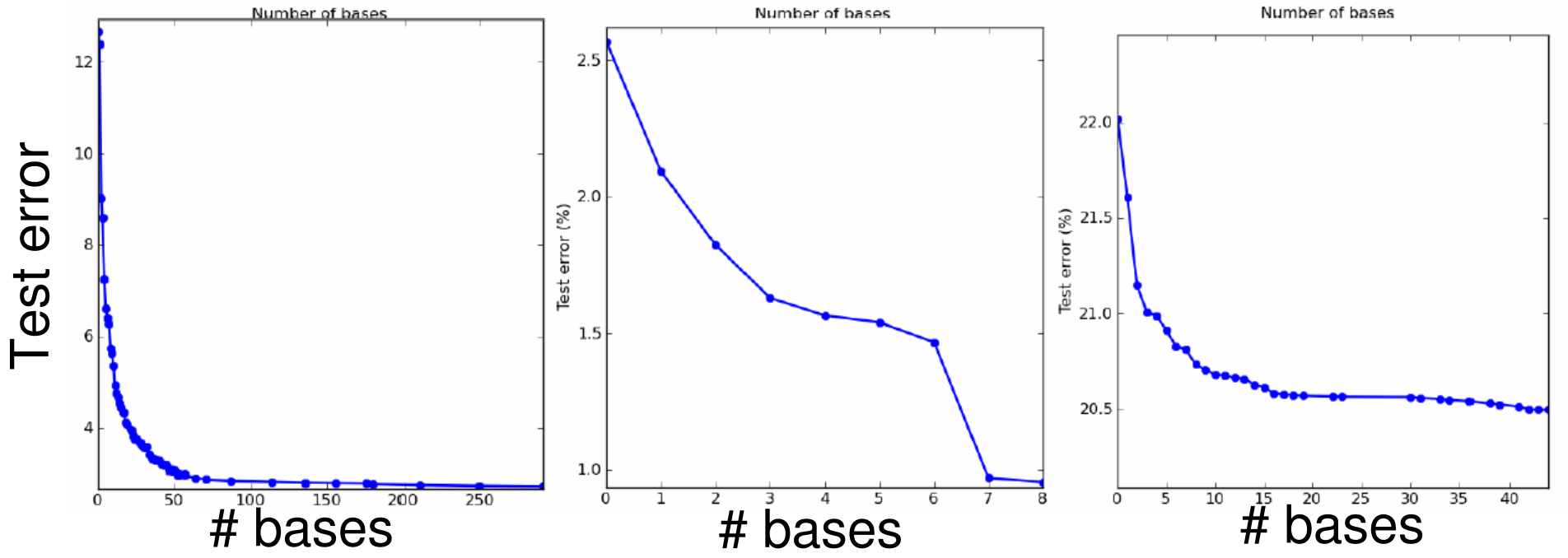


Opamp SR

Bitcell cell_i

Sense amp delay

Test Error vs. Complexity
Large Problems 7-9 (of 12). <30 s!

