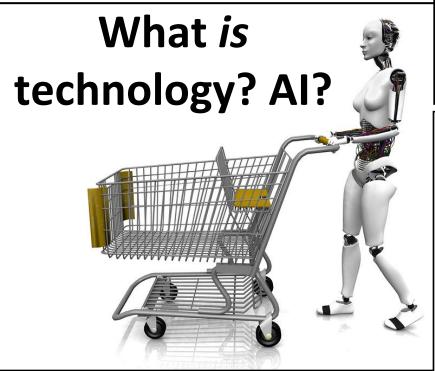
Artificial Intelligence and Symbolic Regression

Trent McConaghy, PhD



Mysteries of the universe..



WTF is genetic programming or symbolic regression? Why should I care?



How *does* Google find furry robots?

What is Al anyway?

What's Artificial Intelligence (AI)?

1. Original:

AI: "A machine that can replicate human cognitive behavior" [Turing test]

2. More recent:

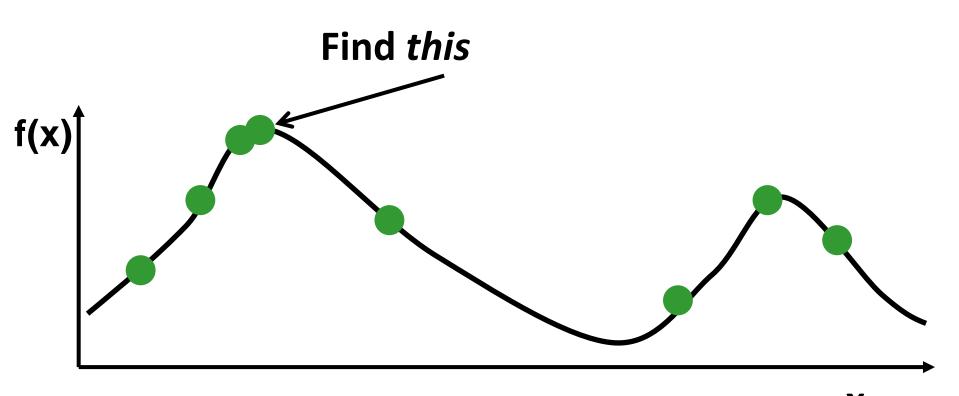
Al: "A machine that can perform a cognitive task, that was previously only possible with a human" [Deep Blue / Chess]

3. Most recent / pragmatic:

Al: "A machine that can perform a non-analytical information processing task, at speed / accuracy / capacity not possible by a human."

Optimization

"Find the x that maximizes f(x)"
(With as few evaluations of f(x) as possible)

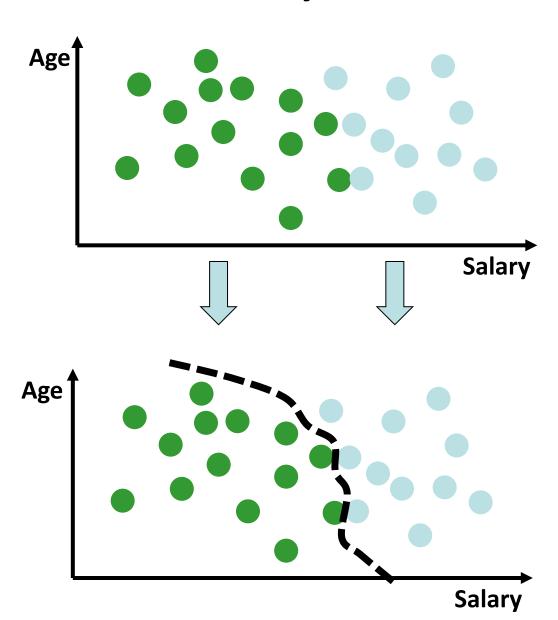


Classification, in 2D

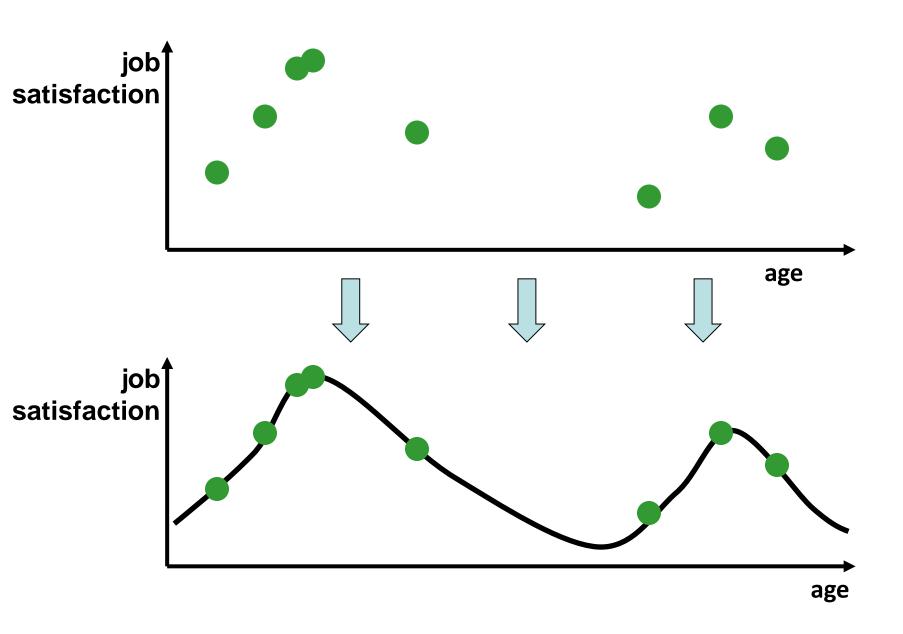
Credit profile:

Paid bills

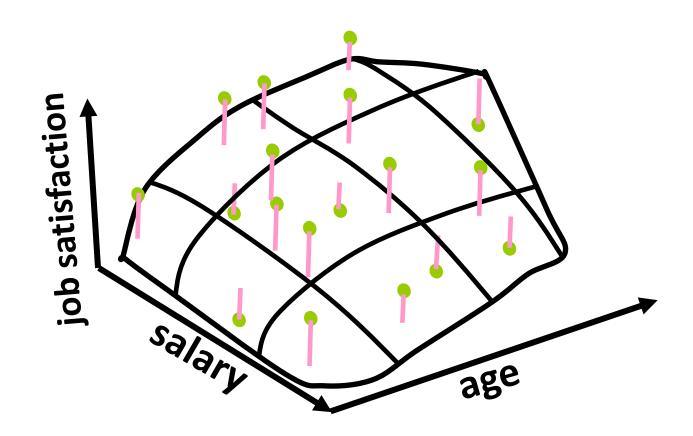
Didn't pay



Regression, in 1D



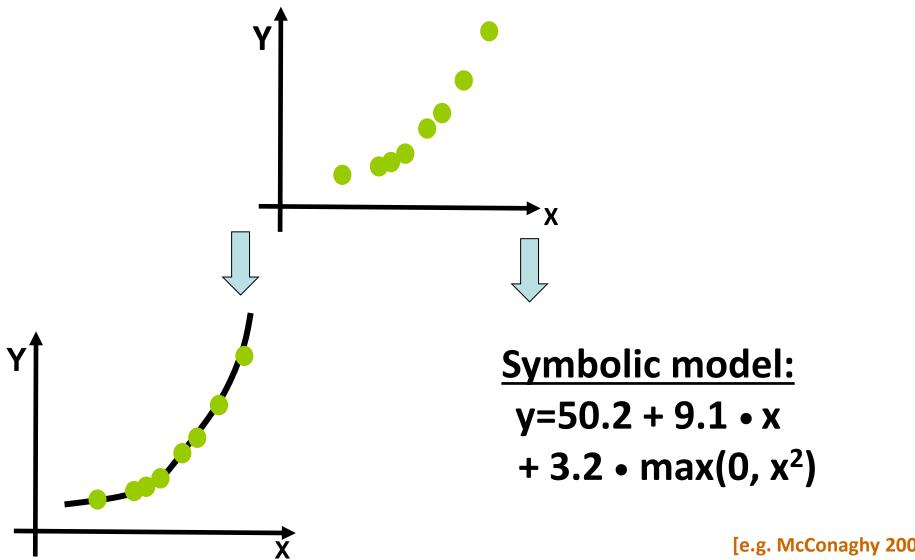
Regression, in 2D



How: Polynomials, splines, neural networks, support vector machines, Gaussian process models, boosted trees, ... [many refs]

Symbolic Regression (SR)

(Like regression, but output a symbolic model too)



[e.g. McConaghy 2005; McConaghy 2011]

Al Has a Toolbox of Ways to Solve...

- Classification Fraud detection, spam filtering ...
- Regression Stock prediction, sensitivity analysis ...
- Whitebox regression Scientific discovery ...
- Optimization Airfoil design, circuit simulation ...
- •Structural synthesis Analog synthesis, robotics ...
- Pattern recognition Face recognition, object recog ...
- System identification Scientific discovery ...
- •Ranking Web search, ad serving, social discovery ...
- Control Auto-driving autos, spacecraft trajectories ...

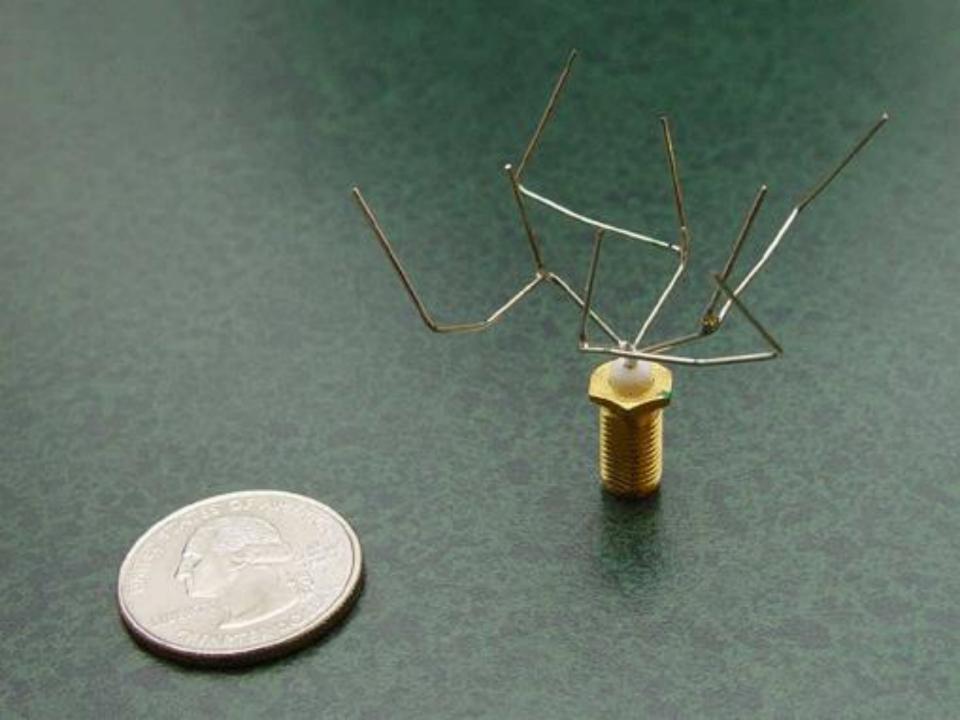
• ...

