

Equilibrium Reconstruction in Stellarators: V3FIT

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Equilibrium Reconstruction

- Use measured diagnostic signals to determine current and pressure profiles, and hence the MHD equilibrium configuration.
- Diagnostics
 - Magnetic Diagnostics: magnetic probes, flux loops, saddle coils, Rogowski coils etc.
 - Microwave Interferometry and Polarimetry
 - Thomson Scattering
 - Motional Stark Effect

Equilibrium Reconstruction

- A classic Inverse Problem
 - Forward problem, determine signals, given parameters.
Known Function $\mathbf{S}(\mathbf{p})$
 - We know (observe) the signals. What are the parameters?
Determine Inverse Function $\mathbf{p}(\mathbf{S})$
 - Use Maximum Likelihood / Least Squares.
- Axisymmetric: EFIT Code.
 - EFIT is *tightly coupled* - the least squares iterations proceed *at the same time* as the equilibrium iterations.
- Non-axisymmetric: V3FIT Code.

V3FIT Code Design Goals

- V3FIT will execute fast enough so that reconstructions can be done between shots.
 - Implies tightly coupled equilibrium and reconstruction iterations.
- V3FIT will be flexible, easy to understand, maintain, and modify.
 - V3FIT will be written in Fortran 95.
 - V3FIT must be written in a modular fashion, with clear and consistent data flow.
- The initial working version of V3FIT will use VMEC as the equilibrium solver, and it will have magnetic diagnostics as the primary signal.
- V3FIT will be designed with future enhancements in mind. Future enhancements include:
 - Adding new diagnostics and signals
 - Changing the equilibrium solver

V3FIT: Variables

- **X**: Equilibrium state. (Quantities that change with each equilibration step.)
 - In VMEC, $\mathbf{X} = (R_{mn}, Z_{mn}, \lambda_{mn})$.
 - *No* implication that \mathbf{X} corresponds to a converged equilibrium.
- **f**: MHD forces. Very small in equilibrium.
- **p**: parameters. Input for Equilibrium Solver. n_p of them.
 - *The parameters are what the Equilibrium Reconstruction will determine.*
 - Pressure profile (VMC: parameterized as power series in s .)
 - Either iota or current profile
 - Iota profile (VMC: Uses iota profile when $n_{cur} = 0$.)
 - Current profile (VMC: Uses current profile when $n_{cur} = 1$.)
 - External currents (free-boundary)
 - Outer surface shape (fixed-boundary)

V3FIT: Variables (cont.)

- **D**: Diagnostics, data that comes from an experiment.
 - Magnetic diagnostics
 - Microwave Interferometry - Polarimetry
 - Motional Stark Effect, Thompson Scattering...
- **S**: Signals, either computed from a *model* [$\mathbf{S}_M(\mathbf{p}, \mathbf{X})$] or *observed* (computed from diagnostics) [$\mathbf{S}_O(\mathbf{p}, \mathbf{D})$]. n_S of them.
 - To reconstruct an equilibrium we minimize the mismatch between observed and equilibrium signals.
 - Computing $\mathbf{S}_M(\mathbf{p}, \mathbf{X})$ is the *forward* problem.
 - Often, the observed signal will be the diagnostic itself, $\mathbf{S}_O(\mathbf{p}, \mathbf{D}) = \mathbf{D}$. This is the case for magnetic diagnostics.

V3FIT: The Inverse Problem

- **ASSUMPTION** - Gaussian Errors

- The probability of observations \mathbf{S}_o is proportional to:

$$f = \exp\left(-\frac{1}{2}(\mathbf{S}_M(\mathbf{p}, \mathbf{X}) - \mathbf{S}_o) \cdot \mathbf{C}^{-1} \cdot (\mathbf{S}_M(\mathbf{p}, \mathbf{X}) - \mathbf{S}_o)\right)$$

- For actual observations $\mathbf{S}_o(\mathbf{p}, \mathbf{D})$, we reinterpret the above probability distribution to be the probability of the parameters \mathbf{p} .