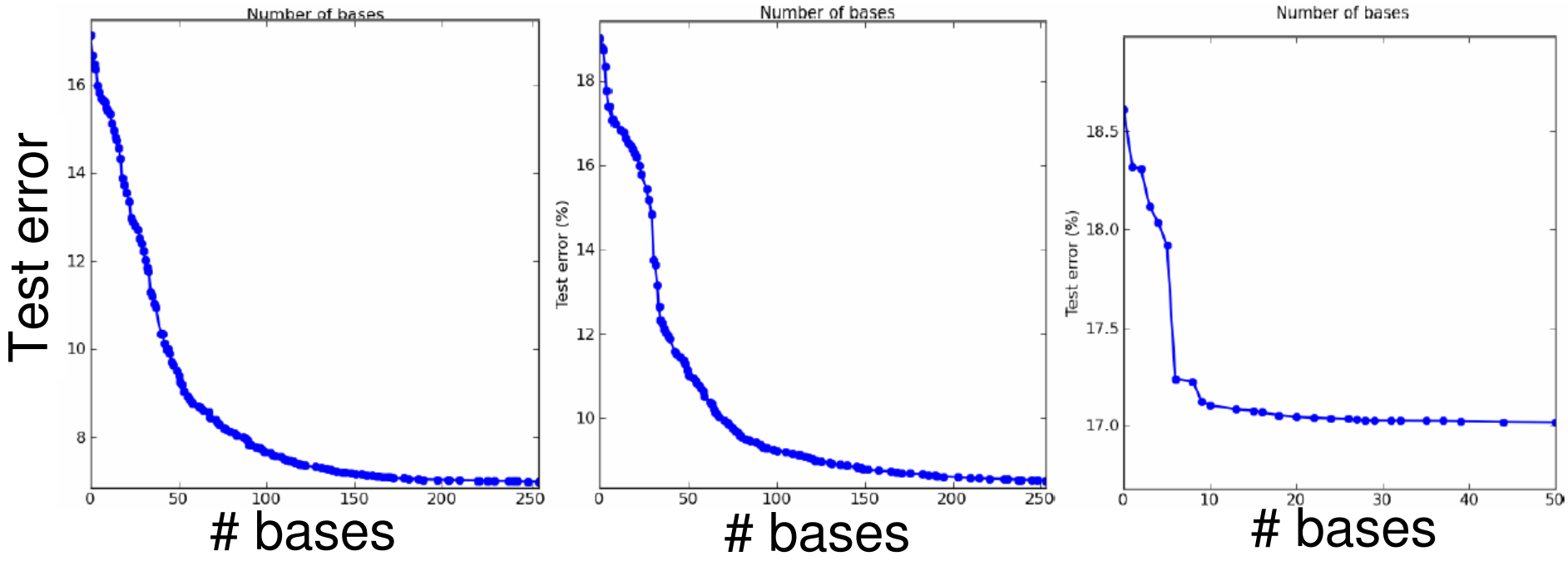


Sense amp PWR

Voltage reference DVREF

Voltage reference power

Test Error vs. Complexity
Large Problems 10-12 (of 12). <30 s!



GMC filter IL

GMC filter ATTEN

Comparator BW

Opamp PM Equations. <30 s!

# Bases	Test error (ϵ_{test}) (%)	Extracted Function
0	15.5	59.6
1	6.8	$59.6 - 0.303 * dxl$
2	6.6	$59.6 - 0.308 * dxl - 0.00460 * cgop$
3	5.4	$59.6 - 0.332 * dxl - 0.0268 * cgop + 0.0215 * dvthn$
4	4.2	$59.6 - 0.353 * dxl - 0.0457 * cgop + 0.0403 * dvthn - 0.0211 * dvthp$
5	4.1	$59.6 - 0.354 * dxl - 0.0460 * cgop - 0.0217 * dvthp + 0.0198 * dvthn + 0.0134 * abs(dvthn) * dvthn$
6	4.07	$59.6 - 0.354 * dxl - 0.0466 * cgop - 0.0224 * dvthp + 0.0202 * dvthn + 0.0135 * abs(dvthn) * dvthn + 0.000550 * DXL$
⋮	⋮	⋮
46	1.0	$(58.9 - 0.136 * dxl + 0.0299 * dvthn - 0.0194 * max(0, 0.784 - dvthn) + \ldots)/(1.0 + \ldots)$

Voltage Reference DVREF. <30 s!

# Bases	Test error (ϵ_{test}) (%)	Extracted Function
0	2.6	512.7
1	2.1	$504/(1.0 + 0.121 * max(0, dvthn + 0.875))$
2	1.8	$503 - 199 * max(0, dvthn + 1.61) - 52.1 * max(0, dvthn + 0.875)$
3	1.6	$496/(1.0 - 0.0447 * max(0, -1.64 - dvthp) * max(0, dvthn + 0.875) - 0.0282 * max(0, -1.90 - dxw) * max(0, dvthn + 0.875) - 0.0175 * max(0, -1.64 - dvthp) * max(0, dvthn + 0.142))$
⋮	⋮	⋮
8	0.9	$476/(1.0+0.105*max(0, dvthn+1.61)-0.0397*max(0, -1.64-dvthp)*max(0, dvthn+0.875)-0.0371*max(0, -1.90-dxw)*max(0, dvthn+0.875)-0.0151*max(0, -1.64-dvthp)*max(0, dvthn+0.142)\ldots)$

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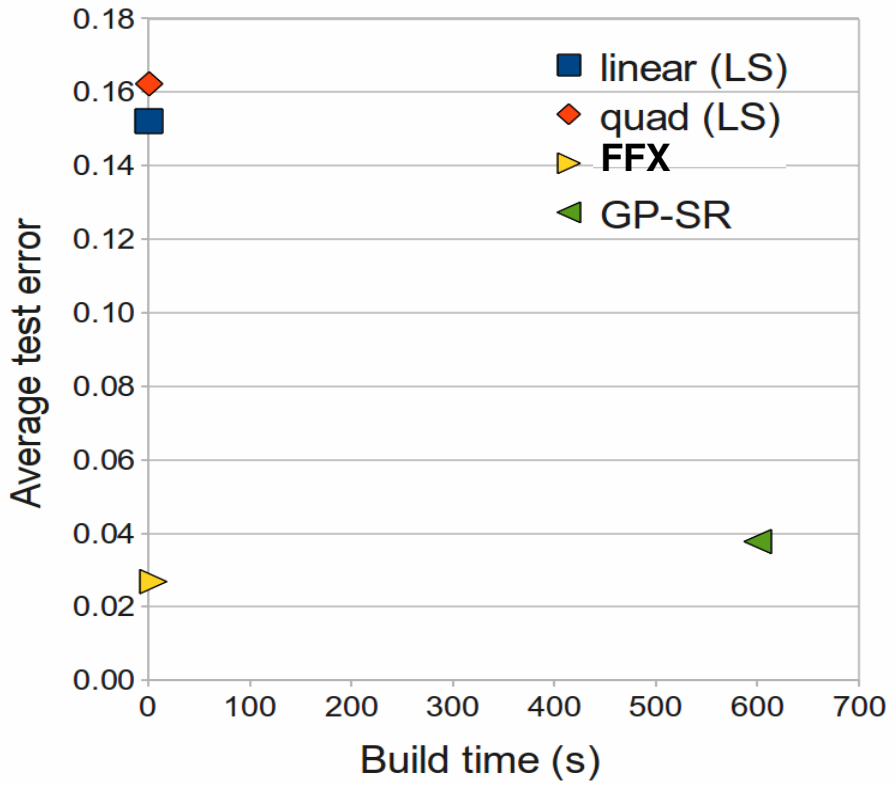
FFX Summary of Results