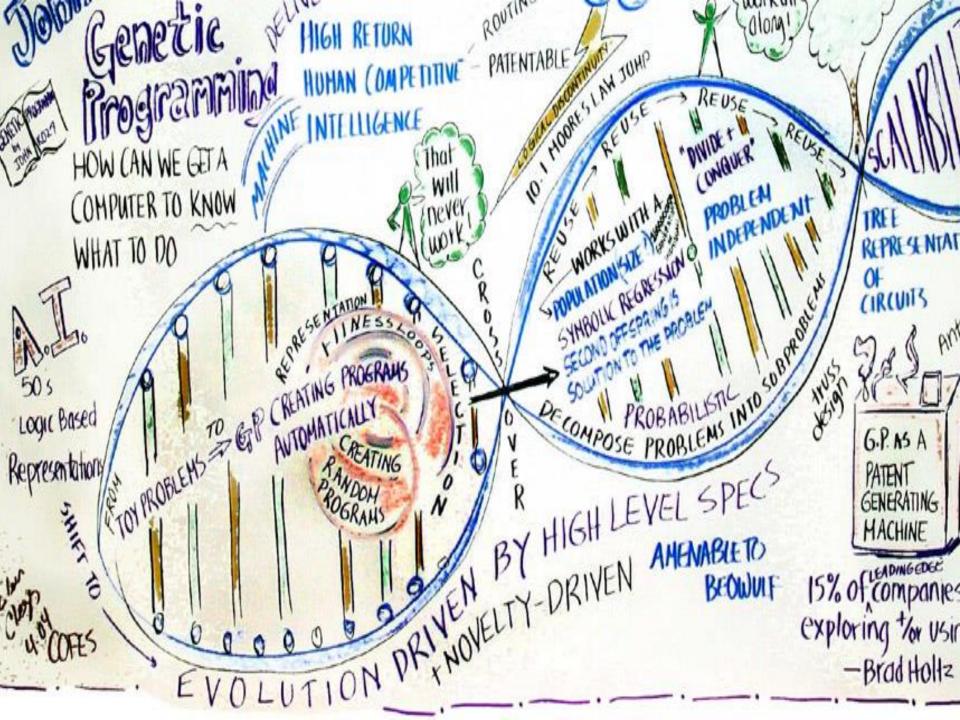
Al Sub-fields

- machine learning
- evolutionary computation
- fuzzy logic
- data mining
- artificial general intelligence
- pattern recognition
- ..
- (nee) nonlinear programming
- (nee) databases
- ..

Genetic Programming (GP):

A branch of a branch of Al But a super-cool one..

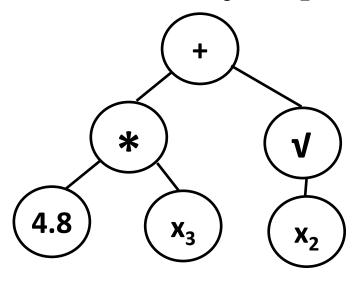




GP for SR

"A function is a tree"

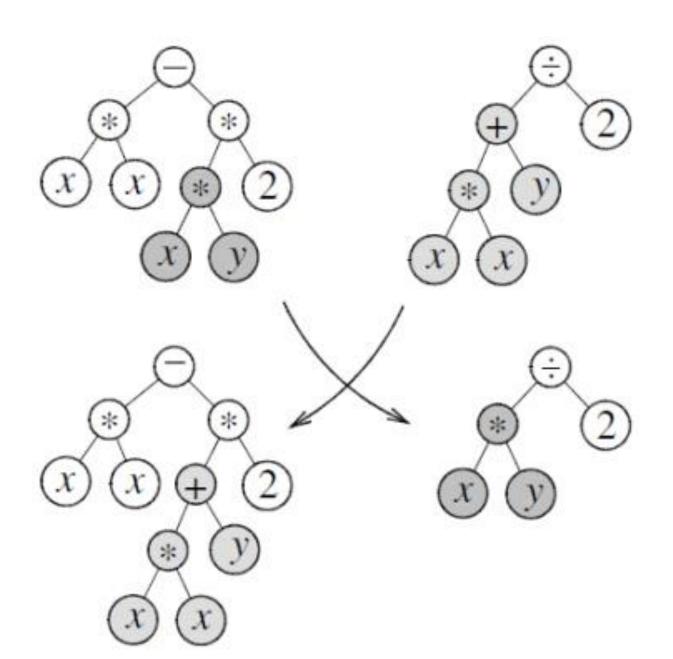
$$f(x) = 4.8 * x_3 + Vx_2$$



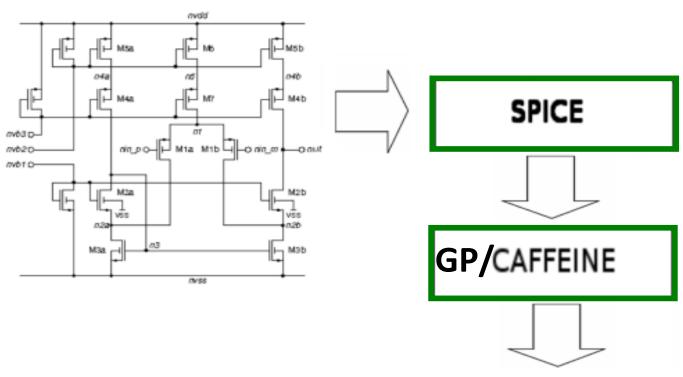
Searches through the space of trees:

- 1. Initial random population; evaluate
- 2. Create children from parents via operators; evaluate
- 3. Select best; goto 2

GP for SR: Crossover Operator



Example: GP for SR on Circuits



Perf.	Expression
A_{LF}	-10.3 + 7.08e-5 / id1
	+ 1.87 * In(-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

What is technology anyway?

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

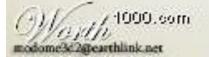
food to cool down

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





























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/ConvexOptimizationl-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/ConvexOptimizationl-Lecture01.pdf

On becoming a "tool"

- 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

Recently, 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

GP SR and Technology

I gave this 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?"

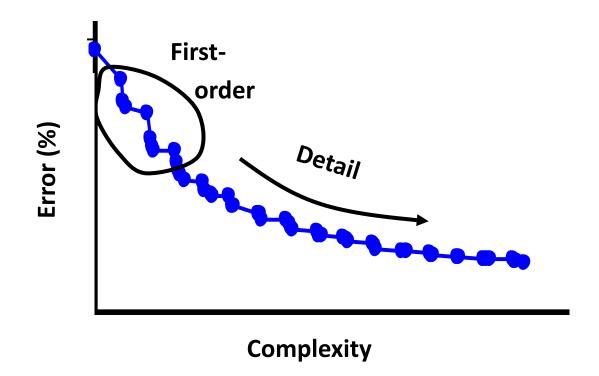
Summary: Aiming for SR* as a Technology



* SR ≠ Shopping Robot

SR Problem Definition

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



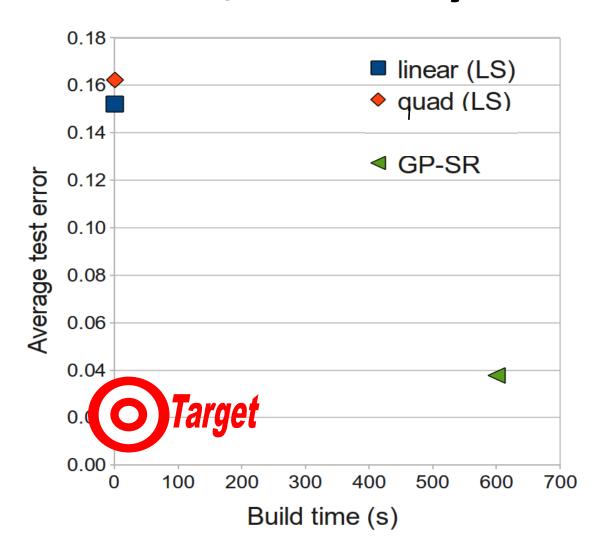
SR Problem Definition

- Given (X,y)
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Desirable Features:

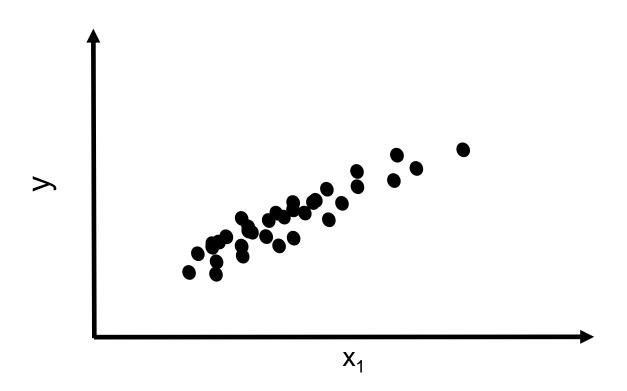
- Scalable (# variables, # samples)
- Fast
- Reliable, consistent results
 - Derandomized → deterministic? (CMAES \rightarrow X/y)
- Ideal: simple algorithm
 - Arch. Altering Ops \rightarrow Push \rightarrow ...
 - FFNNs \rightarrow SVMs
- Ideal: hits global optimum (on problem formulation)

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

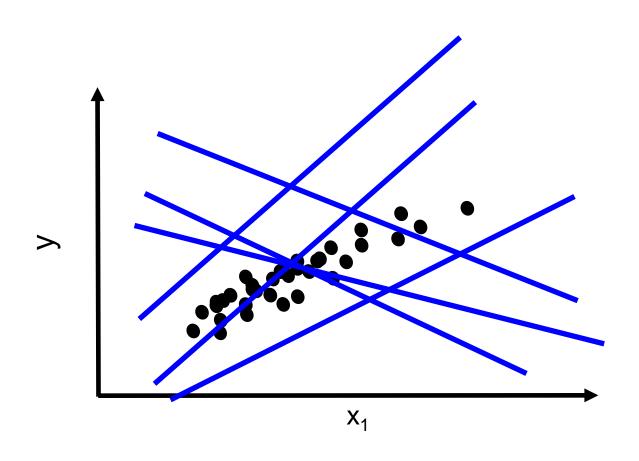


A (Re) Introduction to Regression

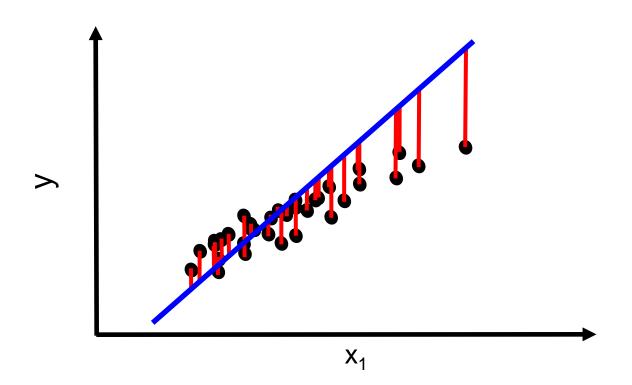
1D Linear Least-Squares Regression



Many possible linear models!