- **Maximum likelihood, -> least squares.**

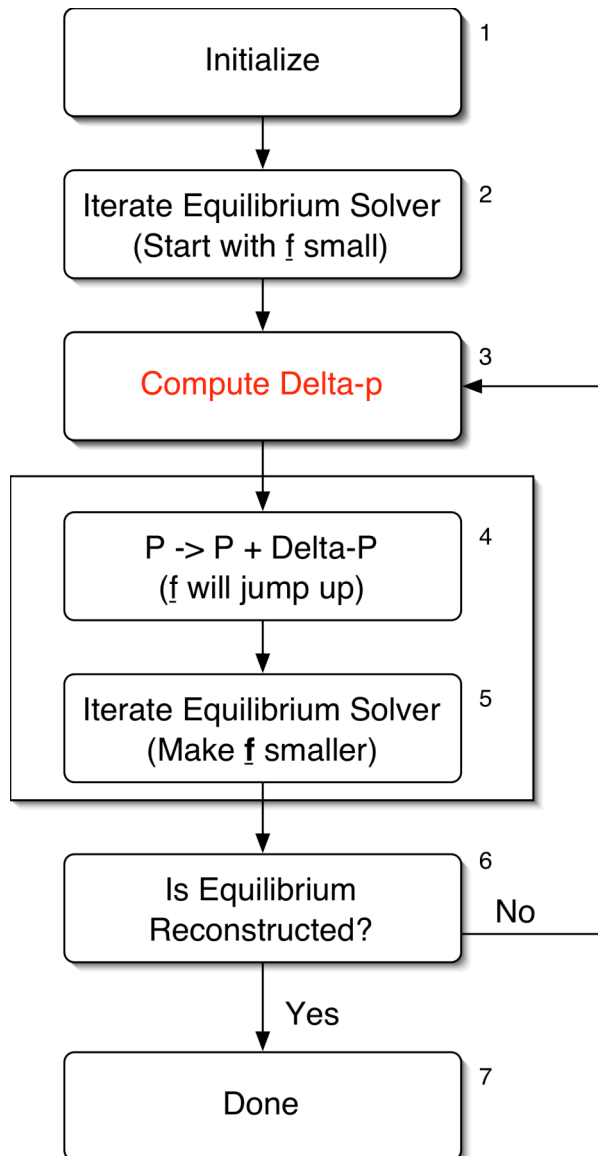
- The *most likely* value of the parameter vector \mathbf{p} will be where the Gaussian distribution function is a *maximum*.
- *Therefore*, to find the most likely value of \mathbf{p} , we minimize chi-squared:

$$\chi^2 = (\mathbf{S}_M(\mathbf{p}, \mathbf{X}) - \mathbf{S}_o) \cdot \mathbf{C}^{-1} \cdot (\mathbf{S}_M(\mathbf{p}, \mathbf{X}) - \mathbf{S}_o)$$