- ≈ as fast as LS-linear:

  <5 s on smaller, <30 s on larger
- As accurate as GP-SR
- Gives error-complexity tradeoffs
- Scalable
- Simple
- Deterministic!
- O(N * n^2) complexity. (Theory!)



*This is **Fast Function Extraction***

Related Work

- Recasting SR from tree towards vector-valued optimization
  - O'Neill and Brabazon 2006
  - McConaghy and Gielen 2006
  - Cerny et al 2008
  - Veerhuis 2009
  - Fonlupt and Robillard 2011
- Doing tree-based search with non-EA:
  - O'Reilly PhD (SA, hillclimb)
- EDAs
  - Derandomize EA search
  - Dispense with mutation, crossover
  - On bitstrings, vectors, trees. Goldberg, Pelikan, Sastry, Looks, Iba, many more; "Modern era" 1999-present.

Related Work

- Vector-based optimization on just SR coefficients
  - Topchy and Punch 2001
  - And many since
- Recasting general tree-valued search into simpler spaces
  - Rothlauf 2006
  - And many more

Related Work

- Linear learning as part of individual's fitness evaluation
  - LS: McConaghy and Leung 1998. Many more!
  - Ridge regression: Nikolaev and Iba 2001
  - PRESS statistic: McConaghy and Gielen 2005
  - GDR: McConaghy and Gielen 2009
- Regularized learning to bias building blocks
  - McConaghy and Gielen 2009

Related Work

- “Popping in” of complexity incrementally
  - Stepwise-forward regression. Linear; nonlinear (eg MARS)
  - Boosting
  - FFNN practice: learn on 1 node. If hit target, stop. Else add 1 node and repeat.
  - NEAT: ≈ like above but automated + tricks
  - More EA references…

But, not *that* related

- FFX has no selection, mutation, crossover
- No “individuals! No population.
- Embarrassingly simple compared to GP
  - Simple enough to develop theory *here*
- Just one (or two) *convex* optimizations
  - SR as one big hill!
  - Therefore globally optimal result
- Threw out randomization completely
  - Deterministic!

Benefits of Deterministic

[Possibly Heretical Comments]

- Same result every time
  - Just like typing “X/y”
  - Just like calling sort()
  - Just like using your telephone
  - Just like typing your keyboard
- Imagine if any of these was stochastic?

- Ease of adoptability
- No “wondering if the next run will get it”

- At the very least: consider that stochastic is not necessarily a virtue!

An FFX-colored view of GP

[Trent's Heretical Comments]

- Doing SR does not have to mean doing GP
- Reconsider other problems traditionally done with "GP".
  - GP may have been the first way. The "most convenient".
    But it's not necessarily the only way!
    Possibility of dramatically different approaches.
  - The approach may even be deterministic! Convex!
  - Possible benefits: speed, scalability, simplicity, adoptability, $?
- Where might GP researchers go from here?
  - Bias to problems that GP is best suited for? Evolvability, …
  - Re-attack GP problems with non-GP approaches
    - Even by trying, you could learn a lot about your domain!
  - Mix the approaches – plenty of fertile ground between GP and {ML, Convex Opt, MC methods, CLP, SAT, …}
  - Use FFX as an off-the-shelf "baseline" in your GP research ☺
    (I'm putting the code online at trent.st)

FFX ≠ Fork Fan Experience

FFX is SR *Technology*: Fast, Scalable, Deterministic

Met my gauntlet:

> "How can SR be scoped so that it becomes another standard, off-the-shelf method in the "toolboxes" of scientists and engineers around the world? Can SR follow in the same vein of linear programming?

> "Scalability is always relative. SR has attacked fairly large problems, but how can SR be improved to solve problems that are 10x, 100x, 1,000,000x harder?"