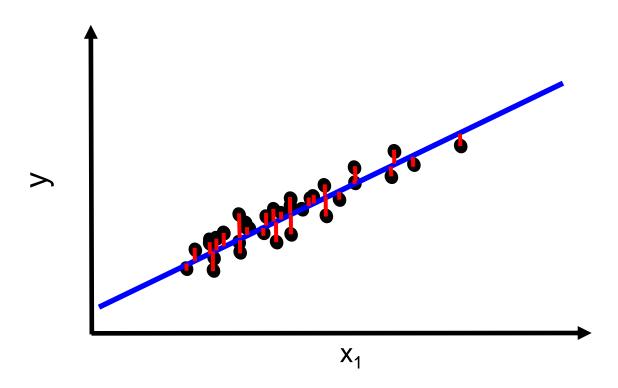


Find linear model that minimizes $\sum (yhat_i-y_i)^2$ for all *i* in training data



Find linear model that minimizes $\sum (yhat_i-y_i)^2$ That is: $[w_0, w_1]^* = argmin \sum (yhat_i-y_i)^2$ where $yhat(x_1) = w_0 + w_1 * x_1$ A CONTRACTOR OF THE PARTY OF TH X_1

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

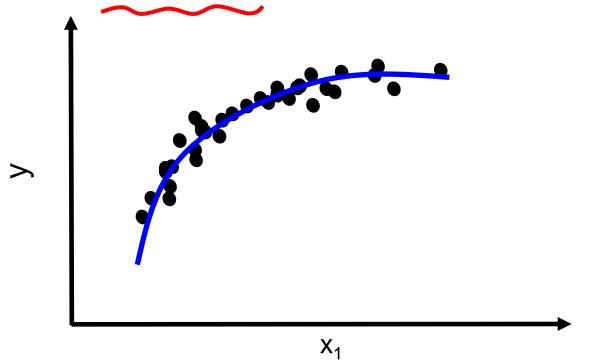


1D Quadratic LS Regression

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

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!

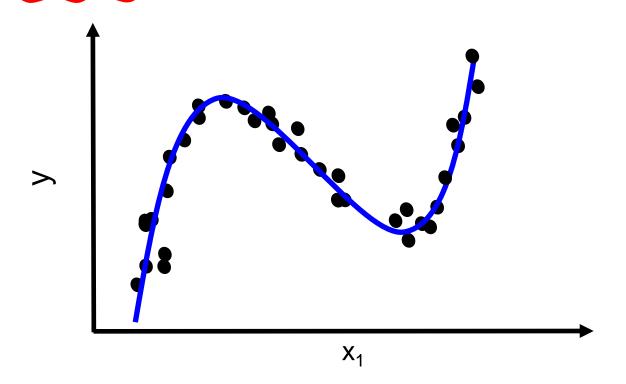


1D Nonlinear LS Regression

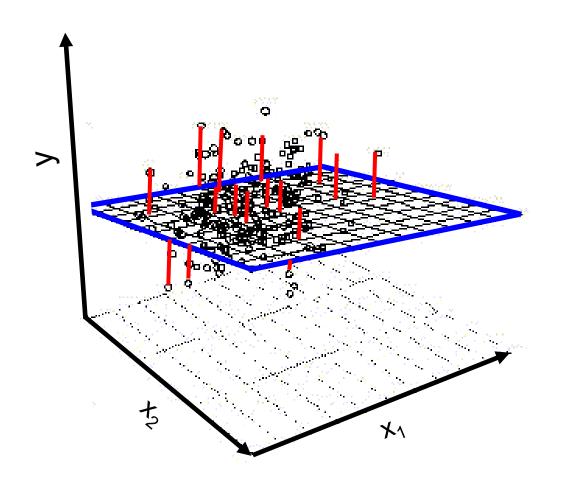
$$[w_0, w_1, w_{sin}]^* = argmin \sum (yhat_i-y_i)^2$$

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!

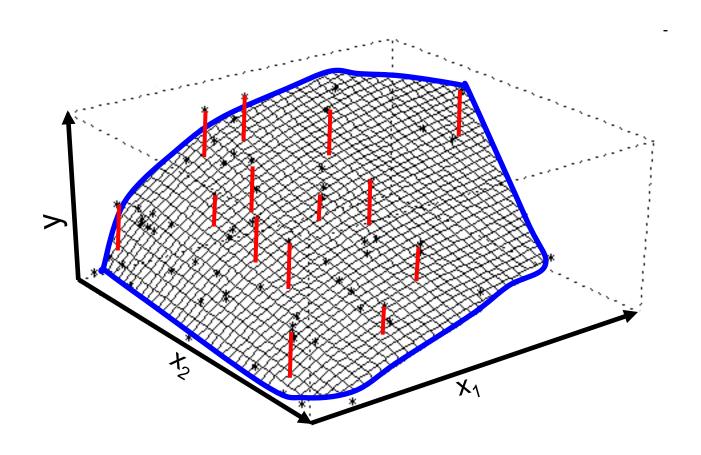


 $[w_0, w_1, w_2]^* = argmin \sum (yhat_i-y_i)^2$ where $yhat(\mathbf{x}) = w_0 + w_1 * x_1 + w_2 * x_2$



2D Quadratic LS Regression

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

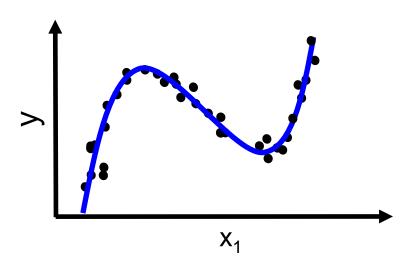


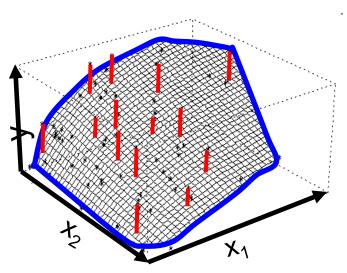
Generalized Linear Model (GLM)

Generalized linear model (GLM) of B basis functions. $yhat(\mathbf{x}) = w_0 + w_1 * f_1(\mathbf{x}) + w_2 * f_2(\mathbf{x}) + ... + w_B * f_B(\mathbf{x})$

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

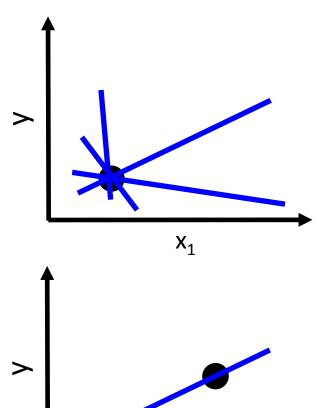
- $yhat(x_1) = w_0 + w_1 * x_1 + w_{11} * x_1^2$
- $yhat(x_1) = w_0 + w_1 * x_1 + w_{sin} * sin(x_1)$
- yhat(\mathbf{x}) = \mathbf{w}_0 + \mathbf{w}_1 * \mathbf{x}_1 + \mathbf{w}_{11} * \mathbf{x}_{12} + \mathbf{w}_{22} * \mathbf{x}_{22} + \mathbf{w}_{12} * \mathbf{x}_1 * \mathbf{x}_2
- polynomials, SVMs, FFNNs, many GP SR. Universal approximator!



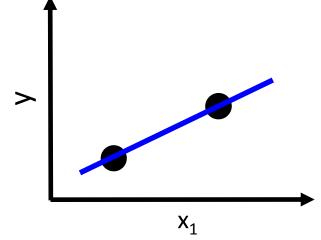


Constraint on LS Regression?

(1D Example)



1 Sample – too few



2 Samples – enough

General rule?

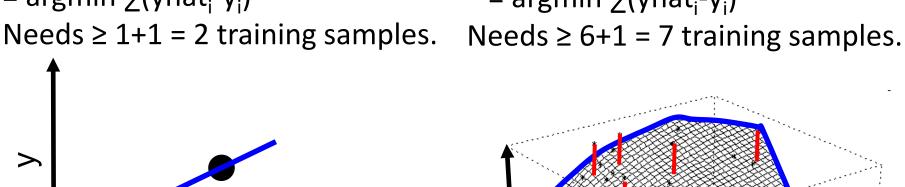
Constraint on LS Regression

General Rule:

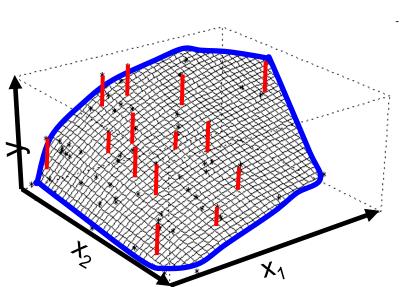
• If *n* variables, need N ≥ n+1 training samples

Examples:

1D Lin: [w₀, w₁]* = argmin ∑(yhat_i-y_i)² Needs ≥ 1+1 = 2 training samples.



2D Quad $[w_0, w_1, w_2, w_{11}, w_{22}, w_{12}]^*$ = argmin $\sum (yhat_i-y_i)^2$



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)*

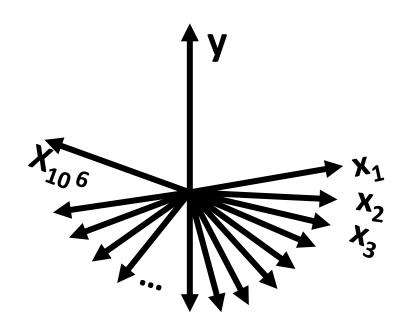
Consider 1M basis functions in a GLM

Q: Can we fit this with LS-learning?

A: Yes! (As long as ≥1M+1 samples)*

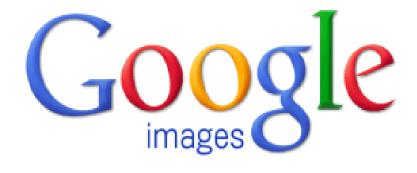
*and no memory issues etc

Regression in 10⁶D?



How?? (and why??)