V3FIT: Two Level Optimizer

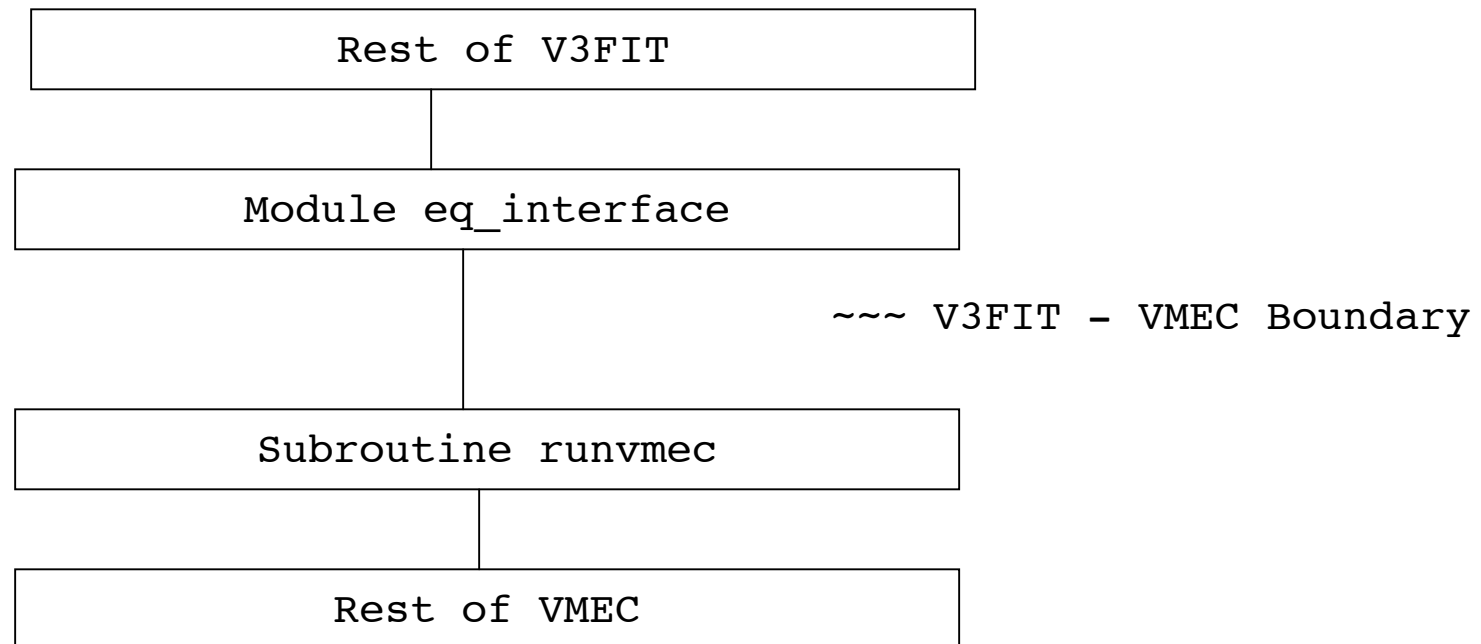
- Upper Level : Reconstruction - change \mathbf{p}
 - Minimize chi-squared by varying \mathbf{p}
 - \mathbf{p} : estimate < 100 parameters
 - \mathbf{S} : estimate about 200 signals
 - Computing the Jacobian is feasible
 - Try standard methods (Levenberg-Marquardt) for optimization.
 - Hope that upper and lower level proceed to convergence at the same time.
- Lower Level: Equilibration - change \mathbf{X}
 - Equilibrium Solver (VMEC, or another solver)
 - Minimize \mathbf{f} by varying \mathbf{X} (for slowly varying \mathbf{p})
 - \mathbf{X} : (100 modes)(100 Radial)(R,Z, λ) = 30,000
 - \mathbf{f} : ~ same number as for \mathbf{X} , = 30,000
 - Hessian $d\mathbf{f}/d\mathbf{X}$ very large ($\sim 10^9$ elements), time consuming to compute.
=> have to be clever (hence VMEC).

V3FIT Flow Chart



- Lots of possibilities for the "Compute Delta-p" step.
 - Jacobian estimation in here
 - Algorithm for Delta-P
- Will need to experiment with how much to iterate equilibrium solver in steps 2 and 5.
- Steps 4 and 5 may be combined: Add Delta-p slowly, over the course of many equilibrium iterations.

V3FIT - VMEC Interface Schematic



- Interaction will occur ONLY through the `eq_interface` module and the `runvmec` subroutine.
- V3FIT needs to have access to the object files of the equilibrium solver.

Modules for Derived Types

- Derived types are implemented in modules (generally with names ending in T)
- The derived types reflect the structure of the problem.
- All have subroutines to construct, destroy, and assign derived types.
- Module `bsc` - Biot-Savart Coil
 - Derived type `bsc_coil` - a magnetic field coil
 - Derived type `bsc_coilcoll` - a collection of `bsc_coil`
 - Subroutines to compute \mathbf{A} , \mathbf{B} , gradients of \mathbf{B} , magnetic flux through a coil, rotate and shift a coil
- Module `diagnostic_T`
 - Derived type `diagnostic_desc` - describe a diagnostic
 - Derived type `diagnostic_data` - carry the diagnostic values
- Module `signal_T`
 - Derived type `signal_desc` - describe a signal
 - Derived type `signal_data` - carry the signal values
 - Derived type `signal_mrf` - Magnetic Response Function

Modules for Derived Types

- Module `eq` - Equilibrium
 - Derived type `eq_param_fix` - Fixed parameters of the equilibrium solver
 - Logical switches
 - Array dimensions
 - Numbers of modes
 - Convergence, iteration parameters
 - Derived type `eq_param_var` - Variable parameters of the equilibrium solver
 - Derived type `eq_state` - Equilibrium state, the X variables
 - Derived type `eq_aux_n` - Variables computable from the state
- Module `model` - The model
 - Right now, just contains a pointer to an `eq_state`
 - Later may need to add on electron density, information about vacuum vessel (for eddy currents), etc.

Other Modules

- Module `eq_interface` - Interface with the equilibrium code (VMEC)
 - Subroutine `eq_init_file`
 - Read a namelist input file, and initialize the equilibrium code.
 - Construct an `eq_param_fix`, `eq_param_var`, and `eq_state`.
 - Subroutine `eq_init_structure`
 - Input an `eq_param_fix`, `eq_param_var`, and `eq_state`
 - Initialize the equilibrium code
 - (Not yet implemented)
 - Subroutine `eq_step`
 - Iterate an `eq_state` for some number of equilibrium iterations
- Module `signal_model` - Computations that need both a signal and a model
 - Subroutine `signal_model_compute`
 - Computes the solution to the forward problem, $\mathbf{S}_M(\mathbf{p}, \mathbf{X})$

Forward Problem - Magnetic Diagnostics

- Compute the magnetic flux through a diagnostic coil
 - Have to integrate over all the source currents.
 - Currents in field generating coils - effectively need mutual inductances
 - Currents in plasma - have to integrate over plasma volume
- Implemented in earlier codes V3RFUN and V3POST
- V3RFUN and V3POST being used to design magnetic diagnostic for NCSX
- Sections of code from V3POST reused in V3FIT

Forward Problem - Microwave Interferometry and Polarimetry

- Signal for Interferometry is phase change along path of microwave - proportional to the electron density

$$\Delta\varphi \propto \int n_e d\ell$$

- Signal for Polarimetry is the change in the angle of polarization of the microwave - proportional to the electron density times the parallel magnetic field.

$$\Delta\alpha \propto \int n_e \vec{\mathbf{B}} \cdot d\vec{\ell}$$

- Coding for solution to forward problem is in progress.
- Will be implemented in existing structure of V3FIT

Status

- V3FIT structural coding is complete
- Modules for Derived Types coded, tested
- Interface with VMEC works.
- Implementation of microwave interferometry-polarimetry in progress
- Next TO DO item - coding of reconstruction algorithm

Extra slides follow

V3FIT: Variables (cont.)

- Why is there a distinction between Diagnostics (\mathbf{D}) and observed Signals (\mathbf{S}_O)?
 - Because for some diagnostics, we can't compute what we expect the diagnostic to be, using the MHD equilibrium information.
 - Example of when an observed signal is NOT the diagnostic:
 - Consider Te data along a chord through the plasma. The values of Te along the chord are the diagnostic.
 - We can't compute the Te measurements we expect from \mathbf{p} and \mathbf{X} , so can't consider the Te values as a signal.
 - However, we can use the Te data to constrain the flux surface geometry so that Te is a flux surface quantity.
 - If λ is a parameter along a chord through the plasma, then an appropriate signal would be $\lambda_{\text{outer}}(\lambda_{\text{inner}})$, suitably discretized.
 - We can calculate both an observed signal $\mathbf{S}_O(\mathbf{D})$ from the Te diagnostic, and an equilibrium signal $\mathbf{S}_E(\mathbf{p}, \mathbf{X})$ from the equilibrium state.