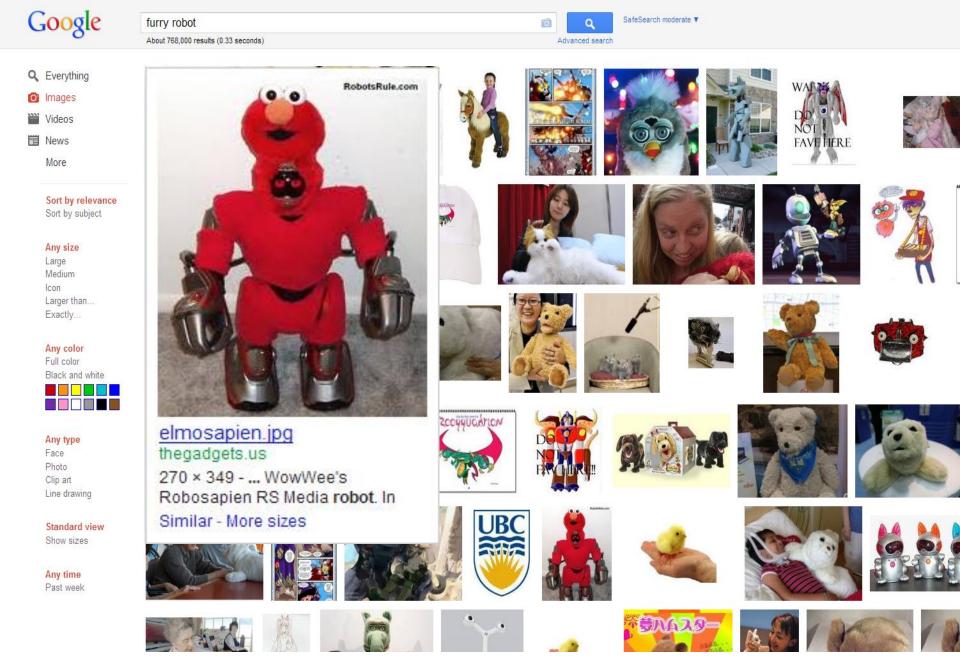
90° turn...



furry robot



Search Images



How does Google find furry robots?



Q Everything Images Wideos ■ News

More

Sort by subject

Any size Large Medium

Larger than... Exactly...

Any color Full color

Any type Face Photo Clip art Line drawing

Standard view Show sizes

Any time Past week





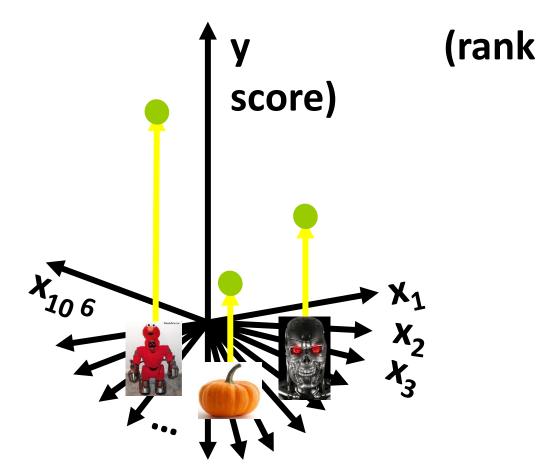


How does Google accurately find furry robots?

Q: How does Google (accurately) find furry robots?

A:

- 1. Treat images as $1000x1000 = 10^6$ input variables (!)
- 2. Do regression on "known" images (furry vs. non)
- 3. Rank the other images. Easy! ©



Q: State of the art in image search? (NIPS '09)

A: BHALR!*

*Big, Hairy, Audacious Linear Regression

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!*

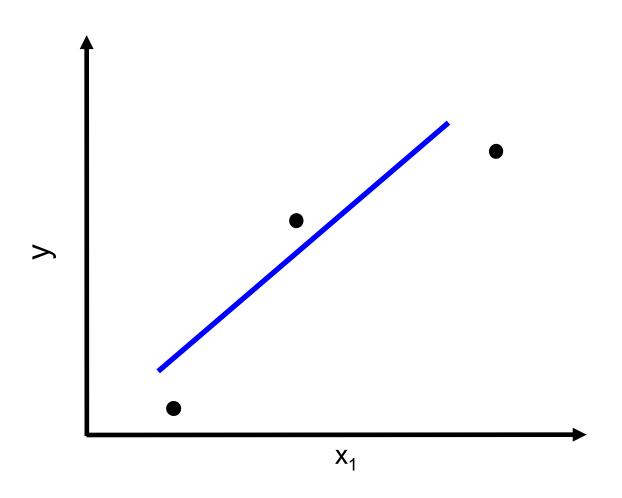
*Big, Hairy, Audacious Linear Regression

1000 pixels x 1000 pixels = 1M input variables 100-1000 samples.

Then apply linear regression or classification

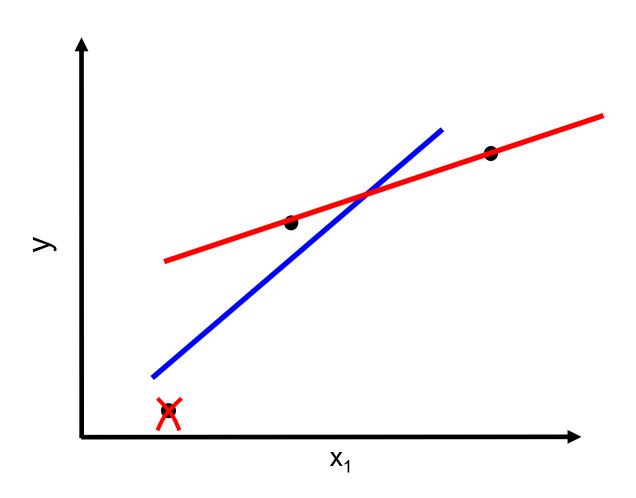
But 100 << 1M. *HOW* ??

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



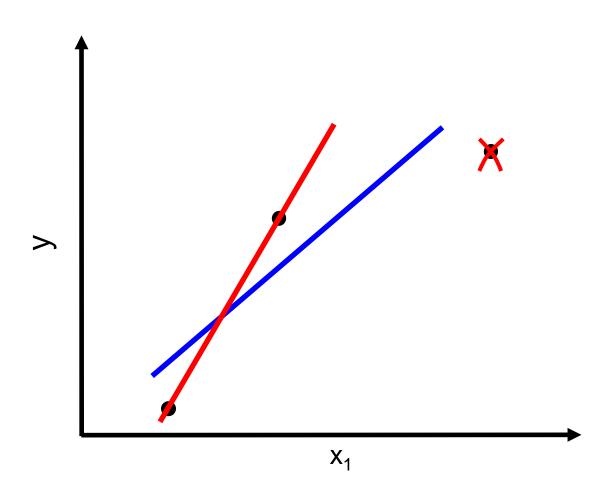
Q: What happens when # samples $N \rightarrow$ # variables n ?

A: Model gets more sensitive!

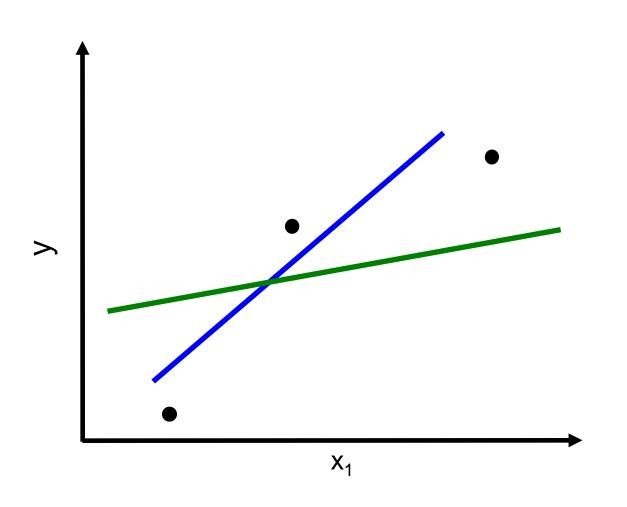


Q: What happens when # samples $N \rightarrow$ # variables n ?

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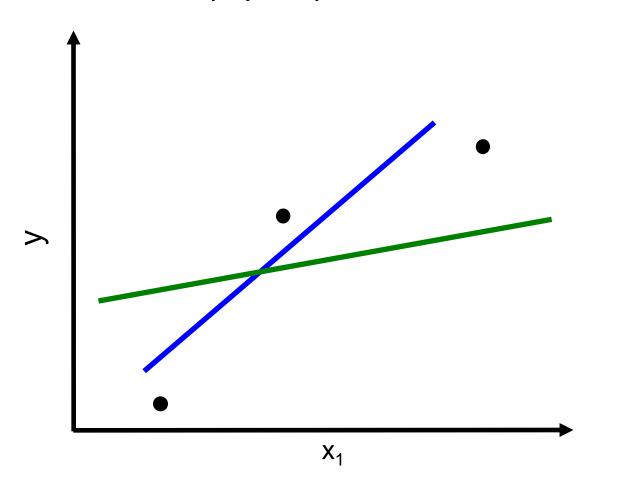


A model that's "less sensitive"



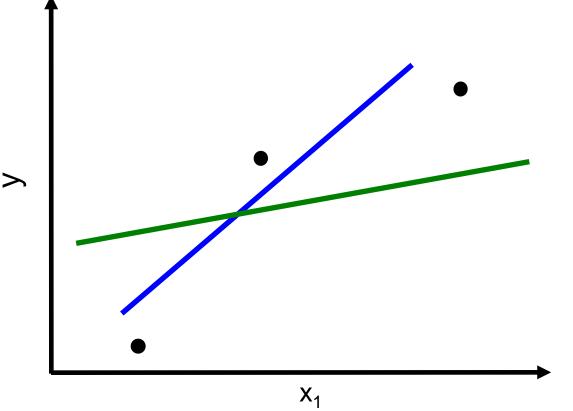
A model that's "less sensitive"

Smaller |dy/dx| means less sensitive



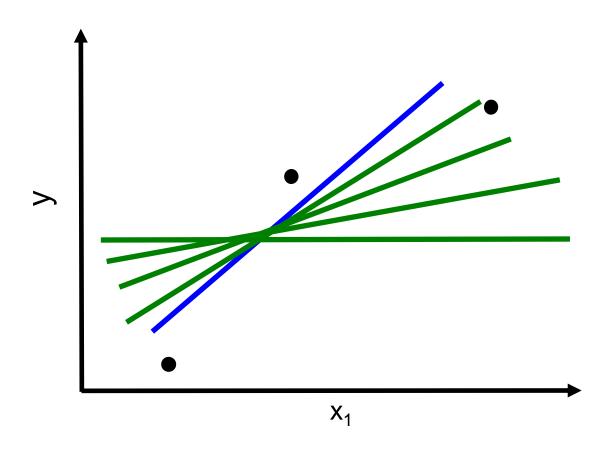
A model that's "less sensitive"

Smaller |dy/dx| means less sensitive i.e. given yhat $(x_1) = w_0 + w_1 * x_1$ A smaller $|w_1|$ means less sensitive or smaller $\sum w_i$ for n > 1 (ignore w_0)



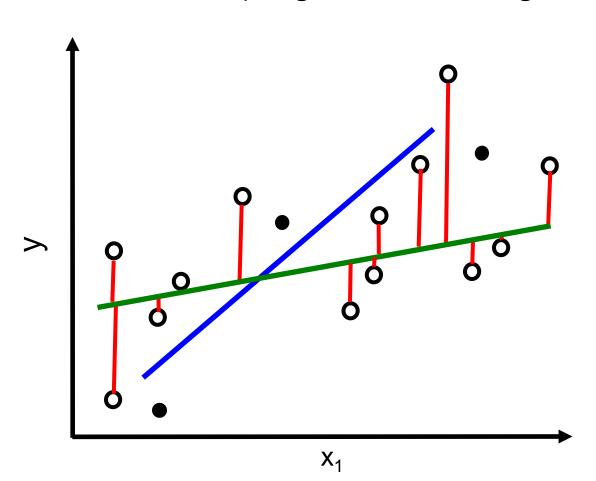
Least-sensitive model has slope of 0
(By definition)

(And also when viewed pragmatically as a model)

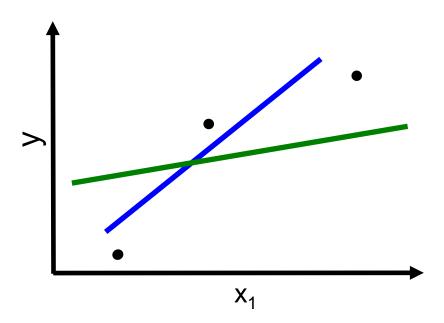


A model that's "less sensitive"

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

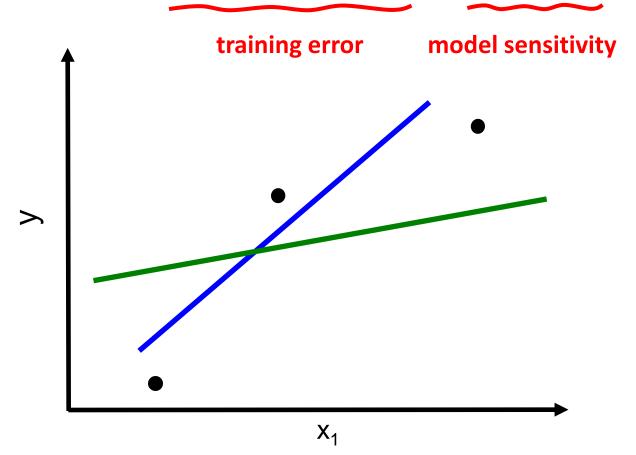


- Aim: minimize *future* prediction error
- Pragmatic Issue: we only have access to training data!
- Trick: minimize sensitivity ≈ minimize future prediction error
- But do consider training data to bias the model (otherwise we end up with a constant useless!)
- So: minimize a combination of training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



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

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



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

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

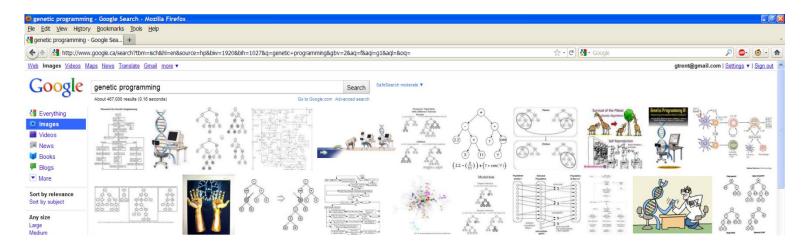
$$\mathbf{w}^* = \operatorname{argmin} \left(\sum (y \operatorname{hat}_i(\mathbf{w}) - y_i)^2 + \lambda * \sum w_i^2 \right)$$
[Ridge Regression]

... [Elastic Net, Gradient Directed Regularization, ...]

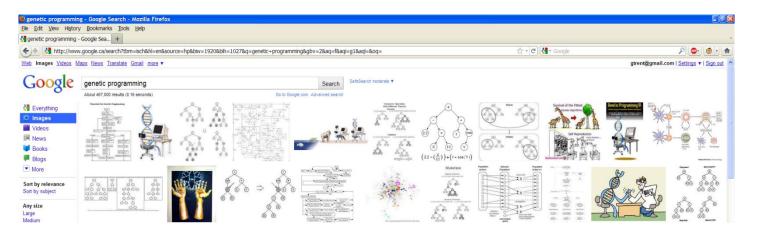
This is regularized linear learning

- 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

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



- 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"

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

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

• Case:
$$\lambda=0$$
 $\sum (yhat_i(\mathbf{w}) - y_i)^2 + \lambda * \sum |w_i|$

...reduces to least-squares

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

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...reduces to least-squares

• Case:
$$\lambda = \infty$$
 $\sum (yhat_i(w) - y_i)^2 + \lambda * \sum |w_i|$

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

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

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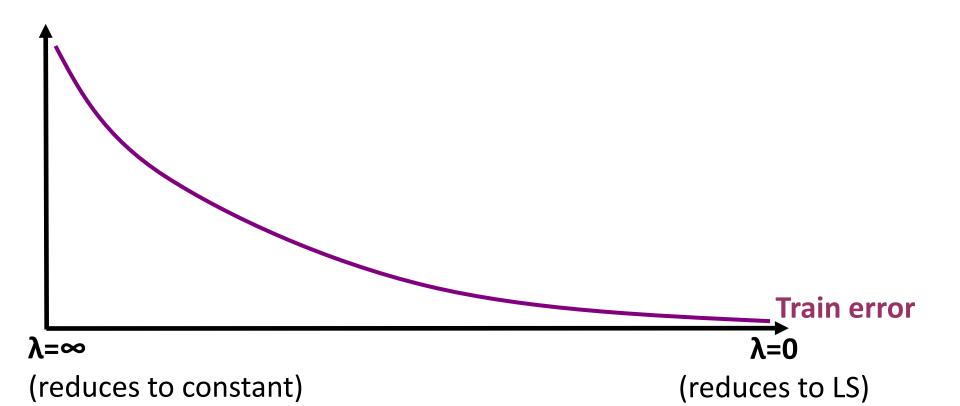
• Case: λ in-between

...is a balance between constant & LS.

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

What is a good value for λ?

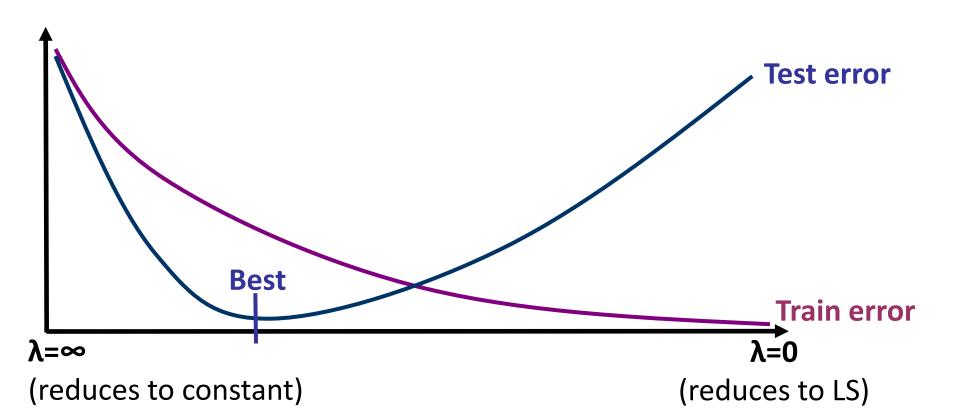
Learn w* at many values of λ



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

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

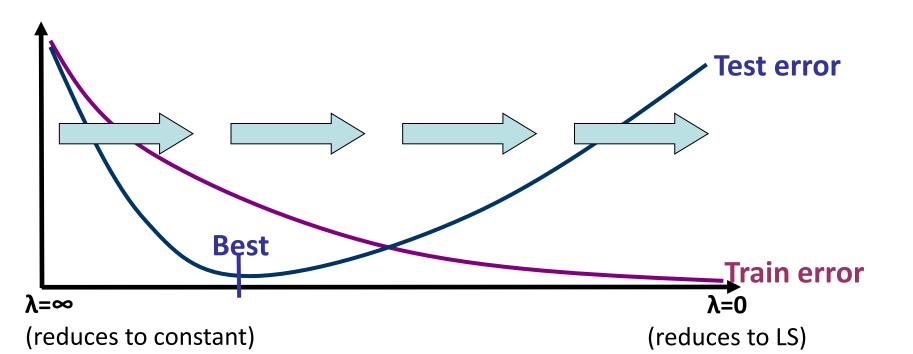
("Best" = best error on a left-out test set.)

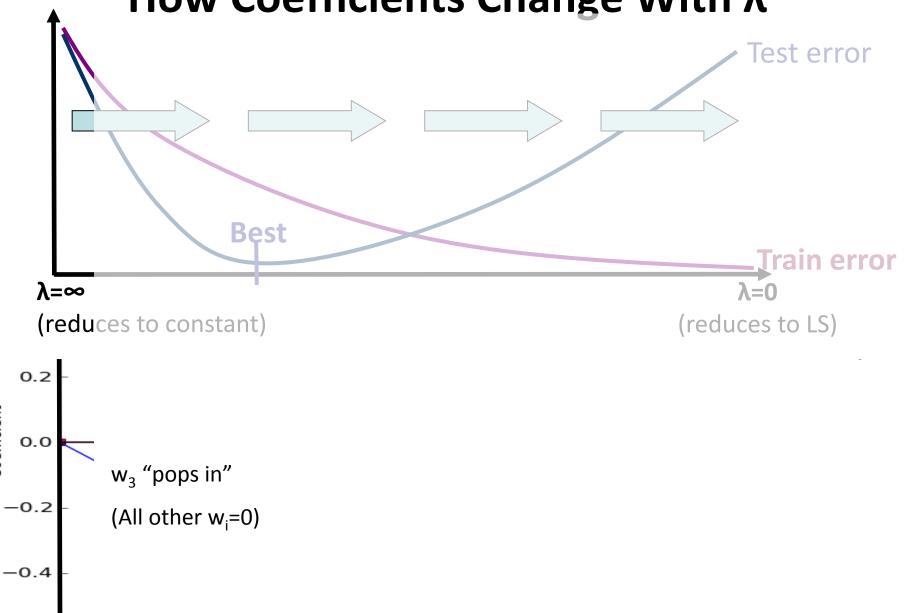


Algorithm

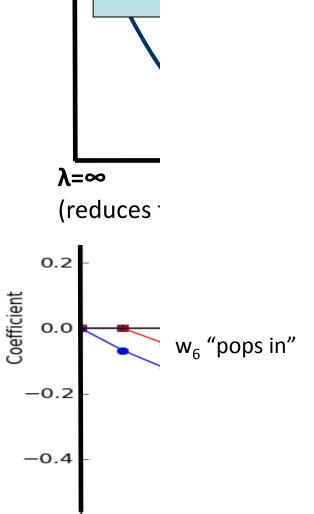
```
\begin{array}{l} \lambda = \text{huge (e.g. 1e40)} \\ \textbf{w} = \textbf{0} \\ \text{while } \lambda > 1\text{e-}10 \\ \lambda = \lambda \ / \ 10 \\ \textbf{w} = \text{solveAt}(\textbf{X}_{\text{train}}, \textbf{y}_{\text{train}}, \lambda, \textbf{w}_{\text{init}} = \textbf{w}) \\ \text{Compute error on test set} \end{array}
```