Correlations between Observations

- The covariance operator \mathbf{C} :
 - Diagonal elements are the variances of the signals: $\mathbf{C}_{ii} = \sigma_i^2$
 - Off-diagonal elements contain information about the correlations between the signals. $\mathbf{C}_{ij} = r_{ij} \sigma_i \sigma_j \quad i \neq j \quad -1 \leq r_{ij} \leq 1$
 - No correlations between the different signals - set the r_{ij} to 0.
 - Note how the covariance operator takes care of the differing dimensions of the signals.
 - Given a probability density $f(\mathbf{x})$, the mean is: $\langle \mathbf{x} \rangle = \int d\mathbf{x} \mathbf{x} f(\mathbf{x})$
 - The Covariance is (in component notation):
$$\mathbf{C}_{ij} = \int d\mathbf{x} (x_i - \langle x_i \rangle)(x_j - \langle x_j \rangle) f(\mathbf{x})$$
 - The normalized Gaussian probability density:
$$f(\mathbf{x}) = \left((2\pi)^N \det(\mathbf{C}) \right)^{-1/2} \exp\left(-\frac{1}{2} (\mathbf{x} - \mathbf{x}_0) \cdot \mathbf{C}^{-1} \cdot (\mathbf{x} - \mathbf{x}_0) \right)$$
has mean \mathbf{x}_0 and covariance \mathbf{C} .
 - Even for a linear problem, the correlations can change the most likely parameter value.

Normalized Variables

- Normalize the parameters and the signals:

$$a_k = p_k / \tilde{p}_k \quad y_{M i}(a_k, \mathbf{X}) = S_{M i}(a_k \tilde{p}_k, \mathbf{X}) / \sigma_i$$

$$y_{O i} = S_{O i} / \sigma_i$$

- Error: $e_i = y_{O i} - y_{M i}(\mathbf{a}, \mathbf{X}) \quad i = 1, n_s$

- chi-squared: $\chi^2 = \sum_{i,j} (y_{M i}(\mathbf{a}, \mathbf{X}) - y_{O i}) w_{ij} (y_{M j}(\mathbf{a}, \mathbf{X}) - y_{O j}) = \mathbf{e} \cdot \mathbf{w} \cdot \mathbf{e}$

- weights $w_{ij} = (\mathbf{C}^{-1})_{ij} \sigma_i \sigma_j$

- Jacobian: $J_{ik} = \frac{\partial y_{M i}(\mathbf{a}, \mathbf{X})}{\partial a_k} \quad i = 1, n_s; k = 1, n_p$

- Gradient:
$$\frac{\partial \chi^2}{\partial a_k} = \sum_{i,j} 2(y_{M i}(\mathbf{a}, \mathbf{X}) - y_{O i}) w_{ij} \left(\frac{\partial y_{M j}(\mathbf{a}, \mathbf{X})}{\partial a_k} \right)$$

$$= -2\mathbf{e} \cdot \mathbf{w} \cdot \mathbf{J} = -2\mathbf{J}^T \cdot \mathbf{w} \cdot \mathbf{e}$$

Minimization

- Following *Numerical Recipes*, 2nd edition, section 15.5.

$$f(\mathbf{a} + \delta\mathbf{a}) \approx f(\mathbf{a}) - 2\boldsymbol{\beta} \cdot \delta\mathbf{a} + \delta\mathbf{a} \cdot \boldsymbol{\alpha} \cdot \delta\mathbf{a}$$

$$\boldsymbol{\beta} = -\frac{1}{2} \nabla f = \mathbf{e} \cdot \mathbf{w} \cdot \mathbf{J} = \mathbf{J}^T \cdot \mathbf{w} \cdot \mathbf{e}$$

$$\beta_k = -\frac{1}{2} \frac{\partial f}{\partial a_k} = \sum_{i,j} (y_{O_i} - y_{M_i}(\mathbf{a}, \mathbf{X})) w_{ij} \left(\frac{\partial y_{M_j}(\mathbf{a}, \mathbf{X})}{\partial a_k} \right)$$

$$\boldsymbol{\alpha} = +\frac{1}{2} \nabla \nabla f = \mathbf{J}^T \cdot \mathbf{w} \cdot \mathbf{J} - \mathbf{e} \cdot \mathbf{w} \cdot \nabla \mathbf{J}$$

$$a_{kl} = +\frac{1}{2} \frac{\partial^2 f}{\partial a_k \partial a_l} = \sum_{i,j} \left(\frac{\partial y_{M_i}(\mathbf{a}, \mathbf{X})}{\partial a_k} \right) w_{ij} \left(\frac{\partial y_{M_j}(\mathbf{a}, \mathbf{X})}{\partial a_l} \right) - (y_{O_i} - y_{M_i}(\mathbf{a}, \mathbf{X})) w_{ij} \left(\frac{\partial^2 y_{M_j}(\mathbf{a}, \mathbf{X})}{\partial a_k \partial a_l} \right)$$

- Following *NR* and everybody else, drop the second derivative term in alpha.

$$\boldsymbol{\alpha} \approx \mathbf{J}^T \cdot \mathbf{w} \cdot \mathbf{J}$$

Minimization (continued)

$$f(\mathbf{a} + \delta\mathbf{a}) \approx f(\mathbf{a}) - 2\boldsymbol{\beta} \cdot \delta\mathbf{a} + \delta\mathbf{a} \cdot \boldsymbol{\alpha} \cdot \delta\mathbf{a}$$

- Two Algorithms

1) Steepest Descent - go downhill fast. Implies $\delta\mathbf{a} = \mu\boldsymbol{\beta}$ $\mu > 0$

2) Hit minimum when gradient is zero, $\nabla f(\mathbf{a} + \delta\mathbf{a}) = -2\boldsymbol{\beta} + 2\boldsymbol{\alpha} \cdot \delta\mathbf{a}$

Set gradient to zero, solve: $\boldsymbol{\alpha} \cdot \delta\mathbf{a} = \boldsymbol{\beta}$

- Levenberg -Marquardt: Clever way to interpolate between these two algorithms.

$$\alpha'_{kl} = \alpha_{kl}(1 + \lambda\delta_{kl}) \quad \delta\mathbf{a} = \boldsymbol{\alpha}'^{-1}\boldsymbol{\beta}$$

- λ small, solving for gradient = 0.
- λ large, matrix diagonally dominant, steepest descent-like step.
- More signals than parameters, use SVD to get approximate inverse.

- Levenberg - Marquardt step (in $\lambda \rightarrow 0$ limit) with SVD minimizes

$$|\boldsymbol{\alpha} \cdot \delta\mathbf{a} - \boldsymbol{\beta}|^2 = |(\mathbf{J}^T \cdot \mathbf{w}) \cdot \mathbf{J} \cdot \delta\mathbf{a} - (\mathbf{J}^T \cdot \mathbf{w}) \cdot \mathbf{e}|^2$$

- n_p equations, n_p deviations $\delta\mathbf{a}$. Expect zero minimum.

Jacobian Calculation and Update

- Consider three types of Jacobian calculations.
 - Separately computable (I don't like this phrase. Got a better one?)
 - Finite Difference
 - Broyden Update

- Illustrative Example. Split the parameter vector into pieces.

$$\mathbf{a} = (\mathbf{a}_{ec}, \mathbf{a}_{cp}, \mathbf{a}_{pp}, \mathbf{a}_{other})$$

- \mathbf{a}_{ec} - all external currents (helical coils, VF coils, correction coils, etc.)
- \mathbf{a}_{cp} - current profile parameters
- \mathbf{a}_{pp} - pressure profile parameters
- \mathbf{a}_{other} - other parameters
- $\hat{\mathbf{a}}_{eck}$ - unit vector in kth slot of external current portion of the \mathbf{a} vector.
- Current, pressure profiles are function of the VMEC radial variable s .

$$I(s) = \sum_{k=1} p_{l(k)} g_k(s) \quad P(s) = \sum_{k=1} p_{m(k)} h_k(s)$$

- g, h are basis functions for profiles. $l(k)$ and $m(k)$ convert index values.
- Assume Signals are magnetic diagnostics.