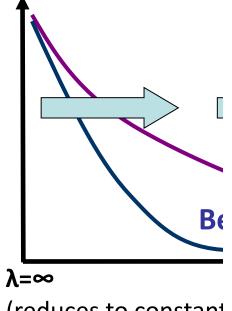
Return w with best test error



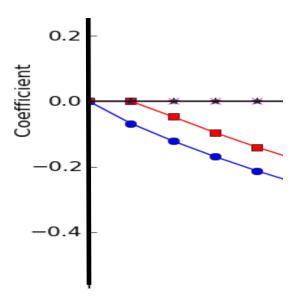


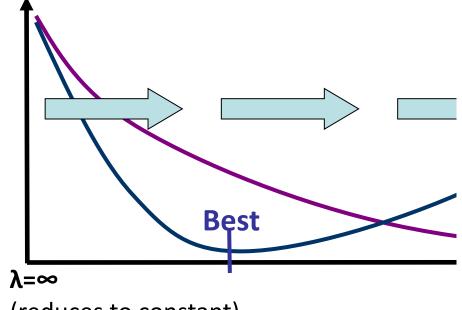
Coefficient



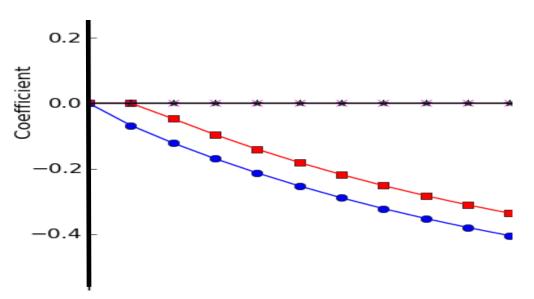


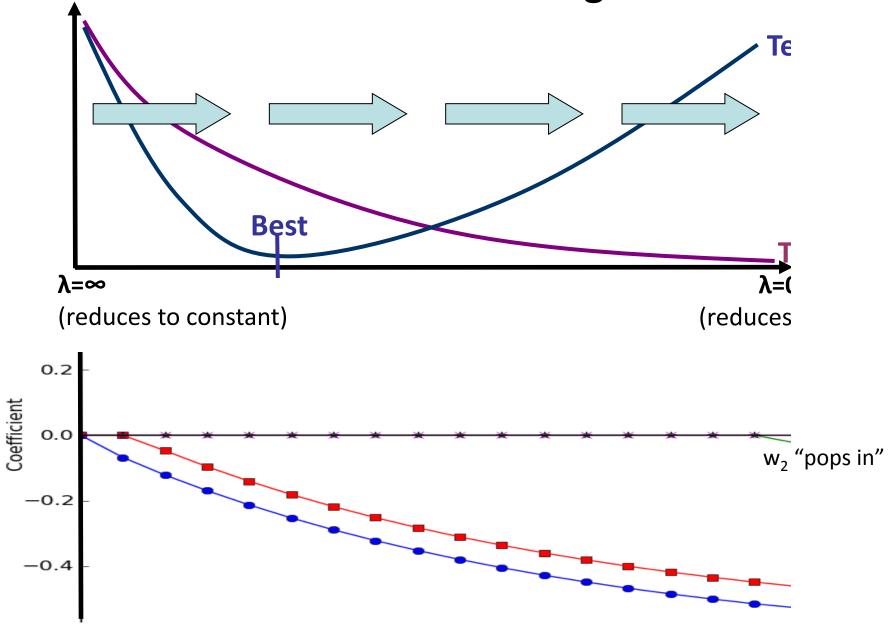
(reduces to constant

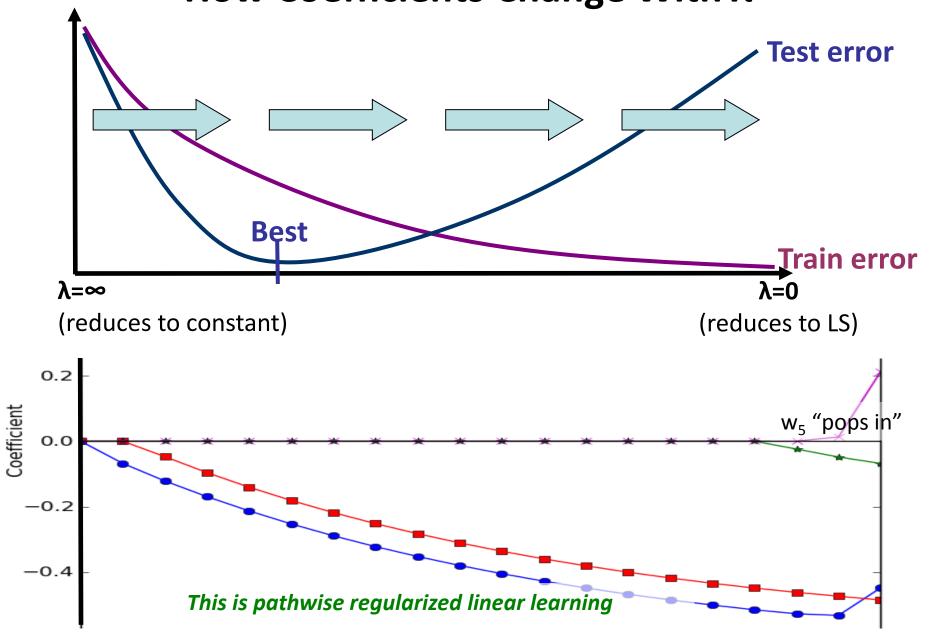




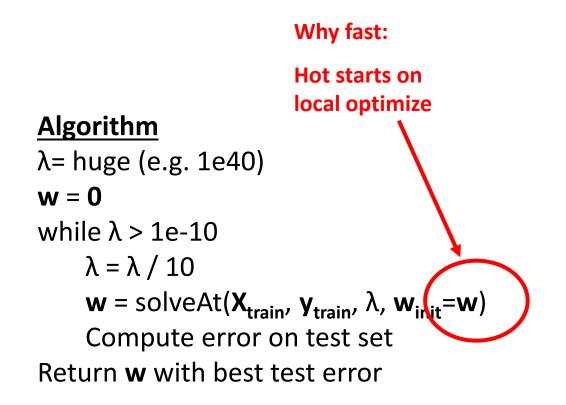
(reduces to constant)

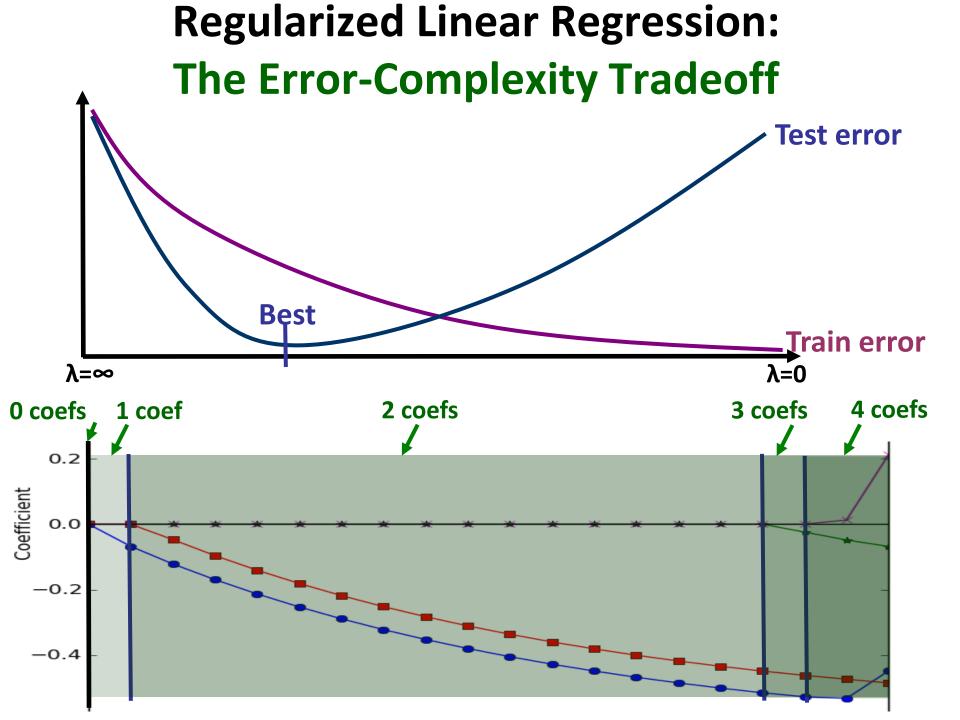




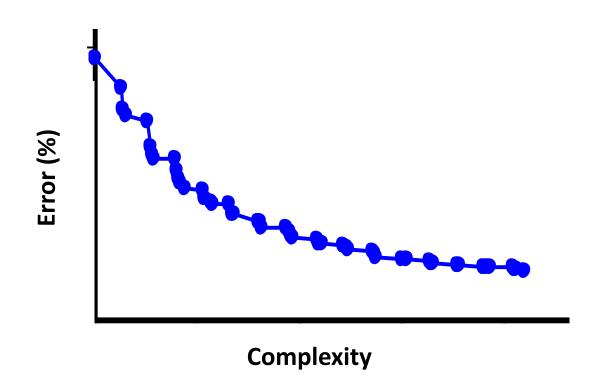


 Cool property #3: solving a full regularized path is ≈ as fast as solving single regularized problem (or a least-squares learning problem)





- 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.

FFX: Fast Function Extraction Technology

FFX Step 1/3: GenerateBases()

```
Inputs: X #input training data
Outputs: B #list of bases
# Generate univariate bases
1. B_1 = \{\}
2. for each input variable v = \{x_1, x_2, \dots\}
       for each exponent exp = \{0.5, 1.0, 2.0\}
3.
           let expression b_{exp} = v^{exp}
4.
           if ok(eval(b_{exp}, X))
              add b_{exp} to B_1
              for each operator op = \{abs(), log_{10}, \dots\}
                   let expression b_{op} = op(b_{exp})
                   if ok(eval(b_{op}, X))
                        add b_{op} to B_1
10.
# Generate interacting-variable bases
11. B_2 = \{\}
12. for i = 1 to length(B_1)
13. let expression b_i = B_1[i]
       for j = 1 to i - 1
14.
           let expression b_i = B_1[j]
15.
           if b_i is not an operator # disallow op() * op()
16.
              let expression b_{inter} = b_i * b_i
17.
              if ok(eval(b_{inter}, X))
18.
19.
                  add b_{inter} to B_2
20. return B = B_1 \cup B_2
```

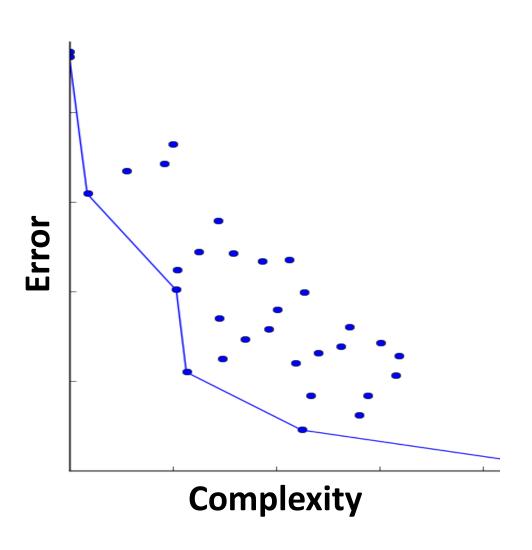
"Replace linear bases with a crazy amount of nonlinear ones"