Jacobian - continued

- The magnetic diagnostic signals are linear in the currents.
- For external current parameters:

$$\frac{\partial y_{M i}}{\partial a_{eck}} \approx S_{M i}((\hat{\mathbf{a}}_{eck}, \mathbf{0}, \mathbf{a}_{pp}, \mathbf{a}_{other}), \mathbf{X}) / \sigma_i$$

- Doesn't depend on approach to equilibrium. Compute once, and don't update.

- For the current profile parameters:

$$\frac{\partial y_{M i}}{\partial a_{cpk}} \approx S_{M i}((\mathbf{0}, \hat{\mathbf{a}}_{cpk}, \mathbf{a}_{pp}, \mathbf{a}_{other}), \mathbf{X}) / \sigma_i$$

- Depends on flux surface shape. Update as the equilibrium iteration proceeds.

- These two are examples of what I call "Separately Computable" Jacobian elements. We use physical knowledge about how the signals depend on the parameters.

Jacobian - Finite Difference

- Define the iteration operator T for the equilibrium solver:
 - Takes a state \mathbf{X}_0 and iterates it with the equilibrium solver m times, using the normalized parameters \mathbf{a} .
 - $T^m(\mathbf{a}, \mathbf{X}_0) = \mathbf{X}_m$
- Jacobian:
$$J \approx \frac{\partial \mathbf{y}_M}{\partial \mathbf{a}} \equiv \frac{\mathbf{y}_M(\mathbf{a} + \delta \mathbf{a}, T^m(\mathbf{a} + \delta \mathbf{a}, \mathbf{X})) - \mathbf{y}_M(\mathbf{a}, T^m(\mathbf{a}, \mathbf{X}))}{\delta \mathbf{a}}$$
 - $m = 0$: fixed geometry. (Probably won't work for pressure profile parameters.)
 - $m \geq 1$: allows geometry to change.
 - $m \rightarrow \text{Infinity}$: Using fully converged equilibria to compute Jacobian. Implemented with STELLOPT.
- How important is accuracy of signal computation?

Jacobian - Broyden Update

- Assume we started at parameter values \mathbf{a}^n , with computed signals $\mathbf{y}_M(\mathbf{a}^n, \mathbf{X}(\mathbf{a}^n))$. A new set of parameters \mathbf{a}^{n+1} are computed, and equilibrium \mathbf{X} 's iterated some more toward convergence, and new signal $\mathbf{y}_M(\mathbf{a}^{n+1}, \mathbf{X}(\mathbf{a}^{n+1}))$ computed. We would like to update the Jacobian \mathbf{J}^n we computed earlier, so that it will satisfy:

$$\mathbf{J}^{n+1} \cdot (\mathbf{a}^{n+1} - \mathbf{a}^n) = \mathbf{y}_M(\mathbf{a}^{n+1}, \mathbf{X}(\mathbf{a}^{n+1})) - \mathbf{y}_M(\mathbf{a}^n, \mathbf{X}(\mathbf{a}^n))$$

- The new Jacobian gets the most recent change correct.
- Best way to do this is the Broyden update:

$$\mathbf{J}_B^{n+1} = \mathbf{J}^n + \frac{(\delta \mathbf{y}_M - \mathbf{J}^n \cdot \delta \mathbf{a}) \otimes \delta \mathbf{a}}{\delta \mathbf{a} \cdot \delta \mathbf{a}}$$

- Root find with Broyden update - similar to secant method in one dimension.

VMEC Flow Diagram