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)
       X_B[i] = \text{eval}(B[i], X)
# Generate \lambda_{vec} = range of \lambda values
3. \lambda_{max} = max(|X^Ty|)/(N*\rho)
                                                                 "Generate set of
4. \lambda_{vec} = logspace(log_{10}(\lambda_{max} * eps), log_{10}(\lambda_{max}), N_{\lambda})
                                                                 models, at increasing
# Main path-following
5. A = \{\}
                                                                 complexity"
6. N_{bases} = 0
7. i = 0
8. a = \{0, 0, \ldots\}
9. while N_{bases} < N_{max-bases} and i < \text{length}(\lambda_{vec})
10. \lambda = \lambda_{vec}[i]
11. a = elasticNetLinearFit(X_B, y, \lambda, \rho, a)
12. N_{bases} = number of nonzero values in a (not counting offset)
13. if N_{bases} < N_{max-bases}
          add a to A
14.
15.
    i = i + 1
```

16. return A

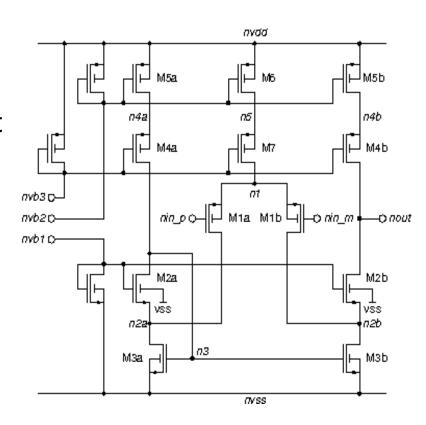
FFX Step 3/3: NondominatedFilter()



FFX Benchmarks

FFX Benchmarks: Experimental Setup

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



FFX Benchmarks: Experimental 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

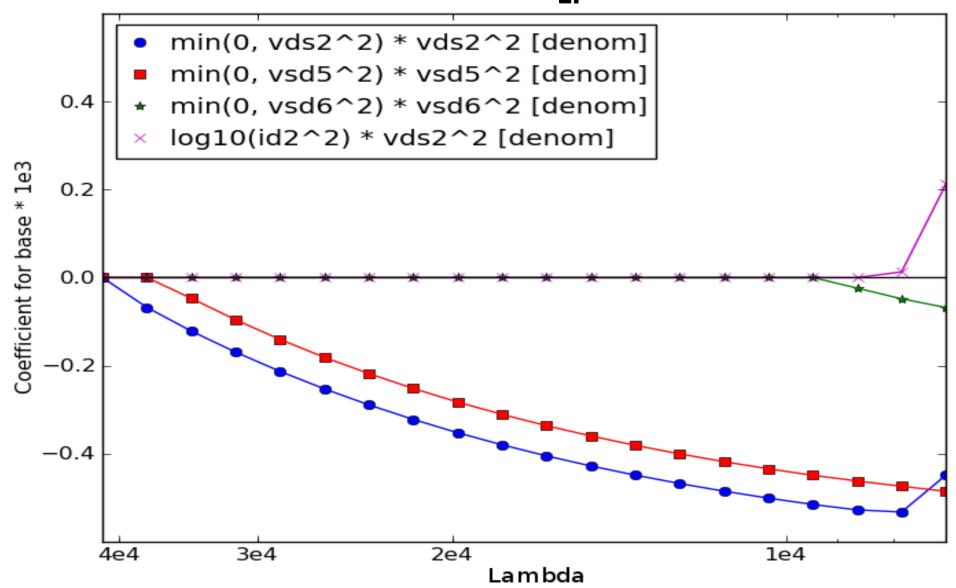
 $v_{sg1}^{0.5},\ abs(v_{sg1}^{0.5}),\ max(0,v_{sg1}^{0.5}),\ min(0,v_{sg1}^{0.5}),\ log_{10}(v_{sg1}^{0.5}),\ v_{sg1},\ abs(v_{sg1}),\ max(0,v_{sg1}),\ min(0,v_{sg1}),\ min(0,$ $log_{10}(v_{sg1}), v_{sg1}^2, \\ max(0, v_{sg1}^2), \\ min(0, v_{sg1}^2), \\ log_{10}(v_{sg1}^2), \\ v_{gs2}^{0.5}, \\ abs(v_{gs2}^{0.5}),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

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

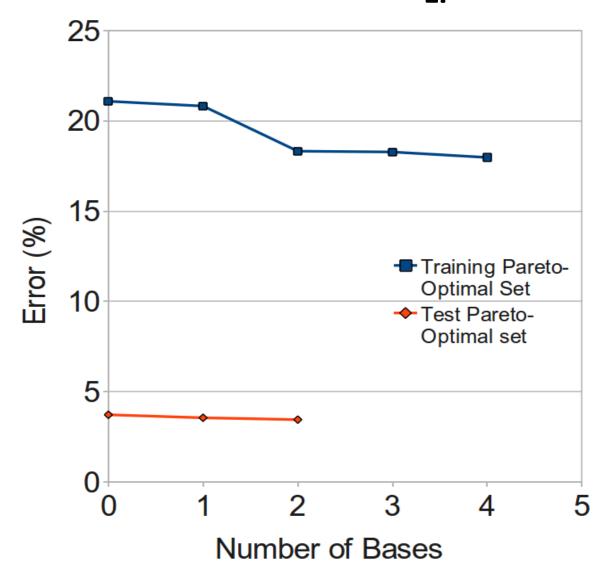
$$\begin{array}{l} log_{10}(i_{b3}^2)*i_{d2}^2, log_{10}(i_{b3}^2)*i_{b1}^{0.5}, log_{10}(i_{b3}^2)*i_{b1}, log_{10}(i_{b3}^2)*i_{b1}^2, log_{10}(i_{b3}^2)*i_{b2}^2, log_{10}(i_{b3}^2)*i_{b2}^{0.5}, log_{10}(i_{b3}^2)*i_{b3}^2, log$$

(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	$\frac{37.379}{1.0 - 6.78e - 5*min(0, v_{ds2}^2) * v_{ds2}^2}$
3.45	$\frac{37.020}{1.0 - 1.22e - 4*min(0, v_{ds2}^2)*v_{ds2}^2 - 4.72e - 5*min(0, v_{sd5}^2)*v_{sd5}^2}$

FFX Functions with Lowest Test Error on 6 Different Problems.

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

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 ≈ 10 minutes on a 1-GHz CPU.

CAFFEINE models with <10% error

Perf.	Expression

-10.3 + 7.08e-5 / id1 A_{IF} + 1.87 * In(-1.95e+9 + 1.00e+10 / (vsg1*vsg3) + 1.42e+9 *(vds2*vsd5) / (vsg1*vgs2*vsg5*id2))

10^(5.68 - 0.03 * vsg1 / vds2 - 55.43 * id1+ 5.63e-6 / id1)

 f_{u}

90.5 + 190.6 * id1 / vsg1 + 22.2 * id2 / vds2 PM

- 2.00e-3 Voffset

SR_D 2.36e+7 + 1.95e+4 * id2 / id1 - 104.69 / id2 + 2.15e+9 * id2

- 5.72e+7 - 2.50e+11 * (id1*id2) / vgs2 + 5.53e+6 * vds2 / vgs2

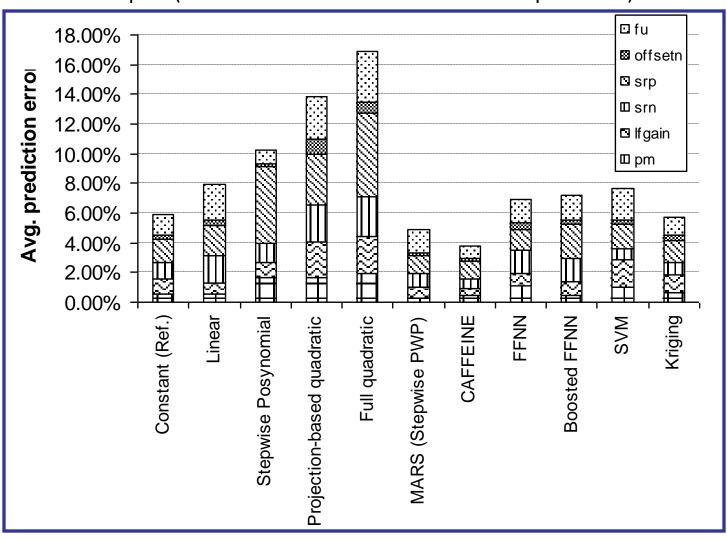
+ 4.63e+8 * id1

+ 109.72 / id1

SR

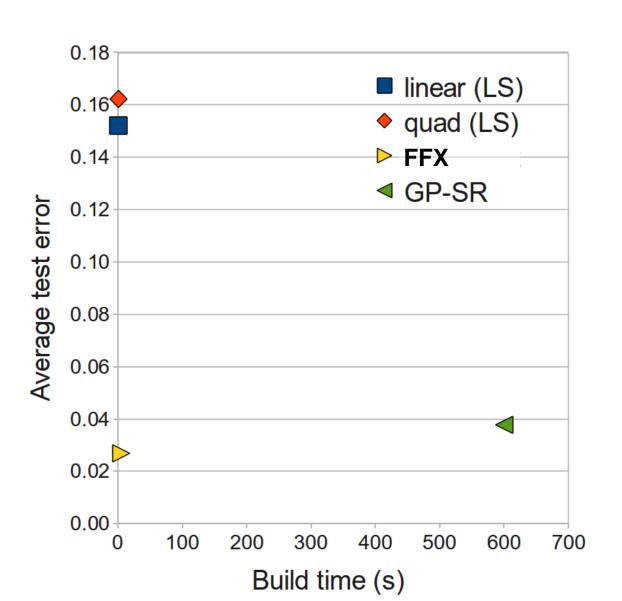
CAFFEINE Prediction Performance

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



Scaling Up FFX?

FFX So Far

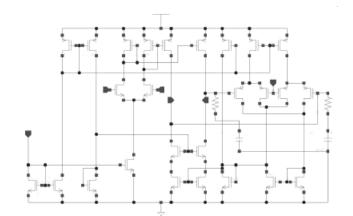
- Problems: 13 input variables, 256 samples
- Results: <5 s, best error
- Pretty good!

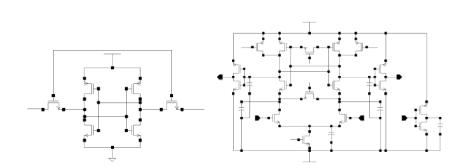
What about 100-1000+ input variables...?

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	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	Boost	Bootstr.		
	(CAFF-	tree	tree	LVSR-	LVSR-
	EINE)	(SGB)	(RF)	GDR	GDR-tune
30T AV	≫10.0	0.6418	0.8183	0.0765	0.1073
30T BW	≫10.0	0.5686	0.7730	0.0378	0.0442
30T PM	≫10.0	0.5894	0.7656	0.0732	0.0693
30T SR	≫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 (\approx 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 $k \le O(\sqrt{n})$ most important basis functions
- 3. Pathwise-learn univariate & combination
- 4. Nondominated filter

Complexity down to O(N*n²)!

Improving FFX

A batch-style riff on MARS.

Revised FFX Algorithm:

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

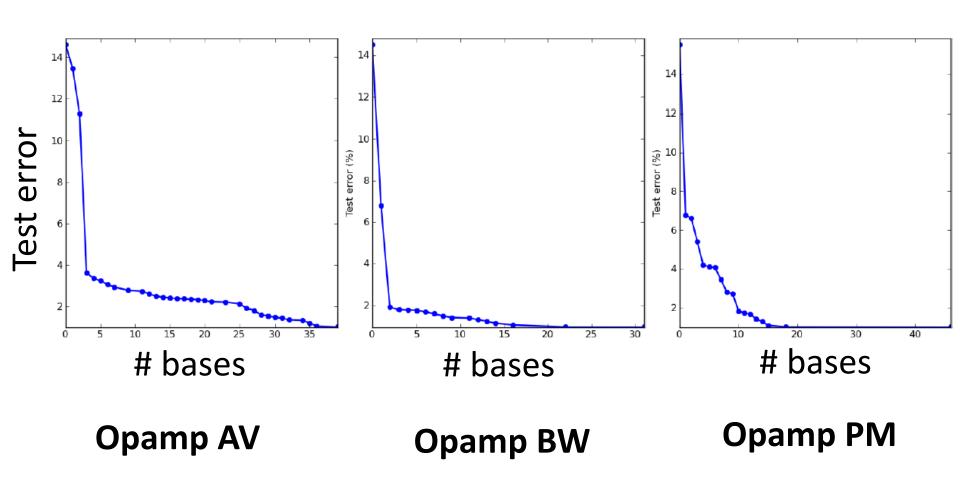
Complexity down to $O(N*n^2)$!

Two more tricks:

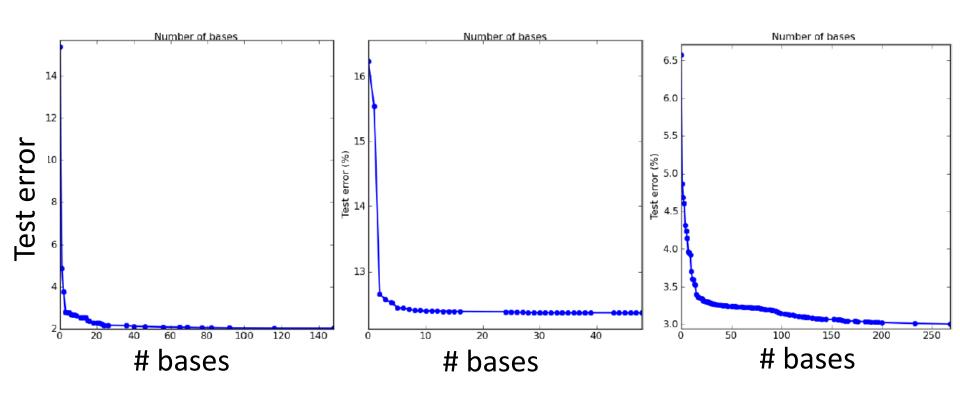
- Add MARS-style "hinge" bases: max(0, x_i-thr), max(0, thr-x_i)
- Repeat steps1-3 six times: maybe interactions, maybe rational, maybe hinge functions, maybe log/abs.

Overall runtime 5-30 s

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



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

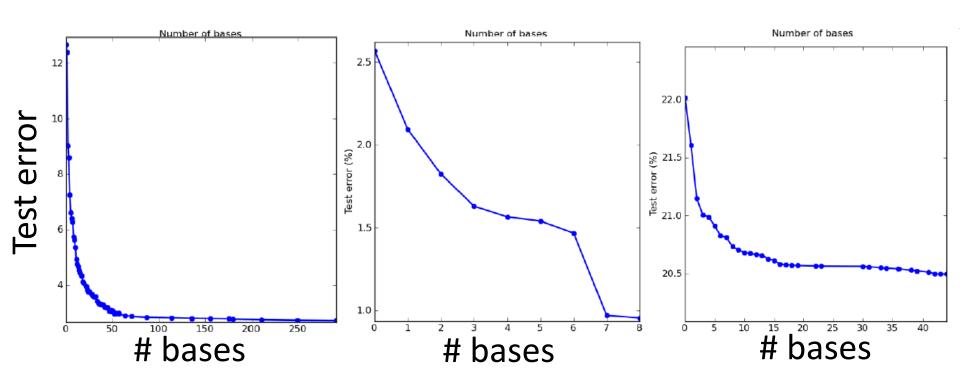


Opamp SR

Bitcell cell_i

Sense amp delay

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

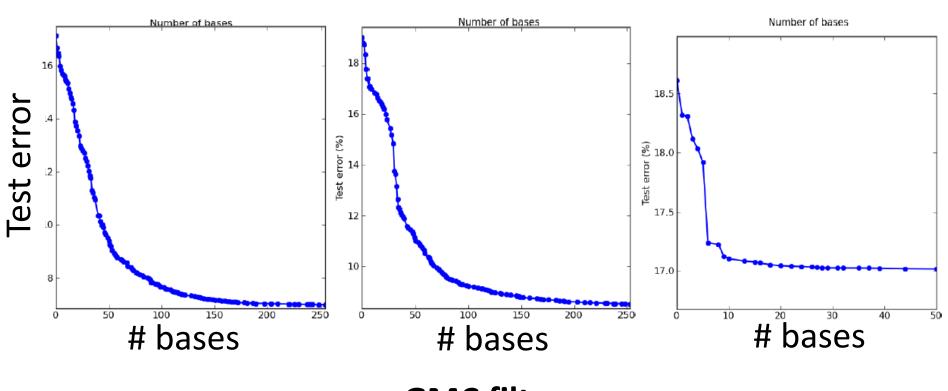


Sense amp PWR

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!

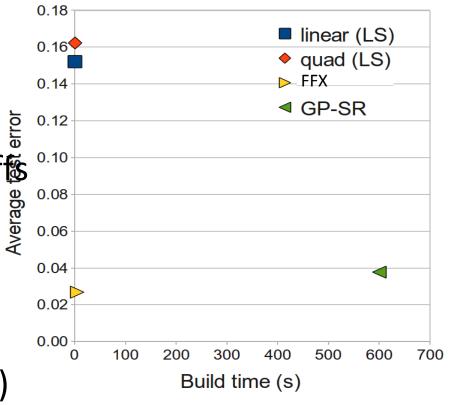
# Bases	Test error (ϵ_{test}) (%)	Extracted Function
0	2.6	512.7
1	2.1	504/(1.0 + 0.121 * max(0, dvthn + 0.875))
2	1.8	503 - 199 * max(0, dvthn + 1.61) - 52.1 * max(0, dvthn + 0.875)
3	1.6	$ \begin{vmatrix} 496/(1.0 - 0.0447*max(0, -1.64 - dvthp) * max(0, dvthn + 0.875) - 0.0282*max(0, -1.90 - dxw) *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

Outline

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

FFX Summary of Results 1/2

- ≈ as fast as LS-linear:
 <5 s on smaller, <30 s on larger
- As accurate as GP-SR
- Gives error-complexity tradeof
- Scalable
- Simple
- Deterministic!
- O(N * n²) complexity. (Theory!)



This is Fast Function Extraction

FFX Summary of Results 2/2

- Has been deployed to industry since 2010
- Off-the-shelf, under-the-hood, no fuss
- Solved >10,000 problems in just one application (Solido HSMC)
- Adopted by others in their research with great success (e.g. De Jonghe, Maricau)
- Now 100K+ variables, 100-10K training pts
- Extended for classification too (beat out 20+ other approaches)

- Field of ML: original intention was SR
- 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.

- 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

- 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

- "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 to an EA Researcher]

- 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"

FFX ≠ Fork Fan Experience

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!

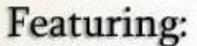
Never burn your tounge again!

Go ahead, be in a hurry.

Never wait for your

food to cool down

ever again.



- * 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





















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

Met my gauntlet:

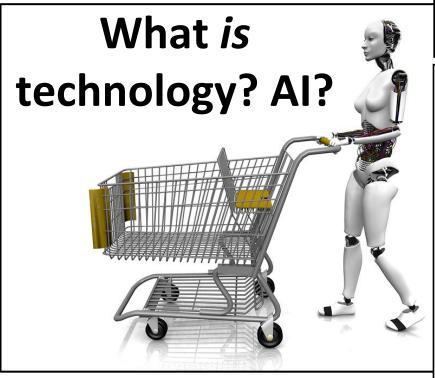
"How can SR be scoped so that it becomes another standard, off-the-shelf method in the "toolboxes" of scientists and engineers around the world? Can SR follow in the same vein of linear programming?

"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?"

Try it out at trent.st/ffx

Conclusion: (Slightly less mysterious) Mysteries of the universe

WTF is genetic programming or symbolic regression? Why should I care?





How *does* Google find furry robots?